# PARTIAL TRANSPOSE OF PERMUTATION MATRICES

Abstract. The main purpose of this paper is to look at the notion of partial transpose from the combinatorial side. In this perspective, we solve some basic enumeration problems involving partial transpose of permutation matrices. Specifically, we count the number of permutations matrices which are invariant under partial transpose. We count the number of permutation matrices which are still permutation matrices after partial transpose. We solve this problem also for transpositions. In this case, there is little evidence to justify a link between some permutations, partial transpose, and certain domino tilings.

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## 1. Introduction

The partial (matrix) transpose is a linear algebraic concept, which can be interpreted as a simple generalization of the usual matrix transpose. The partial transpose can be defined for every square matrix of composite degree. The definition is as follows. Let $p, q$ be two positive integers, $n = pq$ and $M$ be an $n \times n$ matrix with real entries. 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

$$M = \begin{bmatrix} \mathcal{B}_{1,1} & \cdots & \mathcal{B}_{1,p} \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{p,1} & \cdots & \mathcal{B}_{p,p} \end{bmatrix} \quad \text{then} \quad M^{\Gamma_p} = \begin{bmatrix} \mathcal{B}_{1,1}^T & \cdots & \mathcal{B}_{1,p}^T \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{p,1}^T & \cdots & \mathcal{B}_{p,p}^T \end{bmatrix},$$

where $\mathcal{B}_{i,j}^T$ denotes the transpose of the block $\mathcal{B}_{i,j}$, for $1 \leq i, j \leq p$. By taking the adjoint $\mathcal{B}_{i,j}^\dagger$, instead of the transpose $\mathcal{B}_{i,j}^T$, we can easily extend the notion of partial transpose to matrices with complex entries. This is something which we will not need in the present paper. Note that we have defined partial transpose with respect to the parameter $p$. We can also define partial transpose with respect to the parameter $q$, if we look at the blocks of $M$ as the entries of a $p \times p$ matrix. Formally,

$$M^{\Gamma_q} = \begin{bmatrix} \mathcal{B}_{1,1} & \cdots & \mathcal{B}_{p,1} \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{1,p} & \cdots & \mathcal{B}_{p,p} \end{bmatrix}.$$

That is, the block $\mathcal{B}_{i,j}$ in $M$ is the block $\mathcal{B}_{j,i}$ in $M^{\Gamma_q}$ for all $1 \leq i, j \leq p$.

The role of partial transpose is important in the mathematical theory of quantum entanglement. For a general reference on the topic see, *e.g.*, [7]; see [2] for an explanation of the meaning of partial transpose in this context. In particular, the *PPT-criterion* [5, 7, 8], where "PPT" stands for *Positive Partial Transpose*, also called *Peres-Horodecki criterion*, ascertains that 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. Interestingly, it does not matter if the partial transpose is taken with respect to $p$ or to $q$. An important open mathematical problem is to prove that *non-distillable* states have positive partial transpose (see, *e.g.*, [3]).

Looking at partial transpose from the combinatorial point of view is an appealing topic, because it has the potential to uncover rules and patters behind the behavior of entangled states. As a matter of fact there have been a number of recent papers considering entanglement combinatorially [1, 4, 6]. Permutation matrices appear to be a simple, yet rich territory to start with. We will deal with some enumeration problems involving permutation matrices and partial transpose. 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 $\pi : [n] \longrightarrow [n]$, where $[n] = \{1, 2, ..., n\}$. 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 abuse of notation, we write $S_n$ also for the set of all permutations of length $n$.

We will consider the following problems:

- Count the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$.

For example, when $p = q = 2$, we have all together $4 + 4 + 4 = 12$ matrices $P \in S_4$ such that $P^{\Gamma_2} \in S_4$. Among these, 8 are the block-matrices of the forms

$$\begin{bmatrix} * & \mathbf{0} \\ \mathbf{0} & * \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \mathbf{0} & * \\ * & \mathbf{0} \end{bmatrix} . \tag{1}$$

The remaining 4 matrices are the circulant and anti-circulant matrices

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{2}$$

- Count the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} = P$.

For example, when $p = q = 2$, we have all together $4 + 4 + 2 = 10$ matrices $P \in S_4$ such that $P^{\Gamma_2} = P$. Among these, 8 are the block matrices in equation 1. The remaining 2 matrices are the first and the third anti-circulant matrices in equation 2.

We will also consider the number of transpositions which are invariant under partial transpose. This is equivalent to count the number of separable (non-entangled) density matrices of graphs, corresponding to a disjoint union of cycles and isolated vertices [1]. Let us recall that a permutation matrix $P$ is said to be a *transposition* if $P = P^T$ and $P$ is not the identity matrix. Namely, we will address the following:

- Count the number of transpositions $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$.

Section 2 contains solutions to these problems. Section 3 contains a list of open questions.

## 2. Results

We begin by considering the first problem: count the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$. For a permutation matrix $P \in S_{pq}$, let us denote by $\mathcal{P}_{i,j}$ 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 $\mathcal{P}_{i,j}$. For example, given

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

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 $\mathcal{P}_{i,j}$. 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, let us impose the required constraints on $A_{i,j}$ and $B_{i,j}$. We know that $P$ is a permutation matrix if and only if

$$A_{i,j} \cap A_{i,k} = \emptyset, \quad \text{for every } i, j, k \text{ with } j \neq k, \tag{3}$$

$$B_{i,j} \cap B_{k,j} = \emptyset, \quad \text{for every } i, j, k \text{ with } i \neq k, \tag{4}$$

and

$$\bigcup_{j=1}^{p} A_{i,j} = [q], \quad \text{for } i = 1, 2, ..., p, \tag{5}$$

$$\bigcup_{i=1}^{p} B_{i,j} = [q], \quad \text{for } j = 1, 2, ..., p. \tag{6}$$

We need that $P^{\Gamma_p}$ is also a permutation matrix. Therefore, we have

$$A_{i,j} \cap A_{k,j} = \emptyset, \quad \text{for every } i, j, k \text{ with } i \neq k, \tag{7}$$

$$B_{i,j} \cap B_{i,k} = \emptyset, \quad \text{for every } i, j, k \text{ with } j \neq k, \tag{8}$$

and

$$\bigcup_{i=1}^{p} A_{i,j} = [q], \quad \text{for } j = 1, 2, ..., p, \tag{9}$$

$$\bigcup_{j=1}^{p} B_{i,j} = [q], \quad \text{for } i = 1, 2, ..., p. \tag{10}$$

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 the equations (3)–(5), we know that

$$A_{i,j} = \bigcup_{\pi_i = j} A_\pi, \quad B_{i,j} = \bigcup_{\pi_i = j} B_\pi. \tag{11}$$

From (3) and (4), we can write

$$A_\pi \cap A_\sigma = B_\pi \cap B_\sigma = \emptyset, \quad \text{for every } \pi, \sigma \in S_p \text{ with } \pi \neq \sigma. \tag{12}$$

Furthermore,

$$\bigcup_{\pi\in S_p} A_\pi = \bigcup_{\pi\in S_p} B_\pi = [q]. \tag{13}$$

Conversely, given two set partitions $\{A_\pi\}$ and $\{B_\pi\}$ of $[q]$, satisfying the equations (12) and (13), we may define $A_{i,j}$ and $B_{i,j}$ by equation (11). One can easily check that (3)–(10) 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 same. Let $a_\pi$ and $b_\pi$ denote the cardinalities of $A_\pi$ and $B_\pi$, respectively. On the basis of the above observations, we can state the following result:

**Theorem 1.** *Let $Z(p,q)$ the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$. Then*

$$Z(p,q) = \sum_{\substack{\sum a_\pi = \sum b_\pi = q \\ \sum_{\pi_i=j} a_\pi = \sum_{\pi_i=j} b_\pi}} \frac{q!^2}{\prod_\pi a_\pi! b_\pi!} \prod_{i,j=1}^{p} \left( \sum_{\pi_i=j} a_\pi \right)!, \tag{14}$$

*where the sum runs over all nonnegative integers $a_\pi$ and $b_\pi$.*

It may be worth to point out the next corollary:

**Corollary 2.** *The number of permutation matrices $P \in S_{2q}$ such that $P^{\Gamma_2} \in S_{2q}$ is*

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

Now we focuse on the second problem: count the number of permutation matrices $P \in S_{pq}$ such that $P^{\Gamma_p} = P$. We then ask that $\mathcal{P}_{i,j} = \mathcal{P}_{i,j}^T$. Hence, $A_{i,j} = B_{i,j}$. Additionally, given $A_{i,j}$, the number of ways to put 1's in the block $\mathcal{P}_{i,j}$ is exactly the number of transpositions of size $q$, which we denote by $I(q)$. It is well-known that (see, *e.g.*, Example 5.2.10 in [10])

$$I(q) = \sum_{\substack{j=0 \\ j \text{ even}}}^{q} \binom{q}{j} \frac{j!}{2^{j/2}(j/2)!} \tag{15}$$

and $I(q+1) = I(q) + q \cdot I(q-1)$. With the same analysis carried on for Theorem 1, we can directly obtain the number of desired matrices:

**Theorem 3.** *Let $Z_e(p,q)$ the number of permutation matrices $P \in S_{pq}$ such that $P = P^{\Gamma_p}$. Then*

$$Z_e(p,q) = \sum_{\sum a_\pi = q} \frac{q!}{\prod_\pi a_\pi!} \prod_{i,j=1}^{p} i \left( \sum_{\pi_i=j} a_\pi \right), \tag{16}$$

*where the sum runs over all nonnegative integers $a_\pi$, with $\pi \in S_p$.*

When taking $p = 2$, the number of permutation matrices is particularly neat:

**Corollary 4.** *The number of permutation matrices $P \in S_{2q}$ such that $P = P^{\Gamma_2}$ is*

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

Here is the third problem: count the number of transpositions $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$. Let $P$ be the transposition defined by the ordered pairs $(aq+i, bq+j)$, where $0 \le a, b \le p-1$, $1 \le i, j \le q$ and $(a,i) \ne (b,j)$. 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 Id or $P$ itself. In the first case, we must have $P = \mathrm{Id}$, 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

$$\begin{aligned}(aq+i, bq+j) &= (aq+j, bq+i),\\ (bq+j, aq+i) &= (bq+i, aq+j),\end{aligned}$$

or

$$\begin{aligned}(aq+i, bq+j) &= (bq+i, aq+j),\\ (bq+j, aq+i) &= (aq+j, bq+i).\end{aligned}$$

That is, $i = j$ or $a = b$. Hence, the desired transpositions are of type $(aq+i, aq+j)$, with $i \ne j$, or, of type $(aq+i, bq+i)$, with $a \ne b$.

**Theorem 5.** *Let $Z_t(p,q)$ be the number of transpositions $P \in S_{pq}$ such that $P^{\Gamma_p} \in S_{pq}$, or, equivalently, $P^{\Gamma_p} = P$. Then*

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

**Corollary 6.** *The number of transpositions $P \in S_{pq}$ and $p = q+1$ such that $P^{\Gamma_p} = P$ is*

$$Z_t(q+1, q) = q(q+1)(2q-1)/2.$$

*When $p = q$,*

$$Z_t(q,q) = q^3 - q^2.$$

At the end we note that $Z(p,q) = Z(q,p)$ and $Z_t(p,q) = Z_t(q,p)$, which can be seen by the following bijection: Suppose the

$$(ap+i, b(a,i)p + j(a,i))\text{-th}$$

entry of $P$ is 1, then let the

$$((i-1)q + (a+1), (j(a,i)-1)q + (b(a,i)+1))\text{-th}$$

entry of $P'$ be 1. If $P$ is a permutation after partial transpose, then $ap + j(a,i)$ and $b(a,i)p + i$ run over 1 to $n$ for $0 \le a \le q-1, 1 \le i \le p$. Thus, $(i-1)q + (b(a,i)+1)$ and $j(a,i)-1)q + (a+1)$ run over 1 to $n$ also, which implies that $P'$ is a permutation after partial transpose.

While in general $Z_e(p,q) \ne Z_e(p,q)$.

In standard linear notation, a permutation $\pi \in S_n$ can be written as a word of the form $\pi(1)\pi(2)...\pi(n)$. Note that $\sum_{i=1}^n \pi(i) = \sum_{i=1}^n i$. Also, for a permutation matrix $P$, $\sum_{P_{i,j}=1} i = \sum_{i=1}^n i$. The cells in the table below include each permutation $\pi \in S_4$ and the indices of the rows in the associated 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. |

**Proposition 7.** *Let $P \in S_n$, where $n = pq$. Then*

$$\sum_{P^{\Gamma_p}_{i,j}=1} i = n\,(n+1)\,/2.$$

*Proof.* Suppose $P$ is a permutation matrix and the $(ap+i, b(a,i)p+j(a,i))$-th entry of $P$ is 1. Then $b(a,i)$ runs over $0,\ldots,q-1$ $p$ times and $j(a,i)$ runs over $1,\ldots,p$ $q$ times. Thus, $\sum_{a,i} b(a,i) = p\binom{q}{2}$ and $\sum_{a,i} j(a,i) = q\binom{p+1}{2}$. Therefore

$$\sum_{a,i} ap + j(a,i) = p\binom{q}{2} + q\binom{p+1}{2} = \binom{n+1}{2},$$

which completes the proof. □

## 3. Open questions

- Formulate the first two problems for particular classes of permutations. For example, count the number of cyclic permutations $P \in S_{pq}$ such that $P^{\Gamma_p} = P$.
- Formulate the same problems for graphs, that is, general symmetric matrices with entries in the set $\{0,1\}$. When restricted to regular graphs, this problem seems to be amenable to be approached with a direct method similar to the one used in this paper. In fact the adjacency matrix of each $d$-regular graph can be written as a sum of $d$ permutation matrices.
- The number $Z_t(q+1,q)$ is equal to the number of ways of covering a $2q \times 2q$ lattice with $2q^2$ dominoes with exactly 2 horizontal dominoes ([9], Sequence A002414). Is there a bijection between these objects and the permutations of Corollary 6? Pondering this observation, it is tempting to ask if there a relation between certain domino tilings and positivity of partial transpose, at least for some restricted class of matrices.

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