

# Enumeration of matchings in polygraphs\*

Per Håkan Lundow

## Abstract

The 6-cube has a total of 7174574164703330195841 matchings of which 16332454526976 are perfect. This was computed with a transfer matrix method associated with polygraphs. For polygraphs of type  $G \times P_m$  we present a method for compression of the transfer matrix. This compression gives a substantial reduction of the order of the transfer matrix by exploiting the automorphisms of the graph  $G$ . We compute and tabulate matching polynomials of various polygraphs, such as the  $4 \times 4 \times m$ -grid. A Mathematica package, GraFFPack, is demonstrated and used for computation of matching polynomials, permanents and for generating transfer matrices.

## 1 Introduction

A simple graph is denoted  $G = (V, E)$  where  $V$  is the set of vertices and  $E$  is the set of edges. A matching  $M$  is a set of independent edges in  $G$ , i.e. no pair of edges in  $M$  have a vertex in common. A  $k$ -matching is a matching on  $k$  edges and a perfect matching is a matching that covers all the vertices in  $G$ . The matching polynomial of a graph  $G$  on  $n$  vertices is defined as

$$\mu(G; x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k p(G, k) x^{n-2k}$$

where  $p(G, k)$  denotes the number of  $k$ -matchings in  $G$  and we define  $p(G, 0) = 1$ . We overload the notation and define

$$\mu(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} p(G, k)$$

i.e.  $\mu(G)$  is the number of matchings in  $G$ . A 1-factor is a spanning 1-regular subgraph. The edges of a 1-factor then form a perfect matching and the number of 1-factors in a graph  $G$  is denoted  $\Phi(G)$ . In general it is a  $\#P$ -complete problem to compute  $\mu(G; x)$  and also  $\Phi(G)$ , though there are families of graphs such as paths, cycles and complete graphs, for which these functions can be simply expressed. Apart from these instances, general expressions are scarce. It is well-known however, that  $\Phi(G)$  can be computed in polynomial time for planar graphs. Computing the matching polynomial is still harder, becoming

---

\*Revised and updated version of "Computation of the matching polynomial and the number of 1-factors in polygraphs", Research reports, No 12, 1996.

# $P$ -complete even for planar graphs. More information on these matters can be found in Godsil [4] and Lovász and Plummer [14]. For more on complexity classes, see Welsh [22].

In the next section we will state some of the applications of matching theory to physics and chemistry. This is followed by a quick introduction to the subject of actually computing the matching polynomial, the number of matchings and the number of 1-factors in a graph. A family of graphs of interest in chemistry, polygraphs, is presented together with a transfer matrix method to compute their matching polynomials. We then present a new result, a compression of the matrices, which allows us to make these matrices considerably smaller. The algorithms described have been implemented in Mathematica. Some of the Mathematica routines are demonstrated and we give tables of the resulting numbers for some polygraphs along with some recurrence relations.

## 2 Applications of matching theory

There are several connections between matching theory and statistical physics and also chemistry. For example, adsorption of oxygen and hydrogen on a metallic surface can be modelled by a system of monomers-dimers. The question is whether adsorption undergoes a phase transition at some critical temperature. The surface is represented as a grid and it is exposed to a gas consisting of monomers and dimers. Dimers could here correspond to oxygen molecules which cover adjacent vertices on the grid. A set of dimers forms a matching on the grid and the state of the system is then represented by this matching. As partition function one takes the matching polynomial with non-negative coefficients. The paper by Heilmann and Lieb [6] contains a detailed study of this problem.

The Ising model is concerned with the phenomenon of spontaneous magnetization. If a magnetic material is placed in a hot environment it becomes unmagnetized, although below a certain critical temperature the material will regain a degree of its magnetism. We then have a phase transition at this critical temperature. The partition function of the Ising model can be expressed in terms of the 1-factors of a graph with weighted edges, the weight of a 1-factor being the product of its edge-weights. Again we refer the reader to [6] and also Kasteleyn [12]. A nice introduction to the Ising model is given by Cipra [3].

In mathematical chemistry, molecules are viewed as graphs and chemists refer to 1-factors as Kekulé structures. It turns out that the stability of some families of molecules is closely related to the number of 1-factors in their graphs. Several types of polynomials, partition functions and invariants of interest in chemistry have been suggested, many of which are expressed in terms of the numbers  $p(G, k)$ . For example,  $\mu(G)$  is also known as the Hosoya index and has been used to model physicochemical properties such as the boiling point of hydrocarbons. See for example Hosoya [7], Rouvray [17] and Trinajstić [21]. A more general account of combinatorics in statistical physics and chemistry can be found in Chapter 37 and 38 of The Handbook of Combinatorics [5].

### 3 Computation methods

#### 3.1 The matching polynomial

To compute the matching polynomial of a graph  $G$  we need the facts below. We will just state them and refer the reader who requires proofs to [4]. First of all

$$\mu(G; x) = \mu(G - e; x) - \mu(G - u - v; x)$$

where  $e = \{u, v\}$  is an edge of  $G$ . If  $G$  and  $H$  are disjoint graphs then

$$\mu(G \cup H; x) = \mu(G; x) \mu(H; x)$$

Let  $P_n$ ,  $C_n$  and  $K_n$  denote the path, cycle and complete graph respectively on  $n$  vertices. The complementary graph of  $G$  is denoted by  $\overline{G}$ , thus  $\overline{K_n}$  is the empty graph on  $n$  vertices. We have

$$\begin{aligned} \mu(P_n; x) &= \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \binom{n-k}{k} x^{n-2k} \\ \mu(C_n; x) &= \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \frac{n}{n-k} \binom{n-k}{k} x^{n-2k} \\ \mu(K_n; x) &= \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \frac{n!}{(2k)!(n-2k)!} x^{n-2k} \\ \mu(\overline{K_n}; x) &= x^n \end{aligned}$$

We can now give a simple recursive algorithm for computation of  $\mu(G; x)$ : if the maximum degree of the graph is at most 2, then the graph is a union of vertex-disjoint paths and cycles and we can compute the product of their respective matching polynomials. Otherwise, pick a pair of adjacent vertices of high degree, delete these vertices and the edge and make the recursive calls. Though recursive, the method works well for smaller graphs. The running time of the algorithm depends on the number of edges of  $G$ , meaning that dense graphs could be a problem. However, the following formula takes care of that

$$\mu(G; x) = \sum_{k=0}^{\lfloor n/2 \rfloor} p(\overline{G}; k) \mu(K_{n-2k}; x)$$

Thus, if  $G$  is dense (has more than  $n^2/4$  edges, say), then use the algorithm above on  $\overline{G}$  and apply the last formula. To extract  $\Phi(G)$  and  $\mu(G)$  from the matching polynomial we observe that  $\Phi(G) = |\mu(G; 0)|$  and  $\mu(G) = |\mu(G; \mathbf{i})|$ , where  $\mathbf{i}$  is the imaginary unit. In the next section we describe a better way to compute  $\Phi(G)$  when  $G$  is bipartite.

#### 3.2 The permanent

For bipartite graphs, there is a simple non-recursive method to compute  $\Phi$ . Let  $G = (V \cup W, E)$  be a bipartite graph on  $2n$  vertices with bipartition  $(V, W)$ ,

where  $V = \{v_1, \dots, v_n\}$  and  $W = \{w_1, \dots, w_n\}$ . The biadjacency matrix  $B = (b_{i,j})_{n \times n}$  is defined to have entries

$$b_{i,j} = \begin{cases} 1 & \text{if } \{v_i, w_j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

The permanent of an  $n \times n$ -matrix  $B$  is defined as

$$\text{per}(B) = \sum_{\pi} \prod_{i=1}^n b_{i,\pi(i)}$$

where the sum is taken over all permutations  $\pi$  of  $\{1, \dots, n\}$ . If  $B$  is the matrix defined above, then

$$\Phi(G) = \text{per}(B).$$

Thus, counting the 1-factors in a bipartite graph is equivalent to evaluating the permanent of its biadjacency matrix. The permanent, looking deceptively similar to the determinant, shares few of its nice properties. Particularly the property  $\det(AB) = \det(A)\det(B)$  does not hold for permanents. Also, whereas the determinant can be computed in  $O(n^3)$  time, no polynomial-time algorithm is known for the permanent. In fact, it has been shown to be a  $\#P$ -hard problem, making computation of  $\Phi(G)$  a  $\#P$ -complete problem for bipartite graphs as well. A detailed survey on the permanent is found in Minc [15] and a proof of the  $\#P$ -hardness result is sketched in [22].

Evaluation of the permanent, as formulated above, would require  $n \cdot n!$  arithmetic operations. It was shown by Ryser [18] that

$$\text{per}(B) = (-1)^n \sum_{S \subseteq [n]} (-1)^{|S|} \prod_{i=1}^n \sum_{j \in S} b_{i,j}$$

where  $[n] = \{1, \dots, n\}$ . This reduces the number of operations required to about  $n^2 2^{n-1}$ . Nijenhuis and Wilf [16] devised and implemented a method to reduce the number of operations by a factor  $n$ . Their main trick is to order the sets in the first sum in Gray-code order, i.e., so that consecutive sets differ in exactly one element. As it stands then, the permanent can be computed with about  $n2^{n-1}$  operations. Counting the 1-factors in the 6-cube (64 vertices) is thus quite feasible, but the 7-cube (128 vertices) would require immense computer resources with this approach.

There are inequalities for permanents of doubly stochastic matrices (having row and column sums equal to 1) that can be applied to regular bipartite graphs, see [14]. If the bipartite graph  $G$  above is  $k$ -regular then

$$n! \left(\frac{k}{n}\right)^n \leq \Phi(G) \leq (k!)^{n/k}$$

Applied to the 7-cube we get  $3.9280 \cdot 10^{27} \leq \Phi(Q^7) \leq 7.0924 \cdot 10^{33}$ .

### 3.3 Estimating the number of 1-factors

We finish this section by describing a simple probabilistic method for estimating  $\Phi(G)$ , proved in [14]. The adjacency matrix  $A = (a_{i,j})_{n \times n}$  of an oriented graph

$\vec{G}$  on the vertices  $\{v_1, \dots, v_n\}$  has entries

$$a_{i,j} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ -1 & \text{if } (v_j, v_i) \in E \\ 0 & \text{otherwise} \end{cases}$$

Give the graph  $G$  an orientation by randomly orienting every edge with probability  $1/2$  in either direction. It turns out that the expected value of  $\det(A(\vec{G}))$  is  $\Phi(G)$ . This implies a probabilistic method to estimate  $\Phi(G)$ . Just compute

$$\frac{1}{p} \sum_{i=1}^p \det(A(\vec{G}_i))$$

where the sum is taken over  $p$  independently chosen orientations of  $G$ . When  $G$  is bipartite we can gain a factor 8 in running time. Give  $G$  a random orientation  $\vec{G}$  by letting each non-zero entry of the biadjacency matrix  $B$  be positive or negative with equal probability. Observe that if  $G$  is bipartite then

$$A(\vec{G}) = \begin{pmatrix} 0 & B(\vec{G}) \\ -B(\vec{G})^T & 0 \end{pmatrix}$$

and the reader may verify that

$$\det(A(\vec{G})) = (\det(B(\vec{G})))^2$$

This method is also called the Godsil-Gutman estimator. The major drawback with the method is that the number  $p$  which gives a small relative error with a large probability is not necessarily polynomially bounded in  $n$ . Only for a few families of graphs is this known to be the case. However, the very simplicity of the method makes it a first candidate for computing a rough estimate of  $\Phi(G)$ , or at least the number of digits of  $\Phi(G)$ . Karmarkar et al. [13] contains an analysis of the Godsil-Gutman estimator and describes a slightly improved version of it. An implementation of the estimator in Fortran was applied to the 7-cube with  $p = 10^7$  and resulted in the estimate  $\Phi(Q^7) \approx 3.89 \cdot 10^{29}$ .

## 4 Polygraphs

So far we have not discussed how to take advantage of symmetries or recurring structures in a graph when computing matching polynomials. As an example, the reader may have in mind the  $2 \times 2 \times m$ -grid,  $m \geq 1$ , when reading this section. This is just the  $2 \times 2$ -grid, recurring  $m$  times, linked together by edges. Graphs of this kind belong to a family of graphs of interest in theoretical chemistry and are called polygraphs, see Figure 1. They were introduced by Babic et al. [1] who also gave a matrix method for computing their matching polynomials. A polygraph consists of a set of disjoint graphs  $G_1, \dots, G_m$  and a set of binary relations  $X_1, \dots, X_m$ . Let  $X_i \subseteq V(G_i) \times V(G_{i+1})$  for  $i = 1, \dots, m-1$  and  $X_m \subseteq V(G_m) \times V(G_1)$ . For consistency we define  $X_0$  to be identical to  $X_m$ . The polygraph  $\Omega_m$  has vertices  $V(G_1) \cup \dots \cup V(G_m)$  and edges  $E(G_1) \cup X_1 \cup \dots \cup E(G_m) \cup X_m$ . Let  $\Gamma_m$  be the graph  $\Omega_m$  without the edges  $X_m$ . If  $G_1 = \dots = G_m = G$  and  $X_1 = \dots = X_m = X$  we denote  $\Omega_m$  by  $\omega_m$  and call it a

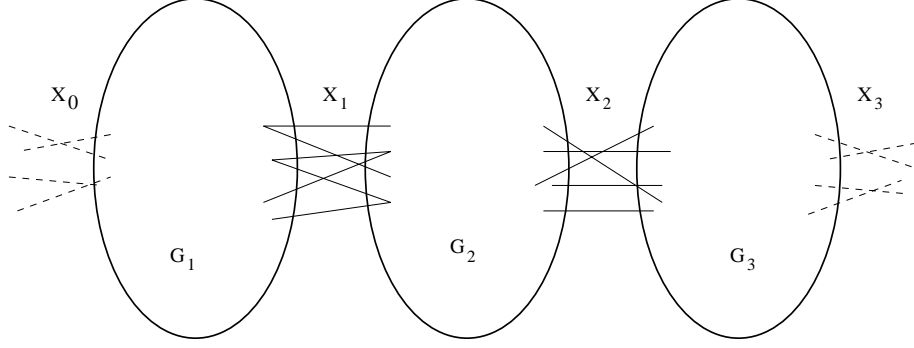


Figure 1: The structure of a polygraph

rotagraph on  $(G, X)$ . Likewise, we denote  $\Gamma_m$  by  $\gamma_m$  and call it a fasciagraph on  $(G, X)$ . Let  $M(X)$  be the set of all matchings in  $X$ . We index these matchings with numbers  $1, 2, \dots, |M(X)|$  and adopt the convention of letting the first matching be the empty set. Let  $W_i^{(k)}$  denote the  $i$ th element in  $M(X_k)$ . If  $W \in M(X)$ , let  $D(W)$  and  $R(W)$  be the domain and range respectively of  $W$ . Define  $\mu(G - A - B; x) = 0$  if  $A \cap B \neq \emptyset$ , where  $A, B \subseteq V(G)$ . Define matrices  $T_k = T_k(G_k, X_{k-1}, X_k)$ ,  $k = 1, \dots, m$  with entries

$$T_k(i, j) = (-1)^{|W_j^{(k)}|} \mu(G_k - R(W_i^{(k-1)}) - D(W_j^{(k)}); x) \quad (1)$$

where the notation  $T_k(i, j)$  refers to the entry in the  $i$ th row and  $j$ th column of the matrix  $T_k$ . Below we repeat some of the results in [1].

$$\begin{aligned} [T_1 \cdots T_m](i, j) &= (-1)^{|W_j^{(m)}|} \mu(\Gamma_m - R(W_i^{(m)}) - D(W_j^{(m)}); x) \\ [T_1 \cdots T_m](1, 1) &= \mu(\Gamma_m; x) \\ \text{tr}(T_1 \cdots T_m) &= \mu(\Omega_m; x) \end{aligned}$$

For rota- and fasciagraphs, we have that  $T_1 = \cdots = T_m = T$  where

$$T(i, j) = (-1)^{|W_j|} \mu(G - R(W_i) - D(W_j); x) \quad (2)$$

We then have

$$\begin{aligned} T^m(i, j) &= (-1)^{|W_j|} \mu(\Gamma_m - R(W_i^{(m)}) - D(W_j^{(m)}); x) \\ T^m(1, 1) &= \mu(\gamma_m; x) \\ \text{tr}(T^m) &= \mu(\omega_m; x) \end{aligned}$$

The formulae become really simple if we want the special cases  $G \times P_m$  or  $G \times C_m$ . Then, for all  $A_i, A_j \subseteq V(G)$  we let

$$T(i, j) = (-1)^{|A_j|} \mu(G - A_i - A_j; x) \quad (3)$$

and so, if we let  $A_1 = \emptyset$ ,

$$\begin{aligned} T^m(1, 1) &= \mu(G \times P_m; x) \\ \text{tr}(T^m) &= \mu(G \times C_n; x) \end{aligned}$$

Of course, after the obvious adjustments, these formulae also holds if we want the number of 1-factors (i.e.  $\Phi$ ) or the number of matchings (i.e.  $\mu$ ), simply delete the sign in front of the entries. Having defined the transfer matrix we can construct recurrence relations for the matching polynomial of  $\omega_m$  and  $\gamma_m$ . Denote the characteristic polynomial of the matrix  $T$  by

$$\Xi(T, \lambda) = \det(\lambda I - T) = \sum_{k=0}^N a_k \lambda^{N-k}$$

where  $N = |M(X)|$  (which is also the order of  $T$ ). Application of the Cayley-Hamilton theorem gives that  $\Xi(T, T) = \mathbf{0}$ , where the  $\mathbf{0}$  represents a zero-matrix of order  $N$ . From this we derive the recursive formulae of order  $N$

$$\begin{aligned} \sum_{k=0}^N a_k \operatorname{tr}(T^{m-k}) &= 0 \\ \sum_{k=0}^N a_k T^{m-k}(1, 1) &= 0 \end{aligned}$$

where  $m \geq N$ . Note that when we are determining  $\mu(\omega_m; x)$  and  $\mu(\gamma_m; x)$ , the coefficients  $a_k$  will be polynomials in  $x$ .

## 5 Compression

Let  $T$  be the transfer matrix for a fasciagraph as defined by Equation (2). Of course we wish the order of  $T$  to be as small as possible, to make matrix computations easy and the recurrence relations short. Unfortunately, though the method described in the previous section *does* take advantage of the recurring structure of the rota- and fasciagraphs, any symmetry in the graph  $G$  is *not* exploited. For example, if the edges in  $X$  are all independent, the matrix  $T$  has order  $2^{|X|}$ , no matter what graph  $G$  we use, empty or complete. In this section we will address this problem. In fact, in a special case we may reduce the order of the matrices by almost a factor the size of the automorphism group of  $G$ . First some notation though.

If  $G$  and  $H$  are graphs, then the Cartesian product  $G \times H$  is defined as the graph having vertices  $V(G) \times V(H)$  and where  $(v, w)$  is adjacent to  $(v', w')$  if and only if

$$v = v' \text{ and } \{w, w'\} \in E(H), \text{ or, } w = w' \text{ and } \{v, v'\} \in E(G)$$

For example,  $P_m \times P_n$  is the  $m \times n$ -grid,  $C_m \times P_n$  is a cylinder and  $C_m \times C_n$  is a torus.

Let  $\operatorname{Aut}(G)$  be the group of automorphisms of  $G$  and let  $A$  be a subset of  $V(G)$  such that  $\alpha(A) = A$  for all  $\alpha \in \operatorname{Aut}(G)$ . The case we are aiming for is the fasciagraph  $\gamma_m$  on  $(G, X)$  where we let  $X = \{(v, v) : v \in A\}$ . Note that if  $A = V(G)$  then  $\gamma_m = G \times P_m$ .

We will now classify the subsets of  $A$  into equivalence classes under the automorphism group according to the following; let  $\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_r$  be the equivalence classes of subsets of  $A$ . That is to say, every  $I \subseteq A$  belongs to some  $\mathcal{A}_k$ , and  $I, J \in \mathcal{A}_k$  if and only if  $J = \alpha(I)$  for some  $\alpha \in \operatorname{Aut}(G)$ . As a convention

we let  $\mathcal{A}_1 = \{\emptyset\}$ . We can now define the compressed matrix  $C$  in terms of the matrix  $T$ . Since the edges in  $X$  are independent, no confusion will arise when we write  $T(I, J)$  instead of  $T(i, j)$  where  $I = D(W_i)$  and  $J = R(W_j)$ .

**Definition 5.1.** The compressed transfer matrix  $C$  is the  $r \times r$ -matrix with entries

$$C(i, j) = \sum_{J \in \mathcal{A}_j} T(I, J) \quad \text{where } I \in \mathcal{A}_i \text{ and } i, j = 1, \dots, r. \quad (4)$$

When calculating  $C(i, j)$  we have to pick a set  $I \in \mathcal{A}_i$ . The following lemma says that it doesn't matter which set we pick, i.e. the matrix  $C$  is well-defined.

**Lemma 5.2.** *Let  $I_1, I_2 \in \mathcal{A}_i$ . Then*

$$\sum_{J \in \mathcal{A}_j} T(I_1, J) = \sum_{J \in \mathcal{A}_j} T(I_2, J) \quad \text{for } i, j = 1, \dots, r$$

*Proof.* Since  $I_1, I_2 \in \mathcal{A}_i$  we can assume that  $I_2 = \alpha(I_1)$  for some permutation  $\alpha \in \text{Aut}(G)$ . It suffices to show that the sets in  $\{I_1 \cup J : J \in \mathcal{A}_j\}$  are equal to the sets in  $\{I_2 \cup J : J \in \mathcal{A}_j\}$  in some, possibly permuted, order. It follows by the definition of the set  $\mathcal{A}_j$  that for all  $\alpha \in \text{Aut}(G)$  and  $J \in \mathcal{A}_j$  there is a  $J' \in \mathcal{A}_j$  such that  $J' = \alpha(J)$ . Thus, for all  $J \in \mathcal{A}_j$  there is a  $J' \in \mathcal{A}_j$  such that

$$I_2 \cup J = \alpha(I_1) \cup \alpha(J') = \alpha(I_1 \cup J')$$

and the lemma follows.  $\square$

**Theorem 5.3.** *If  $I \in \mathcal{A}_i$  then*

$$C^m(i, j) = \sum_{J \in \mathcal{A}_j} T^m(I, J) \quad \text{for } m \geq 1 \text{ and } i, j = 1, \dots, r.$$

*Proof.* By induction on  $m$ . The case  $m = 1$  follows from the definition of the matrix  $C$ . Assume the theorem to be true for  $m - 1$  and show it for  $m > 1$ . We have

$$\begin{aligned} \sum_{J \in \mathcal{A}_j} T^m(I, J) &= \sum_{J \in \mathcal{A}_j} \sum_{K \subseteq A} T^{m-1}(I, K) T(K, J) = \\ &= \sum_{J \in \mathcal{A}_j} \sum_{k=1}^r \sum_{K \in \mathcal{A}_k} T^{m-1}(I, K) T(K, J) = \\ &= \sum_{k=1}^r \sum_{K \in \mathcal{A}_k} T^{m-1}(I, K) \sum_{J \in \mathcal{A}_j} T(K, J) \end{aligned}$$

By the lemma and the definition this is

$$\sum_{k=1}^r \sum_{K \in \mathcal{A}_k} T^{m-1}(I, K) C(k, j)$$

and the induction hypothesis allows us to write this as

$$\sum_{k=1}^r C^{m-1}(i, k) C(k, j) = C^m(i, j)$$

and by the principle of induction the theorem follows.  $\square$



**Corollary 5.4.** *If  $C$  is defined on the matrix  $T$  in Equation (2) then*

$$C^m(1, 1) = \mu(\gamma_m; x) \quad \text{for } m \geq 1.$$

*Proof.* Recall that  $\mathcal{A}_1 = \{\emptyset\}$ .

$$C^m(1, 1) = \sum_{J \in \mathcal{A}_1} T^m(\emptyset, J) = T^m(\emptyset, \emptyset) = T^m(1, 1) = \mu(\gamma_m; x)$$

□

Comparing the orders of  $C$  and  $T$ , how much did we gain? The order of  $T$  is  $N = 2^{|A|}$  since all edges in  $X$  are independent. If we denote by  $r$  the order of  $C$ , then  $r$  is (usually) slightly larger than  $N/|\text{Aut}(G)|$  which is a lower bound on the number of equivalence classes. The exact number can be determined with Polyá's Enumeration Theorem:

$$r = \frac{1}{|\text{Aut}(G)|} \sum_{\pi \in \text{Aut}(G)} 2^{c(\pi, A)}$$

where  $c(\pi, A)$  is the number of cycles in the permutation  $\pi$  that contain elements from  $A$ . In Broersma and Xueliang [2] a reduction of almost a factor 2 of the order of  $T$  was accomplished. They laid slightly less strong restrictions on the binary relation  $X$  (independent edges, though), but the graph  $G$  was restricted to having vertex-set  $\{1, 2, \dots, 2p\}$  and an automorphism  $i \leftrightarrow p + i$ , for  $i = 1, \dots, p$ . The compression described here puts no restrictions on  $G$ , and works better the more automorphisms  $G$  has. Unfortunately we pay with information, since the trace of  $C$  no longer has the meaning it had for  $T$ .

## 6 Further reductions

We assume that we just want to count the 1-factors in  $\gamma_m$ . The order of the matrix  $C$  may then at least be halved to obtain a new, smaller, matrix  $\hat{C}$ . The simplest reduction stems from the fact that a graph on an odd number of vertices does not have a 1-factor. As before we let  $r$  denote the order of  $C$ . Renumber the families of sets that resulted from the classification procedure such that  $\mathcal{A}_1, \dots, \mathcal{A}_s$  contain the subsets of  $A$  of even size, and the remaining classes  $\mathcal{A}_{s+1}, \dots, \mathcal{A}_r$  contain the subsets of odd size. If  $|V(G)|$  is even then  $C(i, j) = 0$  if  $i \leq s$  and  $j > s$ , or,  $i > s$  and  $j \leq s$ . If  $|V(G)|$  is odd, then  $C(i, j) = 0$  if  $i, j \leq s$  or  $i, j > s$ . The matrix  $C$  will then look like

$$\begin{pmatrix} P & 0 \\ 0 & Q \end{pmatrix} \quad \text{for even } |V(G)|, \quad \begin{pmatrix} 0 & R \\ S & 0 \end{pmatrix} \quad \text{for odd } |V(G)|. \quad (5)$$

Here  $P$  is an  $s \times s$ -matrix,  $Q$  an  $(r-s) \times (r-s)$ -matrix,  $R$  an  $s \times (r-s)$ -matrix and  $S$  an  $(r-s) \times s$ -matrix. Assume that  $|V(G)|$  is even and define

$$\hat{C}(i, j) = C(i, j) \quad \text{for } i, j = 1, 2, \dots, s \quad (6)$$

Then  $\hat{C}$  is the upper block  $P$  on the diagonal of  $C$ . The other blocks in  $C$  will not affect this matrix during matrix multiplication, since  $C$  is block diagonal. We have then proved the following

**Proposition 6.1.**

$$\hat{C}^m(i, j) = C^m(i, j) \quad \text{for } m \geq 1$$

We continue with the case when  $|V(G)|$  is odd and define

$$\hat{C}(i, j) = C^2(i, j) \quad \text{for } i, j = 1, 2, \dots, s \quad (7)$$

This means that  $\hat{C}$  is the block product  $RS$ . Note that the upper left block in  $C^m$  will be a zero matrix when  $m$  is odd. A proposition similar to the one above follows.

**Proposition 6.2.**

$$\hat{C}^m(i, j) = C^{2m}(i, j) \quad \text{for } m \geq 1$$

In both the odd and the even case we end up with an  $s \times s$ -matrix, where  $s$  is the number of even non-equivalent subsets of  $A$ . If  $|A|$  is odd then  $s = r/2$  and if  $|A|$  is even then  $s \approx r/2$ . Roughly then, the order of  $\hat{C}$  is half that of  $C$ .

The last case, finally, is when  $G$  is bipartite. Note that a bipartite graph on two sets of unequal size does not contain a 1-factor. Restrict  $G$  to be a bipartite graph on  $2n$  vertices with bipartition  $(V, W)$  and let  $|V| = |W| = n$ . Again we renumber the classes, but this time such that for all  $I \subseteq A$  we have that  $I \in \mathcal{A}_1 \cup \dots \cup \mathcal{A}_s$  if and only if  $|I \cap V| = |I \cap W|$ , that is,  $I$  is a balanced subset of  $V \cup W$ . Then  $C(i, j) = 0$  if  $i \leq s$  and  $j > s$ , or,  $i > s$  and  $j \leq s$ . The matrix  $C$  will then look like the matrix in Equation (5) (in the even case) and so we define

$$\hat{C}(i, j) = C(i, j) \quad \text{for } i, j = 1, 2, \dots, s \quad (8)$$

Correspondingly, Proposition 6.1 follows.

How much did this reduce the order of  $C$ ? If we let  $a_v = |A \cap V|$  and  $a_w = |A \cap W|$ , then the number of sets to classify is

$$a = \sum_{k=0}^{\min(a_v, a_w)} \binom{a_v}{k} \binom{a_w}{k}$$

The order of  $\hat{C}$  is then approximately  $\frac{ar}{N}$ . For the special case when  $A = V \cup W$ , the above sum is

$$a = \sum_{k=0}^n \binom{n}{k}^2 = \binom{2n}{n} \sim \frac{2^{2n}}{\sqrt{\pi n}}$$

by Stirlings formula. We can then estimate the order of  $\hat{C}$  to approximately  $r/\sqrt{\pi n}$ .

Henceforth, when we refer to  $\hat{C}$  we mean that the appropriate reduction method has been applied. If  $G$  is bipartite as above, then we apply the reduction described for the bipartite case, and not merely the reduction in the even case.

## 7 Examples

In this section we apply the methods described above. What the examples also should demonstrate is that the method of polygraphs is very general and unless we can use a compression technique it does not give us good, i.e. short, recursion formulae. It does, however, deliver the *specific* polynomials and numbers

we desire, making tabulations of them fairly easy to carry through, even for rotographs, where the compression technique does not work.

At the same time we give a short demonstration of some of the functions in a Mathematica package, GrafPack, that are relevant to this article. The package is available on the web site [www.math.umu.se](http://www.math.umu.se). Download the entire GrafPack-directory, put it where Mathematica can see it (e.g. under ExtraPackages), start up Mathematica and type `<<GrafPack`Master``. For an introduction to Mathematica, see [23]. The book by Skiena [19] is also recommended.

**Example 7.1.** To compute the matching polynomial of a graph, we use the recursive method described in Section 3.1. The matching polynomial of the 4-cube is produced with the command

```
MatchingPolynomial[Hypercube[4], x]
```

where  $x$  is a variable. This returns the polynomial

$$272 - 3712x^2 + 11648x^4 - 14208x^6 + 8256x^8 - 2496x^{10} + 400x^{12} - 32x^{14} + x^{16}$$

The number of matchings in the 4-cube, 41025, is returned by the command

```
NumberOfMatchings[Hypercube[4]]
```

To obtain the number of 1-factors in the 4-cube, type

```
NumberOfOneFactors[Hypercube[4]]
```

and we receive the constant term, 272, of the polynomial above. Since the 4-cube is bipartite the function computes the permanent of the biadjacency matrix. Had we entered a non-bipartite graph, the function would have used the recursive method of Section 3.1.

The permanent of a square matrix is computed with the Nijenhuis-Wilf method, see Section 3.2. This gives the permanent of the  $10 \times 10$ -matrix with zeroes on the diagonal and ones off the diagonal

```
Permanent[1 - IdentityMatrix[10]]
```

If we want to estimate the number of 1-factors in a fairly large graph, the probabilistic algorithm of Section 3.3 can be used. The command

```
EstimateNumberOfOneFactors[Hypercube[6], 1000]
```

takes the average of 1000 determinants of oriented (bi-)adjacency matrices. The integer should be chosen with care, as large as possible to get a reliable result, modulo how long the user is prepared to wait. In this example, the graph is bipartite so the function will orient only the bi-adjacency matrix. A run returned the estimate  $1.8051 \cdot 10^{13}$ . Being a probabilistic algorithm though, we will receive different results at different runs.

**Example 7.2.** We compute the matching polynomial and the number of 1-factors in the fasciagraph  $\gamma_m = C_4 \times P_m$  using the compression technique. The subsets of  $A = V(C_4) = \{1, 2, 3, 4\}$  sorts into 6 classes under the automorphism group of  $C_4$  and the compressed matrix  $C$  then has order 6. Type

```

g = Cycle[4];
aut = Automorphisms[g];
orb = Orbits[aut, 2];
mat = CompressedTransferMatrixMP[g, orb, x]

```

The variable `orb` contains lists of isomorphic 2-colourings (their ranks to be precise) of the graph. The compressed matrix  $C$ , defined by Equation (4), is returned

$$\begin{pmatrix} 2 - 4x^2 + x^4 & 8x - 4x^3 & -4 + 4x^2 & 2x^2 & -4x & 1 \\ -2x + x^3 & 2 - 3x^2 & 2x & x & -1 & 0 \\ -1 + x^2 & -2x & 1 & 0 & 0 & 0 \\ x^2 & -2x & 0 & 1 & 0 & 0 \\ x & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

We continue the previous sequence of commands:

```

rec = RecursionCoefficients[mat];
r = Length[rec];
Clear[f];
Evaluate[Array[f, r]] = MatrixPower[mat, r, 1, 1, All];
f[m_] := f[m] = Sum[Expand[rec[[i]]*f[m-i]], {i, 1, r}];

```

If we try e.g. `f[7]` then  $\mu(C_4 \times P_7; x)$  is returned.

The matrix for enumeration of matchings is given by

```
mat = CompressedTransferMatrixM[g, orb]
```

If we want  $\Phi(\gamma_m)$ , observe that the graph  $C_4 = (V \cup W, E)$  is bipartite with  $|V| = |W| = 2$ . So we only need to classify those subsets  $I \subseteq V \cup W$  such that  $|I \cap V| = |I \cap W|$ . There are only 6 such sets and they sort into 3 classes. Thus, the matrix  $\hat{C}$  has order 3. This is all taken care of by the next function

```
mat = CompressedTransferMatrix1F[g, orb]
```

The matrix  $\hat{C}$ , defined by Equation (8), is returned

$$\begin{pmatrix} 2 & 4 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

To get a recursive formula for  $\Phi(\gamma_m)$  we proceed as above and receive the following recursive formula

$$\Phi(\gamma_m) = 3\Phi(\gamma_{m-1}) + 3\Phi(\gamma_{m-2}) - \Phi(\gamma_{m-3})$$

We could of course solve this recursive relation to get an explicit formula for  $\Phi(\gamma_m)$ , but we leave this to the enthusiastic reader.

The recursive formulae above corresponds exactly to those obtained by Hosoya and Motoyama [9]. They also gave a recursive formula for  $\Phi(P_2 \times P_3 \times P_m)$ . Typing the last command sequence with `g=GridGraph[2,3]` will return exactly the same formula, namely

$$\begin{aligned} \Phi(\gamma_m) = & 6\Phi(\gamma_{m-1}) + 21\Phi(\gamma_{m-2}) - 42\Phi(\gamma_{m-3}) \\ & - 89\Phi(\gamma_{m-4}) + 68\Phi(\gamma_{m-5}) + 89\Phi(\gamma_{m-6}) - 42\Phi(\gamma_{m-7}) \\ & - 21\Phi(\gamma_{m-8}) + 6\Phi(\gamma_{m-9}) + \Phi(\gamma_{m-10}) \end{aligned}$$

The authors of [9] estimated the order of the recursive formula for the matching polynomial to be approximately 20. This method would return one of order 24 which suits fairly well to their estimate.

We finish this example with a word of warning. Suppose that we replace the graph used above,  $C_4$ , with an odd graph, such as  $P_3$ , and generate the matrix  $\hat{C}$ . Then  $\hat{C}^m(1, 1) = \Phi(P_3 \times P_{2m})$  (!). Note also that the `RecursionCoefficients`-function returns the coefficients  $\{5, -5, 1\}$ , which should be interpreted as

$$\Phi(P_3 \times P_{2m}) = 5 \Phi(P_3 \times P_{2m-2}) - 5 \Phi(P_3 \times P_{2m-4}) + \Phi(P_3 \times P_{2m-6})$$

**Example 7.3.** Let  $G = C_4$  and  $X = \{(1, 1), (2, 2), (3, 3), (4, 4)\}$ . Then  $\omega_m = C_4 \times C_m$ . To compute  $\mu(\omega_4; x) = \mu(Q^4; x)$  type

```
g = Cycle[4];
rel = Table[{i,i},{i, 1, Order[g]}];
mat = TransferMatrixMP[g, rel, rel, x];
Sum[MatrixPower[mat, 4, i, i], {i, 1, Length[mat]}]
```

Here `rel` is the binary relation of edges between the graphs. Note that the built-in function `MatrixPower` has been extended to return particular entries. We could of course obtain recursive formulae for  $\Phi(\omega_m)$  and  $\mu(\omega_m; x)$  as above, but they would be unnecessarily long since they would both have order 16. In [9] a recursive formula for  $\Phi(\omega_m)$  of order 8 was given, and the recursive formula for  $\mu(\omega_m; x)$ , was estimated to have order 10.

**Example 7.4.** In this example we scrutinize the 3-dimensional grids  $P_4 \times P_4 \times P_m$ . Let us first view it as the fasciagraph  $\gamma_m$  on  $P_4 \times P_4$  with relation  $X = \{(1, 1), \dots, (16, 16)\}$ . The matrix  $T$  has order 65536, which would require an enormous amount of computer memory to store. However,  $T$  will be very sparse. Since 16 vertices overlap in  $X$  only  $3^{16}$  of the entries are non-zero and, if we only want 1-factors, fewer still are non-zero. The use of typical sparse matrix methods for computations of powers of  $T$  is of course a justified approach. Compression works well here, the automorphism group of  $P_4 \times P_4$  has 8 elements and the order of  $C$  is 8548. This is still a trifle too big when we are storing polynomials in a computer. The matrix  $\hat{C}$  on the other hand has order 1723, as computations have shown, and this is not too big to treat easily. Note that only the elements  $\hat{C}^m(1, 1)$  are desired, and so only vector-matrix multiplication needs to be performed. This approach does not bring us the matching polynomials of  $\gamma_m$ , but for smaller  $m$  we can use a rotagraph approach. For the case  $m = 4$  we let  $G = P_2 \times P_2 \times P_4$  and  $X = \{(3, 3), (4, 2), (7, 7), (8, 6), (11, 11), (12, 10), (15, 15), (16, 14)\}$ , see Figure 2. The rotagraph on  $(G, X)$  is the cubic grid  $P_4 \times P_4 \times P_4$ . The matrix  $T$  has order 256, which is fairly easily treated. The polynomial is listed in the Tables section. To compute it type

```
g = GridGraph[2, 2, 4];
rel = {{3,3},{4,2},{7,7},{8,6},{11,11},{12,10},{15,15},{16,14}};
mat = TransferMatrixMP[g, rel, rel, x, Verbose->True];
Sum[MatrixPower[mat, 4, i, i], {i, 1, Length[mat]}]
```

Note that adding the option `Verbose->True` as a last argument of the function `TransferMatrixMP` shows the progress of the computations. This makes the waiting for the computations to finish more bearable.

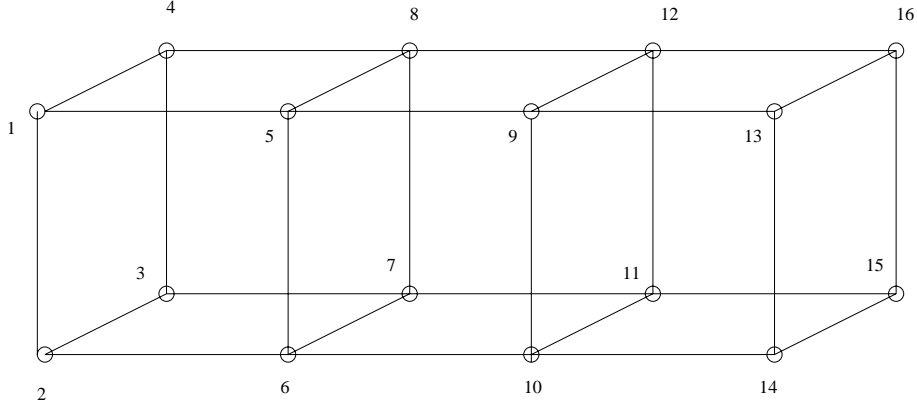


Figure 2: The  $2 \times 2 \times 4$ -grid

**Example 7.5.** We continue here the rotagraph approach from the previous example and describe a method for computing the entries in the transfer matrix. Let  $G = P_2 \times P_2 \times P_4$  and  $X$  be the relation given earlier. We will view  $G$  as a fasciagraph on  $H = P_2 \times P_2$  with the relation  $Y = \{(1, 1), (2, 2), (3, 3), (4, 4)\}$  between each copy of  $H$ , refer to these copies as  $H_1, \dots, H_4$ . Let  $A \subseteq R(X)$  and  $B \subseteq D(X)$  and say that this pair of sets corresponds to the  $(i, j)$ th entry in the transfer matrix  $T$  that we are aiming for. If  $A \cap B \neq \emptyset$  then  $T(i, j) = 0$ , otherwise we wish to compute  $T(i, j) = \Phi(G - A - B)$ . We will do this with transfer matrices though we will forbid the vertices  $A \cup B$ . To do this we define a family of transfer matrices, one for each possible set of vertices that intersect  $V(H_k)$ . Let  $U_k = (A \cup B) \cap V(H_k)$  for  $k = 1, \dots, 4$ . Since  $A \cup B$  intersects each  $H_k$  in at most 3 vertices there are only  $2^3$  different sets  $U_k$ . To compute  $\Phi(G)$ , we would normally use the matrix in Equation (3). Instead we define a modified matrix as follows; for all  $A_i, A_j \subseteq V(H)$  let

$$S_U(i, j) = \begin{cases} \Phi(H - U - A_i - A_j), & \text{if } U \cap (A_i \cup A_j) = \emptyset \\ 0 & \text{otherwise} \end{cases}$$

Now it is easy to see that  $T(i, j) = [S_{U_1} \cdots S_{U_4}](1, 1)$ . If we scale our problem to  $G = P_3 \times P_3 \times P_6$  then we let  $H = P_3 \times P_3$  and produce the necessary  $2^5$  matrices  $S$  in advance, each a  $512 \times 512$  matrix. These matrices will be extremely sparse so sparse matrix methods are very beneficial and there will be no problem in storing them on a computer. This approach was implemented in Fortran to compute  $\Phi(P_6 \times P_6 \times P_n)$  for  $n = 1, \dots, 5$ , (so the case with  $n = 6$  is still difficult) and  $\mu(P_5 \times P_5 \times P_n)$  for  $n = 1, \dots, 5$ , see the Tables section.

**Example 7.6.** The  $n$ -cube, denoted  $Q^n$ , is the graph having the set of binary strings of length  $n$  as vertices. Two vertices are adjacent if their binary strings differ in exactly one position. Note that  $Q^n = Q^{n-1} \times P_2$  and  $Q^n = Q^{n-2} \times C_4$ . We will view  $Q^6$  as the rotagraph  $Q^4 \times C_4$  and proceed to compute  $\Phi(Q^6)$  and  $\mu(Q^6)$ . Note that a transfer matrix for this rotagraph has order  $2^{16} = 65\,536$ . However, the transfer matrix for counting 1-factors has only  $5\,494\,273$  non-zero entries and the matrix for counting matchings has  $3^{16} = 43\,046\,721$  non-zero

entries. Thus storage in a computer memory is possible on a larger workstation by using standard sparse matrix methods. Recall that  $\text{tr}(T^4)$  is the desired number. Again we may use the automorphisms of  $Q^4$  to reduce the amount of work. Let  $\mathcal{A}_1, \dots, \mathcal{A}_{402}$  be the equivalence classes of  $V = V(Q^4)$  and note that every row (and column) of  $T$  corresponds to a subset of  $V$ . Let  $A_i$  be a member of  $\mathcal{A}_i$  for  $i = 1, \dots, 402$ . We have

$$\text{tr}(T^4) = \sum_{I \subseteq V} T^4(I, I) = \sum_{i=1}^{402} |\mathcal{A}_i| T^4(A_i, A_i)$$

Fortran implementations of this approach gave  $\Phi(Q^6) = 16332454526976$  and  $\mu(Q^6) = 7174574164703330195841$ . A smaller example of the sum above is given by the following computation of  $\Phi(Q^4)$ :

```

g = Hypercube[2];
rel = Table[{i, i}, {i, 1, Order[g]}];
aut = Automorphisms[g];
orb = Orbits[aut, 2];
mat = TransferMatrix1F[g, rel, rel];
Sum[
  i = 1 + orb[[k]];
  Length[orb[[k]]]*MatrixPower[mat, 4, i, i],
  {k, 1, Length[orb]}
]

```

Note that the ranks of the 2-colourings are counted from zero but the indices of the matrix are counted from one, which explains the definition of `i`. The number of matchings and the matching polynomials can also be computed this way.

We should remark that the matching polynomial of the 6-cube, for completeness listed in the Tables-section, was computed with a rather different approach; first compute the Ising partition function in two variables and extract the matching polynomial from it. This method will be described in some future paper.

## 8 Tables

*“This process of reduction to cipher is the highest effort man or woman is capable of making. It is the only effort worth making, and it is possible only through ever-increasing self-restraint...”*

Gandhi, 1927.

The matching polynomials and the number of 1-factors has been extensively tabulated for various grids, cylinders and tori. General expressions exist for the number of 1-factors in graphs such as  $P_m \times P_n$ ,  $P_m \times C_n$ ,  $C_m \times C_n$ ,  $P_2 \times P_3 \times P_m$ . The papers by Hosoya et al. [7, 8, 9, 10, 11] contain plenty of tables and general expressions, to which we refer the reader. Fans of integer sequences might want to consult the book by Sloane and Plouffe [20], which also can be reached on the Internet as a searchable database at <http://www.research.att.com/~njas/sequences/>. Below is listed tables of

$p(G, k)$ ,  $\Phi(G)$ ,  $\mu(G)$  and recurrence relations for some fasciagraphs on smaller cycles, grids and hypercubes. They were generated by running a precursor of GrafPack on a Power Macintosh 8100/80. In the tables of  $p(G, k)$ , integers being the number of 1-factors are printed in bold. To simplify the recurrence relations we let  $\mu_m$  denote  $\mu(\gamma_m; x)$  and  $\Phi_m$  denote  $\Phi(\gamma_m)$ . Let also  $r$  denote the order of the compressed matrix  $C$  for matching polynomials and  $\hat{r}$  the order of the compressed (and reduced) matrix  $\hat{C}$  for 1-factors.

Table 1: Order of compressed matrices for some  $G \times P_m$

$G$	$r$	$\hat{r}$	$G$	$r$	$\hat{r}$	$G$	$r$	$\hat{r}$
$P_2 \times P_3$	24	10	$P_2$	3	2	$C_3$	4	2
$P_2 \times P_4$	76	27	$P_3$	6	3	$C_4$	6	3
$P_2 \times P_5$	288	82	$P_4$	10	5	$C_5$	8	4
$P_2 \times P_6$	1072	268	$P_5$	20	10	$C_6$	13	6
$P_3 \times P_3$	102	51	$P_6$	36	14	$C_7$	18	9
$P_3 \times P_4$	1120	274	$P_7$	72	36	$C_8$	30	11
$P_4 \times P_4$	8548	1723	$P_8$	136	43	$C_9$	46	23
$C_3 \times C_3$	26	13	$P_9$	272	136	$C_{10}$	78	26
$Q^3$	22	9	$P_{10}$	528	142	$C_{11}$	126	63
$Q^4$	402	93	$P_{11}$	1056	528	$C_{12}$	224	62

Table 2:  $P_5 \times P_5 \times P_m$

$m$	$\mu$
1	2810694
2	423657524608288
3	42127221925485860896792
4	4435122353330774501960785797973
5	463310369790129032480118384076035223552

Table 3:  $P_6 \times P_6 \times P_m$

$m$	$\Phi$
1	6728
2	53786626921
3	57248060375968384
4	123115692449982216049513
5	216388579168758145017797108072



Table 4:  $C_3 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$	$m = 9$
0	1	1	1	1	1	1	1	1	1
1		3	9	15	21	27	33	39	45
2			18	69	156	279	438	633	864
3			<b>4</b>	107	501	1399	3017	5571	9277
4				36	672	3558	11613	29049	61374
5					285	4338	25029	92109	259956
6					<b>19</b>	2100	28557	175363	709740
7						276	15072	190575	1226919
8							2880	106824	1284651
9							<b>91</b>	25978	752716
10								1818	216951
11									23754
12									<b>486</b>
13									255239
$\mu$	4	32	228	1655	11978	86731	627960	4546684	32919766

Table 5:  $C_4 \times P_m = Q^2 \times P_m = P_2 \times P_2 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$
0	1	1	1	1	1	1	1	1
1		4	12	20	28	36	44	52
2		<b>2</b>	42	142	306	534	826	1182
3			44	440	1672	4248	8680	15480
4			<b>9</b>	588	4863	19774	56333	129644
5				288	7416	55200	235132	728840
6					5470	91200	637914	2810312
7				<b>32</b>	1620	84984	1112668	7465728
8					40553	1208714	13541312	88199495
9						8204	771436	16397296
10					<b>450</b>	261500	12752616	216370582
11						39080	5986432	194313364
12							1681	1532336
13								178272
14								<b>6272</b>
15								8380100
16								788536
$\mu$	7	108	1511	21497	305184	4334009	61545775	873996300

Table 6:  $C_5 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$
0	1	1	1	1	1	1	1
1		5	15	25	35	45	55
2			5	75	240	505	870
3				145	1125	3910	9495
4				<b>9</b>	95	2710	17725
5					3227	48193	286799
6					1645	77405	839930
7					240	69510	1612685
8						31060	1975730
9						5360	1465295
10						<b>176</b>	598928
11							113015
12							6625
13							
14							
15							
16							
17							
$\mu$	11	342	9213	253880	6974078	191668283	5267252351

Table 7:  $C_6 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$
0	1	1	1	1	1	1	1
1	6	18	30	42	54	66	78
2	9	117	363	753	1287	1965	2787
3	<b>2</b>	336	2290	7562	17874	34954	60530
4		420	8139	46938	160887	414792	894189
5		192	16446	187530	987834	3472752	9527094
6		<b>20</b>	18141	487241	4241321	21158661	75753275
7			9870	813486	12846774	95402040	458907006
8			2148	843342	27359544	320645463	2143757547
9			<b>108</b>	509542	40372976	803176510	7768505882
10				160653	40170300	1489152993	21861085377
11				21438	25795320	2015817270	47616569682
12				<b>725</b>	9980480	1949485107	79675739431
13					2078160	1304474898	101182136226
14					188832	576346062	95821362789
15					<b>4480</b>	156728330	66035085642
16						23429940	32011697004
17						1566180	10405152504
18						<b>28561</b>	2112964124
19							239567604
20							12371220
21							<b>179928</b>
$\mu$	18	1104	57536	3079253	164206124	8761336545	467431319920

Table 8:  $P_3 \times P_3 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$
0	1	1	1	1	1	1
1	12	33	54	75	96	117
2	44	436	1260	2525	4231	6378
3	56	2984	16736	50552	113684	215393
4	18	11434	140322	672126	2085694	5054442
5		24766	778452	6277198	27731168	87622530
6		29180	2913096	42480118	276805102	1164755616
7		16984	7361472	211846420	1220333560	12163620462
8		3993	12381180	784200907	12634826746	101433879357
9		<b>229</b>	13428840	2154366513	59027097072	682916407521
10			8893248	4362041263	216913695094	3738673165242
11			3278784	6419477292	626708528128	16712392258753
12			568344	6718664818	1417900872204	61103060700766
13			31344	4835018662	2493032893120	182629834939538
14				2281569082	3367348279396	445089189580448
15				655842108	3437515277416	880370659944042
16				101934041	2593501127101	1403576812451606
17				6870327	1402515949328	1786799130667754
18				<b>117805</b>	520871037067	1793930275383832
19					124842772364	1397774304403158
20					17531745326	827727493314932
21					1217704320	362423901173076
22					28613174	113077255268116
23						23878571601956
24						3164202873629
25						233176559173
26						7654682266
27						<b>64647289</b>
$\mu$	131	90040	49793133	28579431833	16294017491392	9303034425177393

Table 9:  $C_3 \times C_3 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$
0	1	1	1	1	1	1
1	18	45	72	99	126	153
2	99	810	2241	4401	7290	10908
3	180	7518	39678	116316	257106	481731
4	72	38709	442575	2039814	6188463	14778099
5		110817	3254724	25088310	107856216	334725885
6		167448	16056147	223066398	1409411676	5808709002
7		117900	53046918	1456699500	14108774220	79104051891
8		29520	115246440	7029374175	109615427955	858999657429
9		1120	158653112	25022727081	665714322238	7517635432505
10			129944880	65127684555	3168417127554	53381488744872
11			56958480	121909424148	11801137694058	308693456717967
12			10992408	159953324046	34221545160489	1455432762661803
13			585792	141626935710	76569860426940	5588494400657529
14				80001899586	130436645000040	17417917114151796
15				26440161960	166051546684152	43821565164155937
16				4418860545	154011257081100	88290020235183381
17				278666595	100510188513840	140932058555779443
18				<b>2861029</b>	43956690488688	175746115986201690
19					11993327746128	168125848472949201
20					1823418619560	120495553386274359
21					126181749120	62707121963709243
22					2535163200	22712557651235100
23						5392873133377065
24						767195930393457
25						56362288663467
26						1606470279210
27						<b>7537209013</b>
$\mu$	370	473888	545223468	633518934269	735463713700160	853881267896192137

Table 10:  $P_4 \times P_4 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$
0	1	1	1	1
1	24	64	104	144
2	224	1816	4992	9768
3	1044	30208	146940	415368
4	2593	328214	2972395	12430848
5	3388	2456736	43888740	278659560
6	2150	13022504	490410658	4862322484
7	552	49492032	4243096376	67752463152
8	<b>36</b>	135062729	28849000711	767471193606
9		262610832	155554203920	7157834054584
10		357580896	668490123332	55469187090396
11		331384336	2293235516668	359485412847192
12		200032432	6270624556725	1956911884067608
13		73483328	13607937421412	8971759857716256
14		14707328	23264863112266	34682805390128328
15		1308928	31002090496224	113035590354067768
16		<b>32000</b>	31731778597928	310146213937970487
17			24460558393664	714514530994393464
18			13831123293040	1376672261486529068
19			5534768640848	2206488832067036760
20			1490639531680	2921624380278645192
21			250915666208	3168204916452408416
22			23455372800	2783182424023411992
23			980808000	1953962180835361272
24			<b>10885344</b>	1077824850339404286
25				457155298292389608
26				144991813332269700
27				33134934405040272
28				5183929033351776
29				515240510630328
30				28894756833940
31				736291240776
32				<b>5051532105</b>
$\mu$	10012	1441534384	154620656140976	17312701462385916505

Table 11:  $Q^4 \times P_m = C_4 \times C_4 \times P_m$

$k$	$m = 1$	$m = 2$	$m = 3$	$m = 4$
0	1	1	1	1
1	32	80	128	176
2	400	2840	7568	14600
3	2496	59120	274560	759584
4	8256	803580	6848000	27822084
5	14208	7517264	124694656	763504368
6	11648	49715240	1718209088	16311133584
7	3712	235146480	18327675008	278274362192
8	<b>272</b>	795862790	153549653616	3858979023370
9		1910146160	1019460142080	44051088838656
10		3190117800	5389069021056	417676281992856
11		3594554960	22710637612800	3310348880868432
12		2605908220	76162736983680	22024174794317232
13		1129177840	202303330851072	123313091919432144
14		259084440	422310466869504	581630577946974072
15		25108944	685115567624704	2310324639457748096
16		<b>589185</b>	850667743539584	7715963153250311251
17			792016077516800	21604808702631926656
18			538003442426880	50504855552895180056
19			256874061012992	98016417871417039760
20			81810395008768	156788269717168962800
21			16087147553792	204849983435540593552
22			1725682248704	216149310892878810872
23			80406638592	181614258291882122496
24			<b>930336768</b>	119387717864796680906
25				60042777844937606416
26				224430853963359803280
27				5999543286903760304
28				1087639382471943076
29				123724794351752480
30				7805441127361896
31				217782023223920
32				<b>1545853411969</b>
$\mu$	41025	13803794944	3952450882750401	1149377449671217283137

Table 12:  $Q^6 = C_4 \times C_4 \times C_4$

$k$	$p(Q^6, k)$
0	1
1	192
2	17376
3	986240
4	39408480
5	1179696384
6	27488385408
7	511416198144
8	7732531647360
9	96216012236800
10	994137263758848
11	8583228570909696
12	62184244929659648
13	378969619199569920
14	1944655398731796480
15	8398980067449999360
16	30480925212093104640
17	92675048634081607680
18	235053748112782356480
19	494482501391128289280
20	856482708316893954048
21	1210188907641505775616
22	1378948882982541631488
23	1249011213103104491520
24	883258965992225095680
25	476635207372408553472
26	190551239146197909504
27	54258655709480353792
28	10420946627414016000
29	1246585402333593600
30	81808261704974336
31	2333280165691392
32	<b>16332454526976</b>
$\mu$	7174574164703330195841

## 8.1 Recursion formulae

$$\Phi(C_3 \times P_{2m}) = 5\Phi_{2m-2} - \Phi_{2m-4}$$

$$\mu(C_3 \times P_m) = 6\mu_{m-1} + 9\mu_{m-2} - 1\mu_{m-4}$$

$$\mu(C_3 \times P_m; x) = (-5x + x^3)\mu_{m-1} + (-5 + 3x^2 - x^4)\mu_{m-2} + (x + x^3)\mu_{m-3} - \mu_{m-4}$$

$$\Phi(C_4 \times P_m) = 3\Phi_{m-1} + 3\Phi_{m-2} - \Phi_{m-3}$$

$$\mu(C_4 \times P_m) = 14\mu_{m-1} + 6\mu_{m-2} - 46\mu_{m-3} + 18\mu_{m-4} + 2\mu_{m-5} - 1\mu_{m-6}$$

$$\begin{aligned} \mu(C_4 \times P_m; x) &= (6 - 7x^2 + x^4)\mu_{m-1} + (-7 - 6x^2 + 6x^4 - x^6)\mu_{m-2} \\ &\quad + (-8 + 26x^2 - 10x^4 + 2x^6)\mu_{m-3} + (9 - 6x^2 + 2x^4 - x^6)\mu_{m-4} \\ &\quad + (2 + x^2 + x^4)\mu_{m-5} - \mu_{m-6} \end{aligned}$$

$$\Phi(C_5 \times P_{2m}) = 19\Phi_{2m-2} - 41\Phi_{2m-4} + 19\Phi_{2m-6} - \Phi_{2m-8}$$

$$\begin{aligned} \mu(C_5 \times P_m) &= 25\mu_{m-1} + 76\mu_{m-2} - 209\mu_{m-3} - 159\mu_{m-4} + 119\mu_{m-5} \\ &\quad + 40\mu_{m-6} - 3\mu_{m-7} - 1\mu_{m-8} \end{aligned}$$

$$\begin{aligned} \mu(C_5 \times P_m; x) &= (15x - 9x^3 + x^5)\mu_{m-1} + (-19 + 19x^2 - 27x^4 + 10x^6 - x^8)\mu_{m-2} \\ &\quad + (34x - 85x^3 + 69x^5 - 19x^7 + 2x^9)\mu_{m-3} + (-41 + 95x^2 - 39x^4 - 9x^6 \\ &\quad + 6x^8 - x^{10})\mu_{m-4} + (2x - 65x^3 + 39x^5 - 11x^7 + 2x^9)\mu_{m-5} \\ &\quad + (-19 + 11x^2 - 7x^4 + 2x^6 - x^8)\mu_{m-6} + (3x + x^3 + x^5)\mu_{m-7} - \mu_{m-8} \end{aligned}$$

$$\Phi(C_6 \times P_m) = 4\Phi_{m-1} + 16\Phi_{m-2} - 6\Phi_{m-3} - 16\Phi_{m-4} + 4\Phi_{m-5} + \Phi_{m-6}$$

$$\begin{aligned} \mu(C_6 \times P_m) &= 53\mu_{m-1} + 66\mu_{m-2} - 2616\mu_{m-3} + 5076\mu_{m-4} + 5806\mu_{m-5} \\ &\quad - 14388\mu_{m-6} + 1276\mu_{m-7} + 6022\mu_{m-8} - 1420\mu_{m-9} - 424\mu_{m-10} \\ &\quad + 90\mu_{m-11} + 5\mu_{m-12} - 1\mu_{m-13} \end{aligned}$$

$$\begin{aligned} \mu(C_6 \times P_m; x) &= (-12 + 29x^2 - 11x^4 + x^6)\mu_{m-1} + (-32 + 12x^2 + 47x^4 - 49x^6 \\ &\quad + 13x^8 - x^{10})\mu_{m-2} + (71 - 568x^2 + 948x^4 - 714x^6 + 266x^8 - 46x^{10} + 3x^{12})\mu_{m-3} \\ &\quad + (313 - 983x^2 + 1261x^4 - 1339x^6 + 848x^8 - 283x^{10} + 46x^{12} - 3x^{14})\mu_{m-4} \\ &\quad + (40 + 924x^2 - 2103x^4 + 1956x^6 - 812x^8 + 97x^{10} + 34x^{12} - 11x^{14} + x^{16})\mu_{m-5} \\ &\quad + (-601 + 2884x^2 - 4334x^4 + 3559x^6 - 1903x^8 + 823x^{10} - 241x^{12} + 40x^{14} \\ &\quad - 3x^{16})\mu_{m-6} + (-311 + 1132x^2 - 470x^4 + 161x^6 + 259x^8 - 351x^{10} + 153x^{12} \\ &\quad - 32x^{14} + 3x^{16})\mu_{m-7} + (368 - 892x^2 + 1743x^4 - 1764x^6 + 968x^8 - 265x^{10} \\ &\quad + 26x^{12} + 3x^{14} - x^{16})\mu_{m-8} + (251 - 529x^2 + 575x^4 - 205x^6 - 60x^8 + 59x^{10} \\ &\quad - 18x^{12} + 3x^{14})\mu_{m-9} + (-47 - 172x^4 + 130x^6 - 58x^8 + 14x^{10} - 3x^{12})\mu_{m-10} \\ &\quad + (-40 + 28x^2 - 11x^4 + 9x^6 - x^8 + x^{10})\mu_{m-11} + (-5x^2 - x^4 - x^6)\mu_{m-12} + \mu_{m-13} \end{aligned}$$

## References

- [1] D. Babic et al., *The matching polynomial of a polygraph*, Discrete Appl. Math. **15** (1986) 11–24
- [2] H.J. Broersma and Li Xueliang, *On ‘The matching polynomial of a polygraph’*, Discrete Appl. Math. **46** (1993) 79–86

- [3] B.A. Cipra, *An introduction to the Ising model*, Amer. Math. Monthly **94** 937–959
- [4] C.D. Godsil, *Algebraic combinatorics*, Chapman and Hall, 1993
- [5] R. Graham, M. Grötschel and L. Lovasz (editors), *The Handbook of Combinatorics*, Elsevier Science B. V., 1995
- [6] O.J. Heilmann and E.H. Lieb, *Theory of monomer-dimer systems*, Commun. Math. Phys. **25** (1972) 190–232
- [7] H. Hosoya, *On some counting polynomials in chemistry*, Discrete Appl. Math. **19** (1988) 239–257
- [8] H. Hosoya, *Matching and symmetry of graphs*, Comp. and Maths. with Appls. **12B** (1986) 271–290
- [9] H. Hosoya and A. Motoyama, *An effective algorithm for obtaining polynomials for dimer statistics. Application of operator technique on the topological index to two- and three-dimensional rectangular and torus lattices*, J. Math. Phys. **26** (1985) 157–167
- [10] H. Hosoya et al., *Generalized expression of the perfect matching number for  $2 \times 3 \times n$  lattices*, J. Math. Phys. **34** (1993) 1043–1051
- [11] H. Hosoya et al., *Generalized expression for the number of perfect matchings of cylindrical  $m \times n$  graphs*, J. Math. Phys. **32** (1991) 1885–1889
- [12] P.W. Kasteleyn, *Graph theory and crystal physics*, Graph theory and theoretical physics, ed. F. Harary, Academic Press, London, 1967.
- [13] N. Karmarkar et al., *A Monte-Carlo algorithm for estimating the permanent*, SIAM J. Comput. **22** (1993) 284–293
- [14] L. Lovasz and M.D. Plummer, *Matching theory*, North-Holland, 1986
- [15] H. Minc, *Permanents*, Addison-Wesley, 1978
- [16] A. Nijenhuis and H. Wilf, *Combinatorial algorithms*, Academic Press, 1978
- [17] D. H. Rouvray, *The modeling of chemical phenomena using topological indices*, J. Comput. Chem., **8**, (1987) 470–480
- [18] H.J. Ryser, *Combinatorial mathematics*, The Carus mathematical monographs, 1963
- [19] S.S. Skiena, *Implementing discrete mathematics: Combinatorics and graph theory with Mathematica*, Addison-Wesley, 1990
- [20] N.J.A. Sloane and S. Plouffe, *The encyclopedia of integer sequences*, Academic Press, 1995
- [21] N. Trinajstić, *Chemical graph theory*, CRC Press, 1992
- [22] D. J. A. Welsh, *Complexity: Knots, colourings and counting*, Cambridge university press, 1993
- [23] S. Wolfram, *Mathematica: a system for doing mathematics by computer*, Addison-Wesley, 1991