Journal of Mathematical Chemistry 13(1993)133–143

A honeycomb graph perfect matchings enumeration

M. Desainte-Catherine
LaBRI, Université Bordeaux I, 351, cours de la Libération,*
33405 Talence Cedex, France

Received 9 December 1991; revised 3 April 1992

We consider honeycomb graphs with a trapezoidal shape and based on pentagons. We give an exact formula for the number of perfect matchings of these graphs.

1. Introduction

Perfect matchings enumeration is of particular interest in different fields. In quantum-chemical theory, perfect matchings enumeration is used in several resonance theoretic methods [1–5]. Moreover, in statistical mechanics, enumeration of *dimer coverings* is quite equivalent to the solution of the two-dimensional *Ising problem* [6–9]. Uses and methods for enumeration of perfect matchings in honeycomb graphs are reported in refs. [10,11]. The set of methods includes: combinatorial recursion methods, the determinantal method, the Pfaffian method, methods based on graph decomposition, transfer matrix method, correspondences to sets of non-intersecting paths, and others. Our method is of the latter kind and it is inspired by the resolution method for the *Ising problem*. Solving this problem consists in enumerating closed sub-graphs of the lattice (i.e. graphs without vertices of odd degree). This requires the enumeration of the perfect matchings of another lattice, obtained from the original one by a certain transformation. Then, in order to calculate the Pfaffian, which represents the generating function of the perfect matchings, the lattice borders are identified and a cyclic block matrix representing the lattice is obtained.

In this paper, we consider a *honeycomb sublattice* with trapezoidal shape (see fig. 1), based on pentagons. Such a graph can be characterized by two parameters:

- p denoting the number of pentagons,
- n denoting the *height* of the graph, i.e. the number of hexagons stacked on a pentagon plus 1.

* Laboratoire Bordelais de Recherche en Informatique, Unité de Recherche Associée au Centre National de la Recherche Scientifique No. 226.

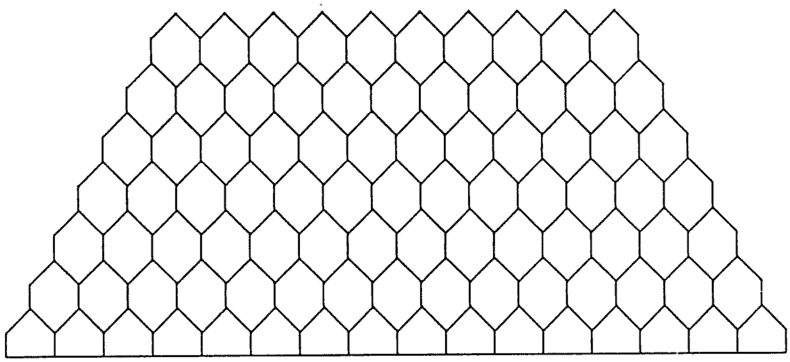


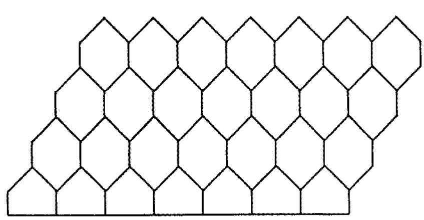
Fig. 1. A honeycomb graph with a trapezoidal shape.

We show that the number of perfect matchings of a pyramid based on $p-1$ pentagons and of height n is equal to

$$\prod_{1\le i\le j\le n} \frac{i+j+p-n}{i+j},$$

where $p-n$ is even, $p>1$ and $n>0$.

Since our lattice involves strong boundary conditions, identification of the borders is impossible. Hence, we have to enumerate directly on a finite sublattice. In a similar way to the resolution methods recalled above, we associate to our honeycomb lattice a square lattice such that the perfect matchings of the first lattice are in bijection with the non-intersecting paths of the second lattice. We have shown in ref. [12] that these paths are also in bijection with certain Young tableaux of which we know the number. We develop a particular case enumerated by the Catalan numbers, and we give a direct and very simple proof, not involving the Young tableaux. The reader will find a survey of other perfect matchings enumerations on different honeycomb graphs in ref. [13]. In particular, the lattice displayed in the scheme below, which is very similar to ours, admits a number of perfect matchings which is a simple binomial.



2. Preliminary definitions

Let $G = \langle A, S \rangle$ be a *graph* where A is the set of edges and S the set of vertices ($A \subseteq S \times S$).

(1) We define the *contraction operation* (see an example in fig. 2) of the edge a within the graph G. The result of this operation is a new graph $G' = \langle A', S' \rangle$ such that: the two extemities s_1 and s_2 of the edge a are replaced by a single vertex s, all the edges which admitted one of the two vertices s_1 or s_2 as an extremity are then connected to the new vertex s.

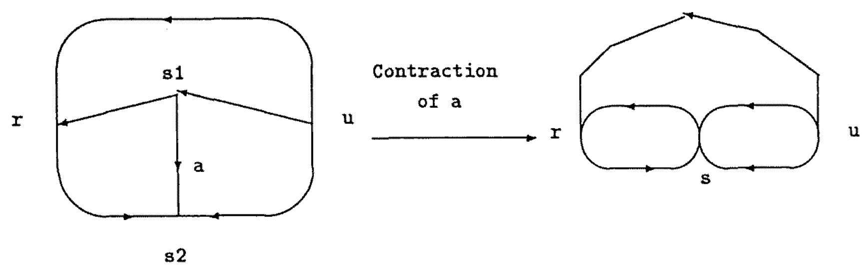


Fig. 2. Example of a contraction.

(2) A *path* w of a graph is a sequence of vertices, $w = (s_1, s_2, \ldots, s_n)$ such that for $1 \le i \le n-1$, (s_i, s_{i+1}) is an edge of G.

(3) *Disjoint paths* or *non-intersecting paths* have no vertices in common.

(4) A *matching* of a graph is a set of disjoint edges.

(5) A *perfect matching* of a graph is a matching such that each vertex of the graph belongs to an edge of the matching.

3. The bijection between perfect matchings and configurations of paths

DEFINITION 3.1

Let $G_{p,n}$ be a honeycomb graph with a trapezoidal shape based on $p-1$ pentagons and of height n, and such that p and n are of the same parity.

Note: The honeycomb graphs with trapezoidal shape, which are drawn as in fig. 1, have four types of edges:

(1) *North* edges, or vertical edges.

(2) *East* edges, or horizontal edges.

(3) *Northeast* edges.

(4) *Northwest* edges.

3.1. THE TRANSFORMATION

The transformation we shall introduce in this subsection is such that there is a bijection between the perfect matchings of the original graph $G_{p,n}$ and the configurations of non-intersecting paths of the transformed graph $G^{\iota}_{p,n}$. Such a bijection is introduced by Klein and Živković [5], between perfect matchings and non-intersecting paths on the same lattice. The bijection is very similar to ours. They remove dimers of the matching from certain edges, and put dimers on other edges so that non-intersecting paths appear. We contract edges (the same as the ones from which Klein and Živković remove dimers), and we obtain a square lattice where the paths are automatically constructed.

We build the graph $G^{\iota}_{p,n}$ by contracting (see section 2) all the Northwest edges of the graph $G_{p,n}$ (see definition 3.1). The transformation is illustrated in fig. 3.

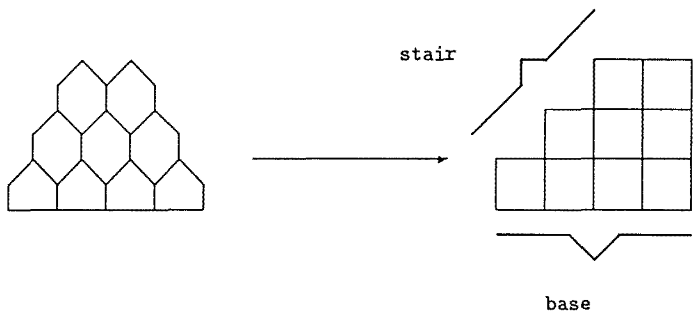


Fig. 3. Transformation of G_4 into G^{ι}_4.

The southern vertices of the graph $G^{\iota}_{p,n}$ will be called the *base vertices*, and the vertices located in the Northwest will be called the *stair vertices*. The number of base vertices of $G_{p,n}$ is equal to p and the number of stair vertices is equal to n. We apply an orientation (indicated in fig. 4) such that every edge is directed toward North or West.

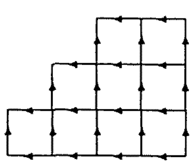


Fig. 4. Orientation of the transformed graph.

Now, we want to show that each perfect matching of $G_{p,n}$ is in bijection with a set of disjoint paths of $G^{\iota}_{p,n}$, joining the base vertices and the stair vertices, respecting the orientation (see example in fig. 5). We apply the transformation to a graph carrying a perfect matching. The dimers carried by a contracted edge all

Fig. 5. A $G_{6,3}$ perfect matching and the corresponding $G^{\prime}_{6,3}$ disjoint paths.

disappear. Other dimers get a vertex in common in pairs, which is the vertex replacing the contracted edge.

Let us give a local definition of the bijection by examining cases of (see fig. 6) the transformation of a contracted edge of $G_{p,n}$ carrying a perfect matching (the other edges remaining unchanged).

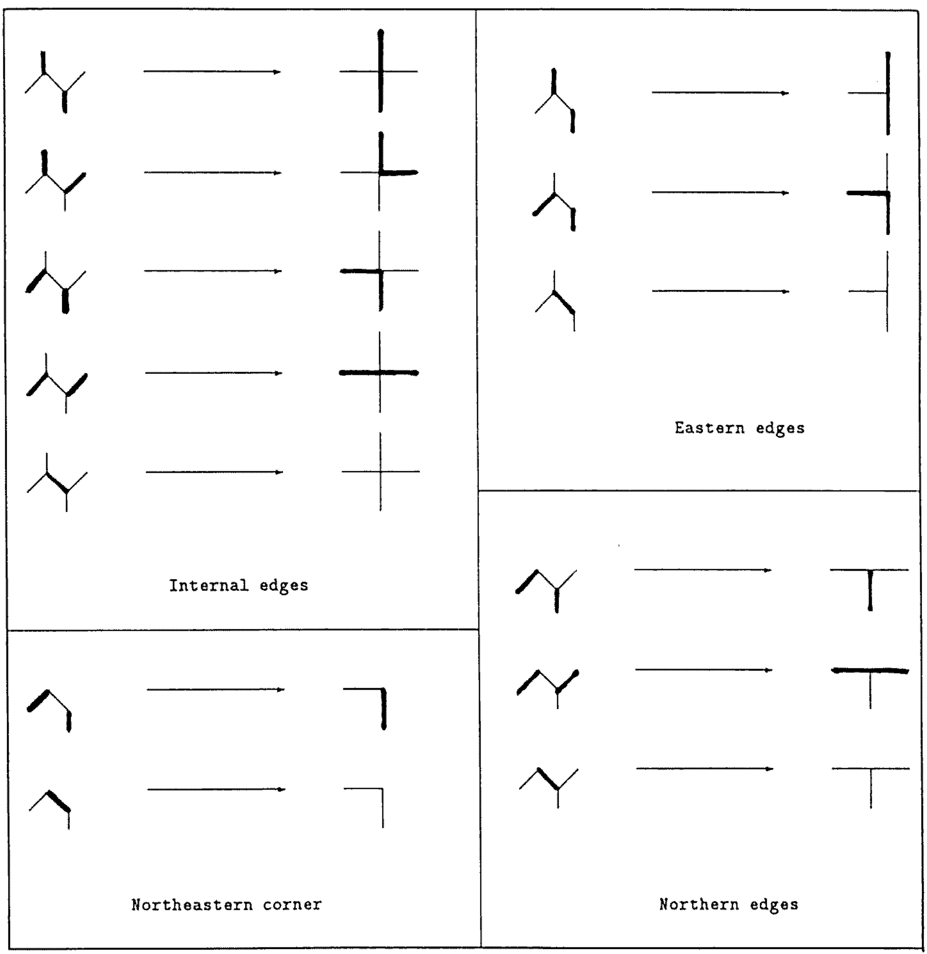


Fig. 6. The different cases of the bijection.

The transformation definition implies:

- On all but the base and the stair vertices of $G^{t}_{p,n}$, the transformed configuration has an even degree. Then the configuration obtained on $G^{t}_{p,n}$ contains a set of paths going from a base vertex to a stair vertex.
- Vertices of degree four do not appear, so the paths of $G^{t}_{p,n}$ are disjoint.
- Each sequence of two consecutive edges of a path goes either Northnorth, Westnorth, Northwest, or Westwest, so the paths respect the graph orientation.
- Every stair or base vertex belongs to a path because they are kept unchanged by the bijective transformation, and they all carry an edge of the $G_{p,n}$ perfect matching.

4. Particular case giving the Catalan numbers

Let us examine the particular pyramid based on p pentagons and of height $p-1$. The top of this pyramid is always composed of two hexagons.

DEFINITION 4.1

Let G_p be a honeycomb graph with trapezoidal shape based on p pentagons and of height $p-1$.

THEOREM 4.2

The number of the honeycomb graph G_p perfect matchings (see section 2) is equal to the Catalan number:

$$M_p = \frac{1}{p+1}\binom{2p}{p}.$$

The proof of the theorem begins with the bijection between the perfect matchings of G_p and the disjoint paths of the transformed graph G^{t}_{p}. Then we prove that the number of those paths are the Catalan number by putting them in bijection with objects counted by those numbers,

Since the number of stair vertices is equal to the number of base vertices minus two, the set of paths of the graph G^{t}_{p} contains paths going from a base vertex to a stair vertex, and one path going from a base vertex to another base vertex. This path is always made of only one edge and will be called *dimer* (which usually denotes a non-directed path). So, let us divide each configuration of disjoint paths into three parts (see fig. 7):

- the dimer,
- the *right-dimer paths*, which are the paths going from a base vertex located on the right of the dimer,

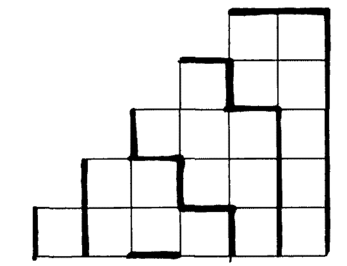


Fig. 7. A configuration of disjoint paths.

- the *left-dimer paths*, which are the paths going from a base vertex located on the left of the dimer.

Notation

Let w be a path and p a step of w. We shall denote by $h(p)$ the *height* of step p, which is equal to the number of North steps preceding p in the path w according to the orientation. Moreover, let us enumerate the paths of the right-dimer set from right to left.

Since the paths are disjoint and respect the graph orientation, the left-dimer paths are all made of vertical steps, without a West step (see fig. 7). Hence, they are determined by the base vertex from which they start. For the same reasons, all the right-dimer paths have two West steps. Thus, a configuration of disjoint paths may be given by

- the number of right-dimer paths,
- the two height sequences of the West step of the right-dimer paths.

PROPOSITION 4.3

There is a bijection between the set of configurations of disjoint paths defined on G_p and the set of all pairs of sequences:

$$((a_i)_{1 \le i \le l}, (b_i)_{1 \le i \le l}), \qquad 0 \le l \le p-1,$$

where l is the number of right-dimer paths, $a_i = h(p_1(w_i))$ and $b_i = h(p_2(w_i))$, where $p_1(w_i)$ and $p_2(w_i)$ are the two West steps of the paths w_i, and $h(p_1(w_i)) \le h(p_2(w_i))$, which satisfy, for $i \in \{1, 2, \ldots, l\}$:

$$\begin{cases} 0 \leq a_i \leq p-1, \\ 0 \leq b_j \leq p-1, \\ a_i \leq b_i, \\ a_i < a_j, \forall i < j, \\ b_i < b_j, \forall i < j. \end{cases} \tag{1}$$

The sequences (a_i) and (b_i) of the proposition have been introduced by Kreweras [14] as "éventails de segments". They are counted by the Catalan numbers.

Let us recall a bijection between those sequences and the so-called Dyck words, using Motzkin words. Let us first recall some definitions and notations:

- An alphabet X is a finite set of letters.
- The free monoid X^* is the infinite set of all the words that can be constructed from X, i.e. the finite sequences of letters of X.
- Concatenation of words is denoted by juxtaposition. If $v = abc$ and $w = ghj$, then the concatenation of v and w is denoted vw and is equal to $abcghj$.
- The length of a word is its number of letters.

DEFINITION 4.4

Let $X = \{x, \bar{x}\}$ and D_n be the set of *Dyck words* of length $2n$ defined by the conditions:

$$\forall u \in X, \ u \in D_n \Leftrightarrow \forall (v, w) \in (X^*)^2, \ \left| \begin{array}{l} u = vw \ \text{(concatenation of } v \text{ and } w\text{)}, \\ |v|_x \leq |v|_{\bar{x}}, \\ |u|_x = |u|_{\bar{x}}, \end{array} \right.$$

where $|u|_x$ means the number of x of the word u.

DEFINITION 4.5

Let $A = \{x, \bar{x}, R, B\}$, M^c be the set of *coloured Motzkin words* defined by the same conditions on x and $\bar{x}$ as the Dyck words for the letters x and $\bar{x}$ (no conditions on the letters R and B). Let M_n^c be the set of coloured Motzkin words with n letters.

LEMMA 4.6

There is a bijection between the couples of sequences satisfying condition (1) and the set M_{p-1}^c.

Proof

Let $i \leq k-1$, and $(a_j)_{1 \leq j \leq l}$ and $(b_j)_{1 \leq j \leq l}$, satisfying (1); then let $u = u_1 u_2 \ldots u_{k-1}$ be the word associated to those sequences by the following bijection:

$$\left|\begin{array}{l}\forall i,\ 1 \le i \le k-1,\\ i \in (a_j)_{1\le j\le l},\ i \in (b_j)_{1\le j\le l} \Rightarrow u_i = R,\\ i \notin (a_j)_{1\le j\le l},\ i \notin (b_j)_{1\le j\le l} \Rightarrow u_i = B,\\ i \in (a_j)_{1\le j\le l},\ i \notin (b_j)_{1\le j\le l} \Rightarrow u_i = x,\\ i \notin (a_j)_{1\le j\le l},\ i \in (b_j)_{1\le j\le l} \Rightarrow u_i = \bar{x}.\end{array}\right.$$

We easily verify that u is a coloured Motzkin word.

LEMMA 4.7

There is a bijection between M_n^c and D_{n+1} (see definitions 4.4 and 4.5).

Proof

This bijection is classical; let us briefly recall it. Let ϕ be the following morphism

$$\phi\ :\ \{R, B, x, \bar{x}\}^* \to \{x, \bar{x}\}^*,$$

such that

$$(y, y') \in \{R, B, x, \bar{x}\},\ \phi(y, y') = \phi(y)\,\phi(y').$$

The morphism ϕ is determined by

$$\phi(R) = x\bar{x}, \phi(B) = \bar{x}x, \phi(x) = xx, \phi(\bar{x}) = \bar{x}\bar{x}.$$

Let w_c be a coloured Motzkin word with n letters; its image w by the bijection is defined by $w = x\phi(w_c)\bar{x}$.

5. Enumeration of perfect matchings in the general case

THEOREM 5.1

The number of $G_{p,n}$ perfect matchings (see section 2) is equal to

$$N_{p,n} = \prod_{1\le i\le j\le n} \frac{1+j+p-n}{i+j}.$$

Proof

In ref. [12] we may find a bijection between the paths obtained by transformation of the graph $G_{p,n}$ and certain Young tableaux with bounded height (see fig. 8). This bijection constructs the tableau from the list of the numbers associated to each vertical step belonging to a path of the configuration (see fig. 8). Note that these

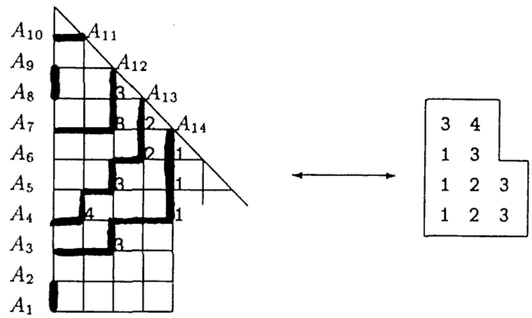


Fig. 8. A path configuration and its associated Young tableau.

numbers are not exactly those introduced as the step heights in the preceding proof. Then the Young tableaux are put in bijection with some fans of Dyck paths, using successive lightings and shadowings of cloud, an intermediate object. Then the final formula is obtained by computing Hankle determinant associated to the Dyck paths (from Gessel–Viennot bijection [15]) using the so-called qd-algorithm from Padé approximants theory.

$$\begin{array}{c}\overbrace{\hspace{7em}}^{p-1}\hspace{22em}\\ \left|\begin{array}{ccccccccccc}
1 & 1 & 1 & \dots & 1 & \binom{p}{1} & \binom{p}{2} & \binom{p}{3} & \dots & \binom{p}{n} \\
 & 1 & 1 & \dots & 1 & \binom{p-1}{1} & \binom{p-1}{2} & \binom{p-1}{3} & \dots & \binom{p-1}{n} \\
 & & 1 & \dots & 1 & .. & .. & .. & .. & .. \\
 & & & .. & .. & .. & .. & .. & .. & .. \\
 & & & 1 & 2 & 1 & 0 & .. & .. & 0 \\
 & & & & 1 & 0 & 0 & .. & .. & 0 \\
 & & & & & & .. & .. & .. & .. \\
 & & & & & & & & .. & .. \\
 & & & & & & & & & 0
\end{array}\right|\end{array}$$

Fig. 9. Pfaffian enumerating the $G_{p,n}$ perfect matchings.

Moreover, a combinatorial interpretation of some Pfaffians involving the configurations of disjoint paths of the graph $G_{p,n}$ is given in refs. [16, 17]. This study provides another expression enumerating the perfect matchings of the graph $G_{p,n}$ involving the Pfaffian of the table represented in fig. 9, which is different from the Pfaffian usually used to enumerate perfect matchings in statistical mechanics.

References

[1] D.J. Klein, G.E. Hite, W.A. Seitz and T.G. Schmaltz, Theor. Chim. Acta 69(1986)409.
[2] M. Randić, S. Nikolić and N. Trinajstić, Croat. Chem. Acta 61(1988)821.

[3] D.J. Klein and N. Trinajstić, J. Mol. Struct. (THEOCHEM) 206(1990)135.
[4] B. Jerman-Blažič, S. Nikolić and N. Trinajstić, J. Mol. Struct. (THEOCHEM) 227(1991)79.
[5] D.J. Klein and T.P. Živković, Subgraph generating functions in chemistry, an example for perfect matchings on honeycomb fragmens, Preprint (1990).
[6] P.W. Kasteleyn, J. Math. Phys. 4 (2)(1963).
[7] M.E. Fisher, J. Math. Phys. 7 (10)(1966)1776.
[8] C.A. Hurst, J. Math. Phys. 5 (1)(1964).
[9] E.W. Montroll, *Applied Combinatorial Mathematics* (Beckenbach/Wiley, New York, 1964).
[10] N. Trinajstić, D.J. Klein and M. Randić, Int. J. Quant. Chem. 520(1986)699.
[11] N. Trinajstić, Rep. Mol. Theor. 2(1990)185.
[12] M. Desainte-Catherine and G.X. Viennot, *Lecture Notes in Mathematics* 1234 (Springer, Berlin, 1986) p. 58.
[13] H. Hosoya, Comp. Math. Appl. 12B(1986)271.
[14] G. Kreweras, Sur les éventails de segments, cahier de BURO 15(1970)3.
[15] I. Gessel and X. Viennot, A combinatorial interpretation of determinants with weighted paths, Preprint.
[16] M. Desainte-Catherine, Couplages et pfaffiens en combinatoire, physique et informatique, thèse de doctorat de l'Université de Bordeaux I, France (1983).
[17] M. Desainte-Catherine and G.X. Viennot, Combinatorial interpretation of pfaffians with configurations of paths, Preprint.