Partial Transpose of Permutation Matrices

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Abstract

The partial transpose of a block matrix $M$ is the matrix obtained by transposing the blocks of $M$ independently. We approach the notion of partial transpose from a combinatorial point of view. In this perspective, we solve some basic enumeration problems concerning the partial transpose of permutation matrices. More specifically, we count the number of permutations matrices which are equal to their partial transpose and the number of permutation matrices whose partial transpose is still a permutation. We solve these problems also when restricted to symmetric permutation matrices only.

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1 Introduction

The partial transpose (or, equivalently, partial transposition) is a linear algebraic concept, which can be interpreted as a simple generalization of the usual matrix transpose. In the present paper, we consider partial transpose from a combinatorial point of view. More specifically, we solve some enumeration problems concerning the partial transpose of permutation matrices.

Even if this notion is a natural one, to the knowledge of the authors, it has never been directly studied by the linear algebra community. On the other hand, partial transpose is an important tool in the mathematical theory of quantum entanglement. For this reason, partial transpose appears often in works contextual with quantum information theory. We will spend a few paragraphs on this, just for taking a snapshot of the scenario in which this notion arises.

Brüll and Macchiavello [3] give an excellent explanation of the meaning of partial transpose in quantum information theory. Its primary use is materialized in the so-called PPT-criterion, where “PPT” stands for Positive Partial Transpose. The criterion, firstly discovered by Peres [13] and the Horodeckis [10] (see also [12]), is as follows: if the density matrix (or, equivalently, the state) of a quantum mechanical system with composite dimension $pq$ is entangled, with respect to the subsystems of dimension $p$ and $q$, then its partial transpose is positive. The converse of the implication is not necessarily true. However, under certain restrictions, for example, when the dimension of the density matrix is six, the PPT-criterion is necessary and sufficient.

There is a number of problems suggested by the PPT-criterion. In particular, in order to shed light onto the structure of the set of density matrices, it would be important to characterize those for which the criterion is valid. An open question of practical importance is to prove or disprove that certain states, which are said to be non-distillable, have positive partial transpose. However, there is strong evidence that there exist non-distillable states with negative partial transpose, which would be then called NPT-bound entangled states. Regarding this topic, see the important references [6, 7], or [4], for an account on recent discussions.

Looking at the notion of partial transpose from the combinatorial point of view is an appealing topic, because it has the potential to uncover patterns in the set of density matrices and indicate connections with other mathematical objects, and this may turn out to be helpful in understanding physical properties. As a matter of fact there have been a number of recent papers...
considering entanglement in discrete settings (see, e.g., [1, 8, 11]).

Here we state and solve some basic enumeration problems involving partial transpose of permutation matrices. Permutations appear in fact to be a simple, yet a rich territory to explore. Enumeration is a good first step towards the quantitative understanding of the structure of a set.

In particular, we count the number of permutations matrices which are equal to their partial transpose and the number of permutation matrices whose partial transpose is still a permutation. We solve these problems also when restricted to symmetric permutation matrices only (i.e., induced by involutions).

Apart from considerations related to symmetry, given that symmetry often predisposes to relations between different combinatorial objects, a further reason to look at involutions comes from [1]. A permutation matrix associated to an involution without fixed points can be seen as the adjacency matrix of the disjoint union of matchings and self-loops. Since the combinatorial Laplacian of any graph is a density matrix after appropriate normalization [1], counting the number of involutions whose partial transpose is a permutation, is equivalent to count the number of these states with positive partial transpose. However, the PPT-criterion is not sufficient also for this extremely restricted class. There actually are disconnected graphs whose Laplacian is entangled even if its partial transpose is positive [9].

The organization of the paper is as follows. In the next section, we give the required definitions and formally state our problems. Section 3 deals with permutations whose partial transpose is a permutation; Section 4 with permutations equal to their partial transpose; Section 5 with involutions whose partial transpose is a permutation.

2 Definitions, statements of the problems and examples

The following is a formal definition of the partial transpose of a matrix:

**Definition 1** Let $M$ be an $n \times n$ matrix with real entries. Let us assume that $n = pq$, where $p$ and $q$ are chosen arbitrarily. Under this assumption, we can look at the matrix $M$ as partitioned into $p^2$ blocks each one $q \times q$. The
partial transpose of $M$, denoted by $M^\Gamma_p$, is the matrix obtained from $M$, by transposing independently each of its $p^2$ blocks. Formally, if

$$M = \begin{pmatrix} B_{1,1} & \cdots & B_{1,p} \\ \vdots & \ddots & \vdots \\ B_{p,1} & \cdots & B_{p,p} \end{pmatrix}$$

then

$$M^\Gamma_p = \begin{pmatrix} B_{1,1}^T & \cdots & B_{1,p}^T \\ \vdots & \ddots & \vdots \\ B_{p,1}^T & \cdots & B_{p,p}^T \end{pmatrix},$$

where $B_{i,j}^T$ denotes the transpose of the block $B_{i,j}$, for $1 \leq i, j \leq p$.

Notice that, by taking the adjoint $B_{i,j}^\dagger$, instead of the transpose $B_{i,j}^T$, the notion of partial transpose can be easily extended to matrices with complex entries. This is something which we will not need here. Note that we have defined partial transpose with respect to the parameter $p$. We could have also defined partial transpose with respect to the parameter $q$, by treating the blocks of $M$ as the entries of a $p \times p$ matrix. Formally,

$$M^{\Gamma_q} = \begin{pmatrix} B_{1,1} & \cdots & B_{p,1} \\ \vdots & \ddots & \vdots \\ B_{1,p} & \cdots & B_{p,p} \end{pmatrix}.$$ 

That is, the block $B_{i,j}$ in $M$ is the block $B_{j,i}$ in $M^{\Gamma_q}$, for all $1 \leq i, j \leq p$. The term “partial transpose” also indicates the actual operation required to obtain the matrix partial transpose as defined here.

We will consider partial transpose of permutation matrices. Let us recall that a permutation matrix of size $n$ is an $n \times n$ matrix, with entries in the set $\{0, 1\}$, such that each row and each column contains exactly one nonzero entry. A permutation of length $n$ is a bijection $\pi : [n] \rightarrow [n]$, where $[n] = \{1, 2, \ldots, n\}$. Given an $n \times n$ permutation matrix $P$, there is a unique permutation $\pi$ of length $n$ associated to $P$, such that $\pi(i) = j$ if and only if $P_{i,j} = 1$. Let us denote by $S_n$ the set of all $n \times n$ permutation matrices. With an innocuous abuse of notation, we write $S_n$ also for the set of all permutations of length $n$.

In standard linear notation, a permutation $\pi \in S_n$ can be written as a word of the form $\pi(1)\pi(2)\ldots\pi(n)$. It may be interesting to point out that a
permutation and its partial transpose share a common property, related to the sum of the row indices. The cells in the table below contain ordered pairs: each left element of the pairs is a permutation $\pi \in S_4$; each right element is the ordered list of the row indices of the one entries in the matrix $P^{\Gamma_2}$:

| 1234, 1234 | 1243, 1243 | 1324, 1414 | 1342, 1432 | 1423, 1441 | 1432, 1432 |
|-------------|-------------|-------------|-------------|-------------|-------------|
| 2134, 2134 | 2143, 2143 | 2314, 4114 | 2341, 4123 | 2413, 1414 | 2431, 1423 |
| 3142, 2314 | 3142, 2323 | 3214, 3214 | 3241, 3223 | 3412, 3412 | 3421, 3421 |
| 4123, 2341 | 4132, 2332 | 4213, 2314 | 4231, 2323 | 4312, 4312 | 4321, 4321 |

**Example 2** If

$$P = \begin{pmatrix}
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0
\end{pmatrix},$$

then

$$P^{\Gamma_2} = \begin{pmatrix}
0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 1 & 1 & 0
\end{pmatrix}.$$  

The matrix $P$ is induced by the permutation $\pi = 3124$. The ordered list of the row indices of the one entries in $P^{\Gamma_2}$ is 2323.

For every permutation $\pi \in S_n$, where $n = pq$, we have

$$\sum_{i=1}^{n} \pi(i) = \sum_{i=1}^{n} i = \sum_{P_{i,j}=1}^{P_{i,j}=1} i = \sum_{P_{i,j}=1}^{P_{i,j}=1} i \quad \text{(1)}$$

$$= n(n + 1)/2.$$  

This is straightforward. Let the $(ap + i, b(a, i)p + j(a, i))$-th entry of $P$ be equal to 1. Then $b(a, i)$ runs $p$ times over $0, \ldots, q - 1$ and $j(a, i)$ runs $q$ times over $1, \ldots, p$. Thus,

$$\sum_{a,i} b(a, i) = p \binom{q}{2},$$

and

$$\sum_{a,i} j(a, i) = q \binom{p + 1}{2}.$$
Therefore
\[
\sum_{a,i} a_p + j(a, i) = p \binom{q}{2} + q \binom{p + 1}{2} = \binom{n + 1}{2},
\]
which validates Eq. (1).

Let us recall that a permutation matrix \( P \) is said to be a involution if \( P = P^T \) and \( P \) is not the identity matrix. We will solve the following problems:

**Problem 3** Count the number of permutation matrices \( P \in S_{pq} \) such that \( P^{\Gamma_p} \in S_{pq} \).

**Example 4** When \( p = q = 2 \), we have all together 12 matrices \( P \in S_4 \) such that \( P^{\Gamma_2} \in S_4 \). Among these, 8 are the block-matrices of the forms
\[
\begin{pmatrix}
* & 0 \\
0 & *
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
0 & * \\
* & 0
\end{pmatrix}.
\] (2)
The remaining 4 matrices are
\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix},
\begin{bmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0
\end{bmatrix},
\begin{bmatrix}
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{bmatrix}.\] (3)

**Problem 5** Count the number of permutation matrices \( P \in S_{pq} \) such that \( P^{\Gamma_p} = P \).

**Example 6** When \( p = q = 2 \), we have all together 10 matrices \( P \in S_4 \) such that \( P^{\Gamma_2} = P \). Among these, 8 are the block matrices in Eq. (2). The remaining 2 matrices are the first and the third matrix in Eq. (3).

**Problem 7** Count the number of involutions \( P \in S_{pq} \) such that \( P^{\Gamma_p} \in S_{pq} \).
Example 8 When \( p = q = 2 \), we have all together 8 involutions \( P \in S_4 \) such that \( P^{\Gamma_2} = P \):

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}
, 
\begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0
\end{pmatrix}
, 
\begin{pmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}
, 
\begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}
, 
\begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
, 
\begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
, 
\begin{pmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}
, 
\begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
.
\]

3 Permutations whose partial transpose is a permutation

We begin with Problem 3. For a permutation matrix \( P \in S_{pq} \), let us denote by \( \mathcal{B}_{i,j} \) the block located in the \( i \)-th row and \( j \)-th column. Let further \( A_{i,j}, B_{i,j} \subseteq [q] = \{1, 2, \ldots, q\} \) be the sets of relative row indices and column indices of the 1’s in the block \( \mathcal{B}_{i,j} \). For example, given

\[
\begin{pmatrix}
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0
\end{pmatrix}
,
\]
we have

\[
A_{1,1} = \{2\}, A_{1,2} = \{1\}, A_{2,1} = \{1\}, A_{2,2} = \{2\},
\]
and

\[
B_{1,1} = \{1\}, B_{1,2} = \{2\}, B_{2,1} = \{2\}, B_{2,2} = \{1\}.
\]

Clearly, \( A_{i,j} \) has the same cardinality as \( B_{i,j} \), which we denote by \( r_{i,j} \). For fixed \( A_{i,j} \) and \( B_{i,j} \), we have \( r_{i,j}! \) ways to place 1’s in \( \mathcal{B}_{i,j} \). Therefore, the number of required matrices equals the number of \( A_{i,j}, B_{i,j} \)'s multiplied by \( \prod_{i,j} r_{i,j}! \). At this stage, we impose the required constraints on \( A_{i,j} \) and \( B_{i,j} \).

We know that \( P \) is a permutation matrix if and only if

\[
A_{i,j} \cap A_{i,k} = \emptyset, \quad \text{for every } i, j, k \text{ with } j \neq k, \quad (4)
\]

\[
B_{i,j} \cap B_{k,j} = \emptyset, \quad \text{for every } i, j, k \text{ with } i \neq k, \quad (5)
\]
We need that $P^F_p$ is also a permutation matrix. Therefore, we have

$$A_{i,j} \cap A_{k,j} = \emptyset, \quad \text{for every } i, j, k \text{ with } i \neq k,$$

(8)

$$B_{i,j} \cap B_{i,k} = \emptyset, \quad \text{for every } i, j, k \text{ with } j \neq k,$$

(9)

and

$$\bigcup_{i=1}^{p} A_{i,j} = [q], \quad \text{for } j = 1, 2, \ldots, p,$$

(10)

$$\bigcup_{j=1}^{p} B_{i,j} = [q], \quad \text{for } i = 1, 2, \ldots, p.$$

(11)

Let

$$A_\pi = \bigcap_{i=1}^{p} A_{i,\pi_i} \quad \text{and} \quad B_\pi = \bigcap_{i=1}^{p} B_{i,\pi_i}, \quad \forall \pi \in S_p,$$

By Eqs. (4)–(6), we know that

$$A_{i,j} = \bigcup_{\pi_i = j} A_\pi, \quad B_{i,j} = \bigcup_{\pi_i = j} B_\pi.$$

(12)

From (4) and (5), we can then write

$$A_\pi \cap A_\sigma = B_\pi \cap B_\sigma = \emptyset, \quad \text{for every } \pi, \sigma \in S_p \text{ with } \pi \neq \sigma.$$

(13)

Furthermore,

$$\bigcup_{\pi \in S_p} A_\pi = \bigcup_{\pi \in S_p} B_\pi = [q].$$

(14)

Conversely, given two set partitions $\{A_\pi\}$ and $\{B_\pi\}$ of $[q]$, satisfying Eqs. (13) and (14), we may define $A_{i,j}$ and $B_{i,j}$ by Eq. (12). One can easily check that Eqs. (4)–(11) hold. The only restriction on the $A_\pi$'s and the $B_\pi$'s is that the cardinalities of $A_{i,j}$ and $B_{i,j}$ should be the equal. Let $a_\pi$ and $b_\pi$ denote the cardinalities of $A_\pi$ and $B_\pi$, respectively. On the basis of the above lines, we can state the following result:
Theorem 9  Let $Z(p, q)$ the number of permutation matrices $P \in S_{pq}$ such that $P^\Gamma \in S_{pq}$. Then

$$Z(p, q) = \sum_{\sum a_\pi = \sum b_\pi = q} \frac{q!^2}{\prod a_\pi! b_\pi!} \prod_{i,j=1}^p \left( \sum_{\pi_i = j} a_\pi \right)!, \quad (15)$$

where the sum runs over all $a_\pi, b_\pi \in \mathbb{Z}$.

The following corollary shows a neat expression for the special case $P \in S_{2q}$:

Corollary 10 The number of permutation matrices $P \in S_{2q}$ such that $P^\Gamma \in S_{2q}$ is

$$Z(2, q) = q!(q + 1)!.$$  

The pattern avoidance language is now a standard tool for characterizing classes of permutations (see [16]). It would be natural to find a characterization of the set of permutations given in Theorem 9 in terms of pattern avoidance.

4 Permutations equal to their partial transpose

We now focus on Problem 5. We then ask that $B_{i,j} = B_{i,j}^T$. Hence, $A_{i,j} = B_{i,j}$. Additionally, given $A_{i,j}$, the number of ways to put 1’s in the block $B_{i,j}$ is exactly the number of involutions of length $q$, which we denote by $I(q)$. It is well-known that (see, e.g., [15], Example 5.2.10)

$$I(q) = \sum_{j=0}^q \binom{q}{j} \frac{j!}{2^{j/2}(j/2)!} \quad (16)$$

and

$$I(q + 1) = I(q) + q \cdot I(q - 1).$$

With the same analysis carried on for Theorem 9 we can directly obtain the number of desired matrices:
Theorem 11 Let \( Z_e(p, q) \) the number of permutation matrices \( P \in S_{pq} \) such that \( P = P^{\Gamma_p} \). Then

\[
Z_e(p, q) = \sum_{a_\pi = q} \frac{q!}{\prod_{\pi} a_\pi!} \prod_{i,j=1}^{p} i \left( \sum_{\pi_i = j} a_\pi \right),
\]

where the sum runs over all \( a_\pi \in \mathbb{Z} \), with \( \pi \in S_p \).

When taking \( p = 2 \), the number of permutation matrices is given in the next corollary:

Corollary 12 The number of permutation matrices \( P \in S_{2q} \) such that \( P = P^{\Gamma_2} \) is

\[
Z_e(2, q) = \sum_{r=0}^{q} \binom{q}{r}^2 I(r)^2 I(q-r)^2.
\]

5 Involution whose partial transpose is a permutation

In this section, we present a solution of Problem 7. Let \( P \) be the involution defined by the ordered pairs \((aq+i, bq+j)\), where \(0 \leq a, b \leq p-1, 1 \leq i, j \leq q\) and \((a, i) \neq (b, j)\). Note that the partial transpose keeps fixed the 1’s in the diagonal. So, the only possible permutation matrices after partial transpose would be the identity matrix \( \text{Id} \) or \( P \) itself. In the first case, we must have \( P = \text{Id} \), since we get back to the original matrix by applying twice the partial transpose operation. Therefore, we only need to consider the second case, that is, when \( P \) remains invariant under partial transpose. Notice that the \((aq+i, bq+j)\)-th and the \((bq+j, aq+i)\)-th entry of the permutation matrix are 1’s. After partial transpose, the \((aq+j, bq+i)\)-th and the \((bq+i, aq+j)\)-th entry are 1’s. Thus we have

\[
(aq+i, bq+j) = (aq+j, bq+i),
\]

\[
(bq+j, aq+i) = (bq+i, aq+j),
\]

or

\[
(aq+i, bq+j) = (bq+i, aq+j),
\]

\[
(bq+j, aq+i) = (aq+j, bq+i).
\]
That is, \( i = j \) or \( a = b \). Hence, the desired involutions are of type \((aq + i, aq + j)\), with \( i \neq j \), or, of type \((aq + i, bq + i)\), with \( a \neq b \). We can then state the following fact:

**Theorem 13** Let \( Z_t(p, q) \) be the number of involutions \( P \in S_{pq} \) such that \( P^{\top} \in S_{pq} \), or, equivalently, \( P^{\top} = P \). Then

\[
Z_t(p, q) = 2p \binom{q}{2} + 2q \binom{p}{2}.
\]

**Corollary 14** The following statements hold true:

- \( Z_t(q + 1, q) = q(q + 1)(2q - 1) \);
- \( Z_t(q, q) = 2(q^3 - q^2) \).

The numbers \( Z_t(q + 1, q)/2 \) are called *octagonal pyramidal numbers*, and count the ways of covering a \( 2q \times 2q \) lattice with \( 2q^2 \) dominoes with exactly 2 horizontal dominoes ([14], Seq. A002414). The numbers \( Z_t(q, q) \) count the possible rook moves on a \( a \times q \) chessboard ([1, 14], Seq. A002414).

To conclude this section, even if these are simple facts, it may be clarifying to remark the following:

**Proposition 15** The following statements hold true for all \( p \) and \( q \):

- \( Z(p, q) = Z(q, p) \);
- In general, \( Z_e(p, q) \neq Z_e(q, p) \);
- \( Z_t(p, q) = Z_t(q, p) \).

**Proof.** While the second point is obvious, the other two can be verified by the following bijection. Suppose that the \((ap + i, b(a, i)p + j(a, i))\)-th entry of \( P \) is 1. Then let the \(((i - 1)q + (a + 1), (j(a, i) - 1)q + (b(a, i) + 1))\)-th entry of \( P^{\top} \) be 1. If the partial transpose of \( P \) is a permutation, then \( ap + j(a, i) \) and \( b(a, i)p + i \) run from 1 to \( n \), for \( 0 \leq a \leq q - 1, 1 \leq i \leq p \). Thus, \((i - 1)q + (b(a, i) + 1)\) and \((j(a, i) - 1)q + (a + 1)\) run from 1 to \( n \) also. This implies that the partial transpose of \( P^{\top} \) is a permutation.

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