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PERFECT MATCHINGS IN RANDOM HEXAGONAL CHAIN GRAPHS

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Abstract

Simple exact formulae are obtained for the expected value of the number of perfect matchings in a random hexagonal chain and for the asymptotic behavior of this expectation.

1. Introduction

A *perfect matching*, sometimes called a *1-factor*, in a graph G is a set of pairwise nonadjacent edges of G that spans the vertices of G. This report deals with some recent findings in connection with perfect matchings in graph-like arrangements of "hexagons" in the plane, or as "structures" realized by arrangements of regular hexagons in the plane. Such structures have interest in the chemistry of benzenoid hydrocarbons, where the perfect matchings correspond to Kekulé structures [1,2] and feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules; see, for example, [3]. For some recent results on the perfect matchings in these hexagonal structures, see [4-8].

In particular, in this note we prove correct a conjecture, stated in [9], concerning the number of perfect matchings in random "linear" arrangements of hexagons.

DEFINITION 1.1: HEXAGONAL GRAPH

A hexagonal graph is a finite connected graph with no cut vertex, no vertex of degree greater than 3, which can be drawn in the plane so that each interior region is bounded by a 6-cycle and such that each pair of interior regions have at most one edge in common. Each interior region in a hexagonal graph is called a hexagonal face. □

Three hexagonal graphs are shown in fig. 1.

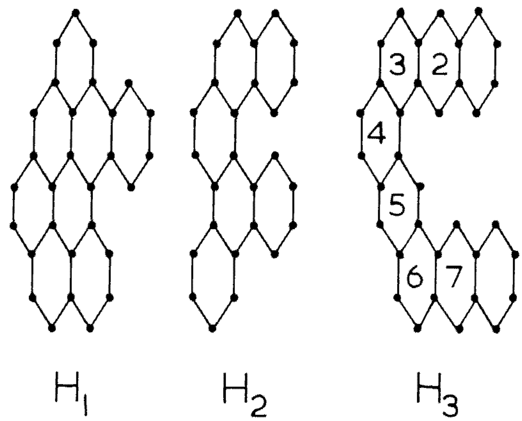

Fig. 1. Three hexagonal graphs.

DEFINITION 1.2: HEXAGONAL SYSTEM

A hexagonal graph H is called a hexagonal system provided H can be embedded in the plane so that each hexagonal face of H is made congruent to a regular unit hexagon. □

All three hexagonal graphs in fig. 1 are also hexagonal systems. We remark that a hexagonal system can also be regarded as any subgraph of a hexagonal (or honeycomb) lattice graph [3] induced by a simple closed Jordan curve in that lattice graph. That is, the union of the boundary and interior is enclosed by a Jordan curve.

DEFINITION 1.3: HEXAGONAL CHAINS

A hexagonal graph (system) is called a hexagonal chain graph (system) provided no hexagonal face is adjacent to more than two other hexagonal faces. □

The hexagonal graph H_3 in fig. 1 is a hexagonal chain graph; H_1 and H_2 are not. The remainder of this report deals only with hexagonal chains (graphs or systems). Clearly, the dual of a hexagonal chain graph, with the external face omitted, is a path graph.

Let H be a hexagonal chain graph with $h \geq 3$ hexagonal faces. Let the hexagonal faces be labelled by $x_1, x_2, \ldots, x_h$ so that x_i and x_{i+1} are adjacent for each $i = 1, 2, \ldots, h-1$. Call x_1 and x_h *terminal* faces. Then, the remaining faces may be either of two types, which we designate *type L* or *type A* according to whether they separate their two adjacent faces by a distance of 2 or 1, respectively. The

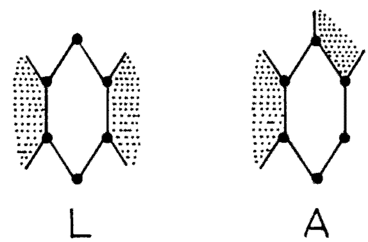

Fig. 2. Two types of non-terminal hexagonal faces.

concept is illustrated in fig. 2. In fig. 1, the non-terminal faces 2, 3, 4, 5, 6, 7 of H_3 are of types L, A, A, L, A, L, respectively.

The number of perfect matchings M_h of a hexagonal chain graph with h faces can be obtained by a recursive method due to Gordon and Davison given in [10], or by the following modified form given in [9,11,12]. Let

$$M_1 = 2, \ M_2 = 3,$$

and then for $i = 3, 4, \ldots, h$,

$$M_i = \begin{cases} 2M_{i-1} - M_{i-2} & \text{if face } i-1 \text{ is of type L,} \\ M_{i-1} + M_{i-2} & \text{if face } i-1 \text{ is of type A.} \end{cases}$$

DEFINITION 1.4: RANDOM HEXAGONAL CHAIN GRAPH

A *random hexagonal chain graph* (of length h) $H(h, p)$ is a hexagonal chain graph with h faces in which each non-terminal face is either of type A with probability p, or type L with probability $1-p$. □

Let $M_{h,p}$ be the number of perfect matching of $H(h, p)$. Then, $M_{h,p}$ is a random variable. Denote the expected value of $M_{h,p}$ by $E(M_{h,p})$.

LEMMA 1.5

For each $i \geq 3$,

$$E(M_{i,p}) = (2 - p)E(M_{i-1,p}) + (2p - 1)E(M_{i-2,p}).$$

Proof

If face $(i-1)$ of $H(h, p)$ is of type A with probability p and of type L with probability $1-p$, then from the Gordon–Davison recursion,

$$E(M_{i,p}) = p(M_{i-1,p} + M_{i-2,p}) + (1-p)(2M_{i-1,p} - M_{i-2,p})$$
$$= (2-p)M_{i-1,p} + (2p-1)M_{i-2,p},$$

$E(E(M_{i,p})) = E(M_{i,p})$ and since $E(M_{i,p})$ is a sum of random variables, it follows that

$$E(M_{i,p}) = (2-p)E(M_{i-1,p}) + (2p-1)E(M_{i-2,p}). \qquad \square$$

In [9,11,13], it is suggested that the function $E(M_{h,p})$ has interest in chemistry, especially concerning its asymptotic behavior with respect to h. The recurrence relation obtained in lemma 1.5 enables us to derive an explicit expression for this function. This is given in the following theorem. In corollary 1.7.1 to this theorem, we show that the value of the limit of $E(M_{h,p})/E(M_{h-1,p})$, as h goes to infinity, is as conjectured in [9]. It is appropriate to note that the form of this limit could be anticipated from [11, (eq. 9)] or [13, eqs. (3.2), (3.3)].

THEOREM 1.7

For each $i \geq 2$ and when $p > 0$,

$$E(M_{i+1,p}) = \left(\frac{2s-3}{s-r}\right) r^i - \left(\frac{2r-3}{s-r}\right) s^i,$$

where $r = (2-p+(p^2+4p)^{1/2})/2$, and $s = (2-p-(p^2+4p)^{1/2})/2$. Or, when $p = 0$, for each $i \geq 0$,

$$E(M_{i+1,0}) = 2 + i.$$

Proof

Let $a_i = E(M_{i+1,p})$, with $i \geq 0$, so that $a_0 = 2$, $a_1 = 3$, and by lemma 1.5

$$a_i = (2-p)a_{i-1} + (2p-1)a_{i-2} \qquad \text{for} \quad i \geq 2.$$

The solution to this recurrence relation is as follows (see, for example, [14, pp. 210–216]): The characteristic equation is

$$x^2 - (2-p)x - (2p-1) = 0$$

and the characteristic roots are

$$r = (2-p+(p^2+4p)^{1/2})/2 \quad \text{and} \quad s = (2-p-(p^2+4p)^{1/2})/2.$$

Case 1: $p > 0$ so that the two roots are distinct. In this case,

$$a_i = \alpha(r)^i + \beta(s)^i.$$

The boundary conditions $a_0 = 2$ and $a_1 = 3$ require

$$\alpha + \beta = 2, \quad \alpha r + \beta s = 3,$$

so that

$$\alpha = \left(\frac{2s-3}{s-r}\right) \text{ and } \beta = -\left(\frac{2r-3}{s-r}\right),$$

which proves the first statement of the theorem.

Case 2: $p = 0$ so that $r = s = 1$. In this case, it is easy to see that $a_i = 2 + i$. □

COROLLARY 1.7.1

If $p > 0$, then

$$\lim_{h\to\infty} \left(E(M_{h,p})/E(M_{h-1,p})\right) = (2-p+(p^2+4p)^{1/2})/2.$$

Proof

$$E(M_{h,p})/E(M_{h-1,p}) = \{\alpha r^{h-1} + \beta s^{h-1}\}/\{\alpha r^{h-2} + \beta s^{h-2}\}$$
$$= \{r + (\beta/\alpha)s(s/r)^{h-2}\}/\{1 + (\beta/\alpha)(s/r)^{h-2}\}.$$

Since $r > s$, it follows that

$$\lim_{h\to\infty} \left(E(M_{h,p})/E(M_{h-1,p})\right) = r = (2-p+(p^2+4p)^{1/2})/2.$$ □

2. LA-sequences for hexagonal chains

Associated with any labelled hexagonal chain graph (or chain system) with length h is a unique ordered sequence of $(h-2)$ symbols from the set {L, A} and comprising the sequence of types of its non-terminal hexagonal faces. This sequence is called the *LA-sequence* of the hexagonal chain (see [1, 15]).

On the other hand, for a given LA-sequence that contains at least two A's, there is more than one associated chain. Specifically, each non-terminal face of type A can have one of two possible orientations with reference to the direction determined by the first two faces of the chain. In view of this, we can augment the LA-sequence of a chain to reflect orientations of the faces of type A by attaching one of the two signs $\{+,-\}$ to each A symbol in an LA-sequence. We call the result an *oriented LA-sequence* (or OLA-sequence) of the hexagonal chain graph (or chain system).

For each (labelled) hexagonal chain graph or chain system, there is an OLA-sequence; furthermore, this is unique up to reversal of all signs. Similarly, for each OLA-sequence, there is an associate hexagonal chain graph. It is not true, of course, that to each OLA-sequence there corresponds a hexagonal chain system, since not every chain graph is a chain system. An obvious example is provided by the OLA-sequence (+A, +A, +A, +A).

DEFINITION 2.1: RANDOM OLA-SEQUENCE

A *random oriented LA-sequence* of length h is an OLA-sequence with $h-2$ entries, each of which is "+A" with probability p_1, or "−A" with probability p_2, or "L" with probability $q = 1 - p_1 - p_2$. The hexagonal chain graph associated with a random OLA-sequence is a random hexagonal chain graph. □

Obviously, since the Gordon–Davison recursion result is invariant to any orientation imposed on non-terminal faces of type A, it immediately follows that the number of perfect matchings in a hexagonal chain graph is independent of any imposed orientation of the graph. Thus, analogues of lemma 1.5 and theorem 1.7 for random OLA-sequences follow by using the replacements $p = p_1 + p_2 = 1 - q$ in those statements.

Note that if all orientations are equiprobable, that is, if $p_1 = p_2 = q = 1/3$, a random OLA-sequence will result in a random hexagonal chain graph with more A faces than in the case where just two equiprobable choices A or L are available (with $p = q = 1/2$). For both probability models, the expected number of perfect matchings is the same for equal values of q.

The effect on $\lim_{h\to\infty}(E(M_{h,p})/E(M_{h-1,p}))$ (see corollary 1.7.1) when there are three *equiprobable* choices, rather than two, is that the limit is then equal to $(2 + (7)^{1/2})/3 = 1.54858377(0)$ rather than 3/2.

Finally, we comment on the number of hexagonal chain graphs. First note that there are 3^{h-2} OLA-sequences of length $h-2$. The OLA-sequence all of whose entries are L corresponds to exactly one hexagonal chain graph. With this one exception, each OLA-sequence and the OLA-sequence obtained by reversing the sign of each A entry correspond to the same labelled hexagonal chain graph. Thus, the 3^{h-2} OLA-sequences correspond to $(3^{h-2}+1)/2$ distinct *labelled* hexagonal chain graphs with h hexagonal faces.

The probability that a random labelled hexagonal chain graph with h hexagons has x non-terminal faces with orientation +A, y with −A, and $z = h - (2 + x + y)$ with orientation L is $2(h-2)!p_1{}^x p_2{}^y q^z/x!y!z!$ when $z \neq h-2$, and q^{h-2} when $z = h-2$.

A similar discussion can be developed for *unlabelled* hexagonal chain graphs.

The problem of enumerating perfect matchings in various generalizations of chain graphs can be reduced to that of enumerating perfect matchings in chain graphs (see [12,16]).

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