Partial transposition on bi-partite system

Y.-J. Han, X. J. Ren, Y. C. Wu, G.-C. Guo

Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei 230026, China

Abstract

Many of the properties of the partial transposition are not clear so far. Here the number of the negative eigenvalues of $\rho^T$ is considered carefully when $\rho$ is a two-partite state. There are strong evidences to show that the number of negative eigenvalues of $\rho^T$ is at most when $\rho$ is a state in Hilbert space $C^N \otimes C^N$. For the special case, $2 \times 2$ system, we use this result to give a partial proof of the conjecture $|\rho^T|^T \geq 0$. We find that this conjecture is strongly connected with the entanglement of the state corresponding to the negative eigenvalue of $\rho^T$ or the negative entropy of $\rho$.

PACS numbers: 03.67.Mn, 03.65.Ud, 03.67.-a
I. INTRODUCTION

Entanglement is one of the most interesting properties of many-body systems. It has many powerful applications, such as quantum communication\cite{1} and quantum computation\cite{2,3}. So it is the cornerstone of quantum information technology\cite{4,5,6}. Although it is very important, unfortunately, it is very difficult to investigate the measurement of entanglement. Sometimes, it is even hard to decide whether a state is entangled or not. Although some useful methods (such as entanglement witness\cite{7,8}, partial transposition\cite{10,11,12}) have been introduced to this problem, it is far from completing this problem even for two-body systems. Partial transposition (PT) is the most powerful tool to detect the entanglement of a state\cite{9}, especially for bipartite systems. The famous Peres-Horodecki criterion\cite{10,11} guarantees that the positive partial transposition (PPT) condition is sufficient and necessary to decide whether a state in Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \mathbb{C}^3$ is entangled or not. But PPT condition is only sufficient (not necessary) for higher dimensional bipartite systems.

There are two reasons for us to consider the PT transformation more carefully in quantum information. One is that we want to know whether the PT method can be generalized and to find the similar method to the higher dimensional Hilbert space, since there are many advantages of this method (such as the convenience of computation). In other words, we want to know the reason why we can or can not extend this method and how if we can. To make these ideas possible, we must carefully investigate the physical significance and mathematical characters of PT transformation. The other reason is that we know little about the PT transformation even in $2 \times 2$ system, since there is no explicitly known mathematical operator corresponding to PT transformation. Many characters (mathematical or physical) of PT are still unclear so far. A simple question of $2 \times 2$ system is introduced by Audenaert et al\cite{13,14}: Prove that

$$\left| \rho^T \right|^T \geq 0$$

for any two-qubit state $\rho$, where $T$ is PT and $\left| . \right|$ is the operator absolute value. This question is clear, but the proof is not found yet. We do not know whether equation(1) is correct or not. In this paper, we devote to a even more simple problem about PT transformation at first: let $\rho$ be a bi-partite state in Hilbert space $\mathbb{C}^N \otimes \mathbb{C}^M$, how many negative eigenvalues are there in $\rho^T$ at most? We find that there are strong evidences showing that the number of the negative eigenvalues of $\rho^T$ is $\frac{N(N-1)}{2}$ at most when $N = M$. Then we give a partial
proof for the problem introduced by Audenaert et al under the assumption that the number of negative eigenvalue of $\rho^T$ (where $\rho$ is a two-qubit state) is 1 at most. At last, we will give our conclusion.

II. THE NUMBER OF NEGATIVE EIGENVALUES OF $\rho^T$

It is well known that the eigenvalues of $\rho^T$ ($\rho$ is a general state in bi-partite system) can be used to detect the entangled property of bi-partite state. When $\rho$ is a separable state, the eigenvalues of $\rho^T$ are positive. But for some entangled states, the eigenvalues of $\rho^T$ may be negative. How many negative eigenvalues can be in $\rho^T$ for different systems? Does the number of the negative eigenvalues have any connection with the entanglement property of $\rho$? These questions are very clear and simple, but their answers are very difficult.

For convenience, we first introduce a useful lemma in matrix analysis [15] before the investigation of these problems. This lemma is about the eigenvalues relations between a Hermitian matrix and its principal submatrix.

Lemma: Let $A$ be a $n \times n$ Hermitian matrix, let $r$ be an integer with $1 \leq r \leq n$, and let $A_r$ be a $r \times r$ principal submatrix of $A$. Then for each integer $k$ such that $1 \leq k \leq n$ we have

$$\lambda_k(A) \leq \lambda_k(A_r) \leq \lambda_{k+n-r}(A),$$

where $\lambda_k(A)$ and $\lambda_k(A_r)$ are the $k$th eigenvalue of $A$ and $A_r$ in increasing order, respectively.

Given this Lemma, we can get the following theory about the number of the negative eigenvalues of $\rho^T$ immediately:

Theorem 1: Let $\rho$ be a bi-partite state in Hilbert space $C^M \otimes C^N$, then the number of the negative eigenvalues of $\rho^T$ is less than $MN - \max(N, M)$.

Proof: Without loss of generality, let $N \geq M$. Suppose the PT operates on the first particle, then using the definition of PT, the $M$ diagonal $N \times N$ blocks of $\rho^T$ (these blocks are $\langle 1_A | \rho^T | 1_A \rangle$, $\langle 2_A | \rho^T | 2_A \rangle$, $\cdots$, $\langle M_A | \rho^T | M_A \rangle$) are the same as the corresponding blocks of $\rho$ (these blocks are $\langle 1_A | \rho | 1_A \rangle$, $\langle 2_A | \rho | 2_A \rangle$, $\cdots$, $\langle M_A | \rho | M_A \rangle$). Since $\rho$ is positive, all these diagonal $N \times N$ blocks are positive.

Let one of the $N \times N$ blocks (such as $\langle 2_A | \rho^T | 2_A \rangle$) be $A_{N \times N}$ and its eigenvalues, arranged in increasing order, be $\{\lambda_1, \lambda_2, \cdots, \lambda_N\}$. In addition, let the eigenvalues of $\rho^T$, also arranged in increasing order, be $\{\hat{\lambda}_1, \hat{\lambda}_2, \cdots, \hat{\lambda}_{N \times M}\}$. It is clear that the block $A_{N \times N}$ is a principal
submatrix of $\rho^T$ (obtained by deleting some $(M - 1)N$ rows and the corresponding columns from $\rho^T$). By the lemma, we can get

$$\hat{\lambda}_k \leq \lambda_k \leq \hat{\lambda}_{k+(M-1)N}$$

(3)

for each integer $k$ such that $1 \leq k \leq N$. Specially, let $k = 1$, we can get

$$0 \leq \lambda_1 \leq \hat{\lambda}_{1+(M-1)N}.$$ 

(4)

That is, $\hat{\lambda}_{1+(M-1)N} \geq 0$. So the number of the negative eigenvalues of $\rho^T$ is $(M - 1)N$ at most.

Q. E. D

Is this the exact limit for the number of the negative eigenvalues of $\rho^T$? When we investigate this problem for $2 \times 2$ system more carefully, we find that it is not the case. We consider the following cases in the two-qubit system to get some concrete idea.

1) $\rho$ is a pure state. It is very clear that $\rho^T$ has 0 negative eigenvalues when $\rho$ is separable and $\rho^T$ has 1 negative eigenvalues when $\rho$ is entangled.

2) $\rho$ is a Bell diagonalized state. So $\rho$ and $\rho^T$ have the forms of

$$\begin{bmatrix}
\alpha_1 & 0 & \beta_1 \\
0 & \alpha_2 & \beta_2 \\
0 & \beta_2^* & \alpha_3 \\
\beta_1^* & 0 & \alpha_4
\end{bmatrix} \quad \text{and} \quad \begin{bmatrix}
\alpha_1 & 0 & \beta_2^* \\
0 & \alpha_2 & \beta_1^* \\
0 & \beta_1 & \alpha_3 \\
\beta_2 & 0 & \alpha_4
\end{bmatrix},$$

(5)

respectively. We can get the relations $\alpha_1 \alpha_4 - |\beta_1|^2 \geq 0$ and $\alpha_2 \alpha_3 - |\beta_2|^2 \geq 0$ by the positive semidefinite of $\rho$. So either $\alpha_1 \alpha_4 - |\beta_2|^2 \geq 0$ or $\alpha_2 \alpha_3 - |\beta_1|^2 \geq 0$. That is, there is a $3 \times 3$ principal submatrix are positive semidefinite in $\rho^T$. So the number of the negative eigenvalue of $\rho^T$ is 1 at most by the similar reason of equation(2).

In fact, to extensively investigate this problem, we use the Monte Carlo method [17] to choose one million random samples and calculate their negative eigenvalues. We find that the number of negative eigenvalues of $\rho^T$ is 1 at most in $2 \times 2$ system. More generally, we use Monte Carlo method to consider the system $N \times M$ and we get the maximal number of
negative eigenvalues of $\rho^T$ in the following table when $N$ and $M$ are small numbers.

| $M \backslash N$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | ... |
|-----------------|---|---|---|---|---|---|---|---|----|-----|
| 2               | 1 | 2 | 3 | 3 | 4 | 4 | 4 | 5 |    |     |
| 3               | 3 | 4 | 4 | 5 | 5 | 6 | 6 | 7 |    |     |
| 4               | 6 | 6 | 7 | 8 | 8 | 8 | 9 |    |    |     |
| 5               | 10| 10| 10| 11| 11| 11|    |    |    |     |
| 6               | 15| 15| 15| 15| 16|    |    |    |    |     |
| 7               | 21| 21| 21| 21| 21|    |    |    |    |     |
| 8               | 28| 28| 28|    |    |    |    |    |    |     |
| 9               | 36| 36|    |    |    |    |    |    |    |     |
| 10              | 45|    |    |    |    |    |    |    |    |     |
| ...             |    |    |    |    |    |    |    |    |    |     |

Table

With this table, we have good reasons to give the following conjecture.

**Conjecture:** The number of the negative eigenvalues of $\rho^T$ is at most $\frac{N(N-1)}{2}$ when $\rho$ is a state in Hilbert space $C^N \otimes C^N$.

Since $\text{PT}$ transformation has no direct geometrical or algebraic meaning, it is difficult to use the powerful geometrical or algebraic tools to completely prove this result even for the simplest case of $2 \times 2$ system. But for this special two-qubit case, we can give some partial results. It is well known that the character of $\rho^T$ is due to the entanglement of $\rho$ in two-qubit case, so the number of the negative eigenvalues of $\rho^T$ is independent of the local unitary. If we use $|0\rangle_1 |0\rangle_2 , |0\rangle_1 |1\rangle_2 , |1\rangle_1 |0\rangle_2$ and $|1\rangle_1 |1\rangle_2$ [where $|0\rangle_1$ and $|1\rangle_1$ are the eigenvectors of $\rho_1 = tr_2(\rho)$, $|0\rangle_2$ and $|1\rangle_2$ are the eigenvectors of $\rho_2 = tr_1(\rho)$] as the basis, and adjust their phase carefully, it is easy to proof that any density matrix $\rho$ of $2 \times 2$ system can be transformed in the following form:

$$
\rho = \begin{bmatrix}
  a_{11} & A & B & \alpha \\
  A & a_{22} & \beta & -B \\
  B & \beta^* & a_{33} & -A \\
  \alpha^* & -B & -A & a_{44}
\end{bmatrix},
$$

(6)
where $A$, $B$, $a_{11}$, $a_{22}$, $a_{33}$ and $a_{44}$ are real numbers. For this density matrix $\rho$, we have the following result:

*Theorem 2:* Let $\rho$ be the form (6), if $AB = 0$ or $\text{Re}(\alpha) = \text{Re}(\beta)$, then $\rho^T$ has 1 negative eigenvalue at most.

Many important states in quantum information are included in this theorem, such as i) Pure states, ii) Bell diagonalized states, iii) Werner states. Though this theorem is not the complete proof of the conjecture of $2 \times 2$ system, it includes enough cases for our use. The proof of this theorem is rather simple.

*Proof:* Since the form of $\rho$ is given as equation (6), then we can get

$$\rho^T = \begin{bmatrix} a_{11} & A & B & \beta^* \\ A & a_{22} & \alpha^* & -B \\ B & \alpha & a_{33} & -A \\ \beta & -B & -A & a_{44} \end{bmatrix},$$

(7)

where the PT transformation operates on the first qubit. For any $3 \times 3$ principal submatrix $A^T$ of $\rho^T$, we have the following interlacing relations [15] between the eigenvalues of $A^T$ and $\rho^T$. Let $\lambda_i (i = 1, 2, 3)$ and $\hat{\lambda}_i (i = 1, 2, 3, 4)$ be the eigenvalues of $A^T$ and $\rho^T$, respectively, and assume that they are arranged in increasing order. Then

$$\hat{\lambda}_1 \leq \lambda_1 \leq \cdots \leq \lambda_3 \leq \hat{\lambda}_4.$$  

(8)

So we can conclude that $\rho^T$ has at most 1 negative eigenvalue if some $3 \times 3$ principal submatrix of $\rho^T$ is positive semidefinite.

Let us consider the $3 \times 3$ principal submatrices of $\rho^T$ and $\rho$. We consider two sets

$$A^T_1 = \begin{bmatrix} a_{11} & A & B \\ A & a_{22} & \alpha^* \\ B & \alpha & a_{33} \end{bmatrix}, A_1 = \begin{bmatrix} a_{11} & A & B \\ A & a_{22} & \beta \\ B & \beta^* & a_{33} \end{bmatrix},$$

(9)

and

$$A^T_2 = \begin{bmatrix} a_{11} & A & \beta^* \\ A & a_{22} & -B \\ \beta & -B & a_{44} \end{bmatrix}, A_2 = \begin{bmatrix} a_{11} & A & \alpha \\ A & a_{22} & -B \\ \alpha^* & -B & a_{44} \end{bmatrix}.$$  

(10)

Since $\rho$ is positive, all the principal submatrix of $\rho$ are positive. Specially, $\begin{bmatrix} a_{11} & A \\ A & a_{22} \end{bmatrix}$ is positive too. Now we only need calculate the determinates of $A^T_1$ and $A^T_2$ under the condition.
that \( A_1 \) and \( A_2 \) are positive. Simple calculations can get

\[
\text{Det}(A_1) - \text{Det}(A_1^T) = 2AB \text{Re}(\beta - \alpha) + a_{11}(|\alpha^2| - |\beta^2|),
\]

(11)

\[
\text{Det}(A_2) - \text{Det}(A_2^T) = 2AB \text{Re}(\beta - \alpha) + a_{11}(|\beta^2| - |\alpha^2|).
\]

(12)

Now, using the conditions that \( AB = 0 \) or \( \text{Re}(\alpha) = \text{Re}(\beta) \), we can get

\[
\text{Det}(A_1) - \text{Det}(A_1^T) = a_{11}(|\alpha^2| - |\beta^2|),
\]

(13)

\[
\text{Det}(A_2) - \text{Det}(A_2^T) = a_{11}(|\beta^2| - |\alpha^2|).
\]

(14)

Obviously, \( \text{Det}(A_1) - \text{Det}(A_1^T) \) or \( \text{Det}(A_2) - \text{Det}(A_2^T) \) is no more than 0. That is, \( \text{Det}(A_1^T) \geq \text{Det}(A_1) \) or \( \text{Det}(A_2^T) \geq \text{Det}(A_2) \). So \( A_1^T \) or \( A_2^T \) is positive semidefinite. This is the end of the proof.

Q. E. D.

But for the higher dimensional situations, the similar result is rather difficult to be obtained. There are a lot of things to do to completely prove our conjecture.

III. PARTIAL PROOF OF \( |\rho^T|^T \geq 0 \) IN TWO-QUBIT SYSTEM

If the number of negative eigenvalue of \( \rho^T \) (\( \rho \) is in \( 2 \times 2 \) system) is really at most 1, we can give a partial proof of equation (1). Obviously, when the two-qubit state \( \rho \) is separable, the equation (1) is correct. But our result show that when the entanglement of the eigenvector corresponding to the negative eigenvalue of \( \rho^T \) is sufficient high (which connected with the condition about the negative entropy of \( \rho \)) the equation is true too.

For any Hermitian matrix \( H \), we can make a expansion

\[
H = H_+ - H_-
\]

(15)

where \( H_+ \) and \( H_- \) are positive semidefinite and \( H_+H_- = H_-H_+ = 0 \). So assume

\[
\rho^T = A - \rho_-
\]

(16)

where \( \text{Rank}(A) = 3 \), \( A\rho_- = 0 \), \( \rho_- = |\Psi\rangle \langle \Psi| \) and \( |\Psi\rangle = \alpha |00\rangle + \beta |11\rangle \) (where \( |\Psi\rangle \) is not normalized and we have used proper local unitary transformations to make \( \alpha \) and \( \beta \) positive real number) at the present situation. Now we can describe our result as the following
Theorem 3: Let \( \rho \) be a two-qubit density matrix, its partial transposition \( \rho^T \) have only one negative eigenvalue \( E \) and the corresponding eigenvector is \( |\Psi \rangle = \alpha |00\rangle + \beta |11\rangle \) (where \( |\Psi \rangle \) is not normalized, \( \alpha \geq \beta \) and \( \alpha^2 + \beta^2 = |E| \)). If \( \alpha \) and \( \beta \) satisfy the conditions:

\[ \alpha \beta = 0 \quad (17) \]

or

\[ 1 \leq \frac{\alpha}{\beta} \leq \sqrt{\sqrt{2} + 1}. \quad (18) \]

Then \( |\rho^T|^T \geq 0. \)

**Proof:** Using the equation (16), we can rewrite \( \rho^T \) and \( \rho \) in explicit form as follows

\[
\rho^T = A - \rho_- = \begin{bmatrix}
A_{11} - \alpha^2 & A_{12} & A_{13} & A_{14} - \alpha \beta \\
A_{21} & A_{22} & A_{23} & A_{24} \\
A_{31} & A_{32} & A_{33} & A_{34} \\
A_{41} - \alpha \beta & A_{42} & A_{43} & A_{44} - \beta^2
\end{bmatrix}
\]

and

\[
\rho = A^T - \rho_- = \begin{bmatrix}
A_{11} - \alpha^2 & A_{12} & A_{31} & A_{32} \\
A_{21} & A_{22} & A_{41} - \alpha \beta & A_{42} \\
A_{13} & A_{14} - \alpha \beta & A_{33} & A_{34} \\
A_{23} & A_{24} & A_{43} & A_{44} - \beta^2
\end{bmatrix},
\]

where we have supposed that the PT transformation operates on the first qubit. Since \( \rho \) is a density matrix of a state, it is positive semidefinite. On the other hand, from the formula (18), we can get \( |\rho^T|^T = A + \rho_- \). So we can express \( |\rho^T|^T \) as follows

\[
|\rho^T|^T = A^T + \rho_- = \begin{bmatrix}
A_{11} + \alpha^2 & A_{12} & A_{31} & A_{32} \\
A_{21} & A_{22} & A_{41} - \alpha \beta & A_{42} \\
A_{13} & A_{14} + \alpha \beta & A_{33} & A_{34} \\
A_{23} & A_{24} & A_{43} & A_{44} + \beta^2
\end{bmatrix}.
\]

If \( \alpha \) or \( \beta \) is equal to zero, that is \( \alpha \beta = 0 \), it is clear that \( |\rho^T|^T \) is positive semidefinite. Without loss of generality, let \( \beta = 0 \), then \( \rho \) and \( |\rho^T|^T \) are the same except the element \((1,1)\). Since \( \rho \) is positive semidefinite, the 3-by-3 principal submatrix

\[
A_{\text{sub}} = \begin{bmatrix}
A_{22} & A_{41} & A_{42} \\
A_{14} & A_{33} & A_{34} \\
A_{24} & A_{43} & A_{44}
\end{bmatrix}
\]

8
is positive semidefinite. In order to prove the positive semidefinite of \( |\rho^T|^T \), we need only consider the determinate of \( |\rho^T|^T \). Simple calculation can find that

\[
\text{Det}(|\rho^T|^T) - \text{Det}(\rho) = 2|\alpha^2| \text{Det}(A_{sub}) \geq 0. \tag{23}
\]

Since \( \rho \) is positive semidefinite, then \( \text{Det}(|\rho^T|^T) \) is positive and \( |\rho^T|^T \) is positive semidefinite. From now on we assume neither \( \alpha \) nor \( \beta \) is equal to 0.

Now we can consider the condition between \( A \) and \( \rho_- \): \( A\rho_- = 0 \). This condition can be expressed by the elements of \( A \) and \( \rho_- \) as

\[
\begin{align*}
\alpha A_{11} + \beta A_{41} &= 0, \\
\alpha A_{41} + \beta A_{44} &= 0.
\end{align*} \tag{24}
\]

These equations imply that \( \frac{A_{11}}{A_{44}} = \frac{\beta^2}{\alpha^2} \). With equation (23), we can delete the elements \( A_{14} \) and \( A_{41} \) from equation (19) and (20). We rewrite \( \rho \) and \( |\rho^T|^T \) as

\[
\rho = \begin{bmatrix}
A_{11} - \alpha^2 & A_{12} & A_{31} & A_{32} \\
A_{21} & A_{22} & -\frac{\alpha}{\beta}(A_{11} + \beta^2) & A_{42} \\
A_{13} & -\frac{\alpha}{\beta}(A_{11} + \beta^2) & A_{33} & A_{34} \\
A_{23} & A_{24} & A_{43} & A_{44} - \beta^2
\end{bmatrix}, \tag{25}
\]

and

\[
|\rho^T|^T = \begin{bmatrix}
A_{11} + \alpha^2 & A_{12} & A_{31} & A_{32} \\
A_{21} & A_{22} & -\frac{\alpha}{\beta}(A_{11} - \beta^2) & A_{42} \\
A_{13} & -\frac{\alpha}{\beta}(A_{11} - \beta^2) & A_{33} & A_{34} \\
A_{23} & A_{24} & A_{43} & A_{44} + \beta^2
\end{bmatrix}. \tag{26}
\]

Now we introduce Shur product (also called Hardmard product) \( [A_{ij}] \in M_{m,n} \) and \( B = [b_{ij}] \in M_{m,n} \). This Shur product is given as \( A \circ B = [a_{ij}b_{ij}] \in M_{m,n} \). It can be proved that \( A \circ B \) is positive semidefinite if \( A \) and \( B \) are positive semidefinite. Using the definition of Shur product, we can get the relations between \( |\rho^T|^T \) and \( \rho \). That is, \( |\rho^T|^T = \rho \circ S \), where \( S \) is defined as

\[
S = \begin{bmatrix}
\frac{A_{11} + \alpha^2}{A_{11} - \alpha^2} & 1 & 1 & 1 \\
1 & 1 & \frac{A_{11} - \beta^2}{A_{11} + \beta^2} & 1 \\
1 & \frac{A_{11} - \beta^2}{A_{11} + \beta^2} & 1 & 1 \\
1 & 1 & 1 & \frac{A_{11} + \beta^2}{A_{11} - \beta^2}
\end{bmatrix}. \tag{27}
\]
we have used the relations between $A_{11}$ and $A_{44}$ to delete $A_{44}$. We have known that $\rho$ is positive semidefinite. Since Shur product have the property that $A \circ B$ is positive semidefinite if $A$ and $B$ are positive semidefinite, we need only to consider when $S$ is positive semidefinite under the condition $\rho \geq 0$.

At first, we need to get the relations of $A_{11}$, $\alpha$ and $\beta$ by $\rho \geq 0$, that is

$$A_{11} \geq \alpha^2,$$  \hspace{1cm} (28)

$$A_{11} \geq \frac{\beta^4}{\alpha^2},$$  \hspace{1cm} (29)

$$A_{22}A_{33} - \frac{\alpha^2}{\beta^2} (A_{11} + \beta^2)^2 \geq 0,$$  \hspace{1cm} (30)

$$A_{11} - \alpha^2 + \frac{\alpha^2}{\beta^2} A_{11} - \beta^2 + A_{22} + A_{33} = 1.$$  \hspace{1cm} (31)

The last conditions is given by the condition $\text{tr}(\rho) = 1$. Using conditions (27.3) to delete $A_{22}$ and $A_{33}$ in (27.4), then the condition (27.4) can be rewritten as

$$A_{11} - \alpha^2 + \frac{\alpha^2}{\beta^2} A_{11} - \beta^2 + 2 \frac{\alpha}{\beta} (A_{11} + \beta^2) \leq 1.$$  \hspace{1cm} (32)

That is

$$\left(\frac{\alpha + \beta}{\beta}\right)^2 A_{11} \leq 1 + (\alpha - \beta)^2.$$  \hspace{1cm} (33)

Without loss of generality, let $\alpha \geq \beta$, then the conditions of $A_{11}$, $\alpha$ and $\beta$ can be reduced to (27.1) and (29). In order to make these two inequalities are consistent, it requires

$$\alpha^2 \leq \frac{1 + (\alpha - \beta)^2}{(\alpha + \beta)^2} \beta^2.$$  \hspace{1cm} (34)

We can rewrite this condition in another way if let $k = \frac{\alpha}{\beta}$, that is

$$\beta^2 \leq \frac{1}{k^2(k+1)^2 - (k-1)^2}.$$  \hspace{1cm} (35)

In fact, this condition is about the negative eigenvalue of $\rho^T$

$$|E| = \alpha^2 + \beta^2 \leq E_1 = \frac{1 + k^2}{k^2(k+1)^2 - (k-1)^2}.$$  \hspace{1cm} (36)

Now we turn back to consider matrix $S$. Using conditions (27.1) and (27.2), all of the $1 \times 1$ and $2 \times 2$ principal submatrices of $S$ are positive semidefinite. We need only to consider $\det(S_{3 \times 3})$ and $\det(S)$ where we choose a 3-by-3 principal submatrix as

$$S_{3 \times 3} = \begin{bmatrix} \frac{A_{11} + \alpha^2}{A_{11} - \alpha^2} & 1 & 1 \\ 1 & 1 & \frac{A_{11} - \beta^2}{A_{11} + \beta^2} \\ 1 & \frac{A_{11} - \beta^2}{A_{11} + \beta^2} & 1 \end{bmatrix}.$$  \hspace{1cm} (37)
Simple Calculation can show that
\[
\det(S_{3 \times 3}) = \frac{4 \nu [(2 \mu - \nu)A_{11} + \mu \nu]}{(A_{11} - \mu)(A_{11} + \nu)^2},
\]
where \(\mu = \alpha^2\) and \(\nu = \beta^2\) for simplicity. It is easy to verified that \(\det(S_{3 \times 3}) \geq 0\) since we have let \(\alpha \geq \beta\) and \(A_{11} \geq \alpha^2\). It is also easy to get the determinate of \(S\) as
\[
\det(S) = -\frac{8 \nu [(\mu - \nu)^2A_{11} - 2 \mu \nu^2]}{(A_{11} - \mu)(A_{11} + \nu)^2(\mu A_{11} - \nu^2)}.
\]
(39)

For the same reason of \(\det(S_{3 \times 3})\), to make \(\det(S) \geq 0\), it is sufficient to make \((\mu - \nu)^2A_{11} - 2 \mu \nu^2 \leq 0\). This requirement is,
\[
A_{11} \leq \frac{2 \mu \nu^2}{(\mu - \nu)^2}.
\]
(40)

In order to make requirement (36) possible, \(\alpha\) and \(\beta\) must satisfy the condition \(\mu \leq \frac{2 \mu \nu^2}{(\mu - \nu)^2}\). That is,
\[
1 \leq \frac{\mu}{\nu} \leq \sqrt{2} + 1
\]
(41)

where we have considered the relation between \(\alpha\) and \(\beta\).

Now we have to compare the conditions (29) and (36). If
\[
\frac{1 + (\alpha - \beta)^2}{(\alpha + \beta)^2} \leq \frac{2 \alpha^2 \beta^4}{(\alpha^2 - \beta^2)^2},
\]
then the requirement (36) will be automatically guaranteed by the conditions (27.1) and (29) (positive semidefinite of \(\rho\)). That is, \(S\) will be positive semidefinite for \(\rho \geq 0\). This condition is also about the negative eigenvalue of \(\rho^T\)
\[
|E| = \mu + \nu \geq E_2 = \frac{(1 + k^2)(k - 1)^2}{2k^2 - (k - 1)^4}.
\]
(43)

So we have two conditions about the negative eigenvalue, conditions (32) and (39), coming from the positive semidefinite of \(\rho\) and \(S\), respectively. In order to make these two conditions consistent, it will require that
\[
\frac{1}{k^2(k + 1)^2 - (k - 1)^2} \geq \frac{(k - 1)^2}{2k^2 - (k - 1)^4}.
\]
(44)

this inequality gives the same constraint on the parameter \(k\) as condition (37). In another word, inequality (40) is automatically satisfied under the condition (37).

So when the eigenvector corresponding to the negative eigenvalue of \(\rho^T\) satisfies condition \(1 \leq k \leq \sqrt{2} + 1\) which implies the condition of negative eigenvalue about \(E_2 \leq |E| \leq E_1\), the formula \(|\rho^T|^T = \rho \circ S\) is positive semidefinite.
This is the end of the proof.
Q. E. D.

When the density matrix $\rho$ is separable, this theorem is trivial. Our theorem shows that the entanglement of the eigenvector corresponding to negative eigenvalue of $\rho^T$ is concerned with the formula (1). When the entanglement is zero or sufficiently high, this formula is true. As a matter of fact, the conditions (17.1) and (17.2) are concerned with the entanglement of $|\Psi\rangle$. Equation (17.1) means that the state is a product state and the entanglement is zero. Equation (17.2) means that the state is near the maximal entangled state where $\alpha = \beta$ and the entanglement is rather high. Our theorem also shows that this formula is related with the negative entropy of the density matrix $\rho$. We know that the negativity[18] of a state $\rho$ is defined as $N(\rho) = (|\rho^T|_1 - 1)/2$ (another measurement, logarithmic negativity, is defined as $E_N = \log_2 |\rho^T|_1$). It is easy to show $N(\rho) = \sqrt{|E|}$. So it is clear that the condition of equation (40) is just for the negativity of state $\rho$. In our case, the negativity is bounded by the formula of $k$ (in another word, the entanglement of $|\Psi\rangle$). So the negativity of $\rho$ and the entanglement of $|\Psi\rangle$ are connected. We cannot determine which aspect is the key quantity concerned with the formula (1).

IV. SUMMARY

In this paper, we discussed the mathematical property of partial transposition which is a famous operator in quantum information. More concretely, we consider the number of the negative eigenvalues of $\rho^T$. Through Monte Carlo random method, we find that there are good reasons to conjecture that the maximal number of negative eigenvalues of $\rho^T$ (where $\rho$ is a quantum state in $C^{N\times N}$ Hilbert space) is $\frac{N(N-1)}{2}$. This conjecture is clear, but it is hard to prove even for the two-qubit system. We just prove it under some special case, but this special case have included many often used cases. How to completely prove this result is still a big challenge for us. There are some reasons for its difficulty. One is that the PT transformation has no direct relations with some known geometrical or algebraic operators. So we can’t use their powerful tools. The other is that the eigenvalues of $\rho^T$ are invariants under global unitary in the whole Hilbert space. But $\rho$ and $\rho^T$ are related by their local elements, these relations are not invariants under global unitary.

When the state $\rho$ is separable, it is easy to see that $|\rho^T|^T \geq 0$ since the operator $|.|$ does
nothing on $\rho^T$. We have shown that it is also true when the entanglement of the eigenvector corresponding to the negative eigenvalue of $\rho^T$ is sufficiently high (or the negative entropy of $\rho$ satisfy some condition). But to complete this proof is beyond the technique introduced in this paper. $|.|$ is only concerned with the eigenvalues of $\rho^T$, but PT transformation is concerned with the elements of $\rho$. So it is hard to find the direct relations between $\rho$ and $|\rho^T|^T$. In other words, it is hard to prove the positive semidefinite of $|\rho^T|^T$ by the positive semidefinite of $\rho$. There are some evidences that we need consider all of the elements of $\rho$ to complete the proof. But it is hard to deal with so many variables. So it may be necessary to introduce some new techniques to this problem.

V. ACKNOWLEDGMENT

This work was funded by the National Fundamental Research Program (2001CB309300), the Innovation Funds from Chinese Academy of Sciences (CAS), China Postdoctoral Science Foundation(2005038012) and Chinese Academy of Sciences K. C. Wong Post-doctoral Fellowships.

[1] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, England, 2000).
[2] P. W. Shor, Proceedings 35th Annual symposium on foundations of computer science, (IEEE Press, Los Alamitos, CA, 1994).
[3] L. K. Grover, Phys. Rev. Lett. 79, 325 (1997).
[4] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin and W. K. Wootters, Phys. Rev. A. 54, 3824(1996).
[5] V. Vedral and M. B. Plenio, Phys. Rev. A, 57, 1619 (1998).
[6] V. Vedral, Rev. Mod. Phys. 74, 197 (2002).
[7] M. Lewenstein, B. Kraus, J. I. Cirac and P. Horodecki, Phys. Rev. A 62, 052310 (2000).
[8] M. Lewenstein, B. Kraus, J. I. Cirac and P. Horodecki, Phys. Rev. A 63, 044304 (2001).
[9] W. Dür, J. I. Cirac and R. Tarrach, Phys. Rev. Lett. 83, 3562 (1999); W. Dür and J. I. Cirac, Phys. Rev. A 61, 042314 (2000); W. Dür and J. I. Cirac, Phys. Rev. A 62, 022302 (2000).
[10] A. Peres, Phys. Rev. Lett. 77, 1413 (1996).

[11] M. Horodecki, P. Horodecki and R. Horodecki, Phys. Lett. A 223, 1 (1996).

[12] P. Horodecki, Phys. Lett. A 232, 333 (1997).

[13] K. Audenaert, B. De Moor, K. G. H. Vollbrecht and R. F. Werner, Phys. Rev. A 66, 032310 (2002).

[14] O. Krueger and R. F. Werner, quant-ph/0504166.

[15] R. A. Horn, C. R. Johnson, Matrix Analysis, (Cambridge University Press, Cambridge, England, 1985).

[16] R. V. Kadison, J. R. Ringrose, Fundamentals of the theory of operator algebras, American Mathematical Society, 1997.

[17] D. P. Landau and K. Binder, A guide to Monte Carlo Simulations in Statistical Physics, (Cambridge University Press, Cambridge, England, 2005).

[18] G. Vidal and R. F. Werner, Phys. Rev. A 65, 032314 (2002).