

## On Matching Polynomials of a Simple Hexagonal Lattice

S.A. Wahid

Department of Mathematics and Computer Sciences, The Centre for Graph Polynomials,  
 The University of the West Indies, St. Augustine, Trinidad and Tobago

**Abstract:** A recurrence relation is derived for the matching polynomial of a 2 x n hexagonal lattice. Explicit formulae are then obtained for the first ten and the final four coefficients.

**Key words:** Polynomial, hexagonal lattice, coefficients

### INTRODUCTION

The graphs considered here are all finite and without loops or multiple edges. By a matching in a graph  $G$ , we mean a spanning subgraph of  $G$  whose components are nodes and edges. We define a defect- $d$  matching to be a matching with  $d$  component nodes, see Berge<sup>[1,2]</sup> and Little<sup>[3]</sup>. We denote the number of defect- $d$  matchings in  $G$  by  $N_d(G)$ . A perfect matching is a defect-0 matching. Let  $G$  be a graph with  $p$  nodes. We associate the weights  $w_1$  and  $w_2$  with each node and edge respectively. With each matching in  $G$ , we associate the monomial  $w_1^{2k}w_2^k$  i.e., the product of the weights of the components. Then the matching polynomial of  $G$  is 
$$M(G;w_1,w_2) = \sum_k \alpha_k w_1^{p-2k} w_2^k$$

where  $\alpha_k$  is the number of matchings in  $G$  with  $k$  edges and the summation is taken over all values of  $k$ . The basic properties of matching polynomials can be found in Farrell<sup>[4]</sup>. A monomer-dimer covering of a molecule is equivalent to a matching in a graph.

The importance of monomer-dimer coverings in statistical mechanics have been examined by Heilmann and Lieb<sup>[5]</sup>.

The acyclic polynomial which is obtained from the matching polynomial by putting  $w_1 = x$  and  $w_2 = -1$  has been shown to be a useful tool in mathematical chemistry, see Gutman<sup>[6,7]</sup> and Aihara<sup>[8]</sup>.

We denote by  $A_n$  the lattice formed by concatenating two layers of hexagons.

### MATERIALS AND METHODS

The following results given in<sup>[4]</sup> are the essential methods used to reduce a graph. By applying this reduction process we can set up recurrences for matching polynomials of graphs. They are useful in the material which follows.

**The fundamental reduction process:** Let  $G$  be a graph having an edge  $e$ . Let  $G'$  be the graph obtained from  $G$  by deleting  $e$  and  $G''$ , the graph obtained from  $G$  by removing the nodes at the ends of  $e$ . Then

$$M(G;w_1,w_2) = M(G';w_1,w_2) + w_2 M(G'';w_1,w_2).$$

**The component theorem:** If  $G$  consists of two components  $R$  and  $S$ , then  $M(G;w_1,w_2) = M(R;w_1,w_2) M(S;w_1,w_2)$ .

We use generating functions to solve the system of recurrences that are obtained by using (a) and (b). The following result (c) is used to find the first three coefficients.

(c) Let  $G$  have  $p$  nodes and  $q$  edges. Then in  $M(G;w_1,w_2)$ ,  
 (i)  $a_0 = 1$ ,  $a_1 = q$  and

(ii)  $a_2 = \binom{q}{2} - \beta$ , where  $\beta$  is the number of paths of length 2 in  $G$ .

It is easy to find  $\beta$  by choosing two edges at each node in all different ways i.e.,

$$\beta = \sum_{i=1}^p \binom{v_i}{2}, \text{ where } v_i \text{ is the valency of node } i \text{ in } G.$$

The successive coefficients are found by first obtaining a recurrence for the hexagonal lattice  $A_n$ . Once an expression for a coefficient is found, we use these formulae to generate the value of the successive coefficient.

### RESULTS

**The matching polynomial of  $A_n$  written as a recurrence:** We apply the reduction process as stated in result (a) initially to the graph  $A_n$  and all reduced graphs that are shown in Fig. 1.

In so doing the following recurrences are obtained that are valid for  $n \geq 1$ .

**Lemma 1**

- (I)  $A_n = B_{n-1} + w_2 C_{n-1}$ .
- (ii)  $B_n = w_1 D_n + w_2 E_n$ .
- (iii)  $C_n = w_1 F_n + w_1 w_2 G_{n-1} + w_2^2 w_1 D_{n-1} + w_2^2 J_{n-1} + w_2^3 C_{n-1} + w_2^3 G_{n-1}$ .
- (iv)  $D_n = w_1 C_n + w_2 w_1 K_n + w_2^2 w_1 A_n + w_2^2 D_{n-1}$ .
- (v)  $E_n = w_1 F_n + (w_2^2 + w_2 w_1^2) A_n + w_2^2 w_1 M_{n-1}$ .
- (vi)  $F_n = w_1 P_n + 2w_2 w_1 A_n + w_2^2 M_{n-1} + w_2^2 Q_{n-1}$ .
- (vii)  $G_n = w_1 J_n + (w_2 w_1^2 + w_2^2) K_n + w_2^2 w_1^2 A_n + w_2^3 w_1 D_{n-1}$ .
- (viii)  $J_n = w_1 C_n + w_2 R_n$ .
- (ix)  $K_n = w_1^2 A_n + w_2 w_1 M_{n-1} + w_2 w_1 D_{n-1} + w_1 w_2^2 R_{n-1} + w_2^3 K_{n-1}$ .
- (x)  $M_n = (w_1^2 + w_2) R_n + w_2 w_1 K_n + w_2 w_1 P_n + w_2^2 w_1 A_n + w_2^3 M_{n-1}$ .
- (xi)  $P_n = w_1^2 A_n + w_2 w_1 M_{n-1} + w_2 w_1 J_{n-1} + w_2^2 w_1 F_{n-1} + w_2^3 P_{n-1}$ .
- (xii)  $Q_n = w_1 C_n + w_2 F_n$ .
- (xiii)  $R_n = w_1 K_n + (w_2 w_1^2 + w_2^2) J_{n-1} + w_2^2 w_1^2 F_{n-1} + w_2^3 w_1 P_{n-1}$ .

We then use standard techniques of generating functions to get the following recurrence in  $A_n$ .

**Theorem 1**

$$A_n = (w_1^6 + 8w_2 w_1^4 + 17w_2^2 w_1^2 + 8w_2^3) A_{n-1} - (3w_2^2 w_1^8 + 28w_2^3 w_1^6 + 84w_2^4 w_1^4 + 88w_2^5 w_1^2 + 28w_2^6) A_{n-2} + (3w_2^4 w_1^{10} + 32w_2^5 w_1^8 + 126w_2^6 w_1^6 + 228w_2^7 w_1^4 + 191w_2^8 w_1^2 + 56w_2^9) A_{n-3} - (w_2^6 w_1^{12} + 12w_2^7 w_1^{10} + 61w_2^8 w_1^8 + 172w_2^9 w_1^6 + 281w_2^{10} w_1^4 + 224w_2^{11} w_1^2 + 70w_2^{12}) A_{n-4} + (3w_2^{10} w_1^{10} + 28w_2^{11} w_1^8 + 102w_2^{12} w_1^6 + 176w_2^{13} w_1^4 + 151w_2^{14} w_1^2 + 56w_2^{15}) A_{n-5} - (3w_2^{14} w_1^8 + 20w_2^{15} w_1^6 + 52w_2^{16} w_1^4 + 56w_2^{17} w_1^2 + 28w_2^{18}) A_{n-6} + (w_2^{18} w_1^6 + 4w_2^{19} w_1^4 + 9w_2^{20} w_1^2 + 8w_2^{21}) A_{n-7} - w_2^{24} A_{n-8}, (n \geq 9).$$

A Table of coefficients of  $M(A_n; w_1, w_2)$  for  $n = 1$  to  $9$  is given below. We note that  $A_1$  is the path on four nodes.

Theorem 1 is now used to give the number of  $k$ -matchings ie. the coefficients of matching polynomials.

**Number of  $k$ -matchings in  $A_n$ :** As mentioned before, the number of defect  $-k$  matchings in  $G$  is written as  $N_k(G)$  and the number of  $k$ -matchings is  $\alpha_k(G)$ . We state the formulae for  $\alpha_k(A_n)$  for the first three values of  $k$ .

**Theorem 2**

$$\begin{aligned} \alpha_0(A_n) &= 1, & n \geq 1 \\ \alpha_1(A_n) &= 8n - 5, & n \geq 1 \\ \text{and } \alpha_2(A_n) &= 32n^2 - 58n + 29, & n \geq 2. \end{aligned}$$

Table 1: Coefficients of matching polynomials

n	Coefficients of $M(A_n; w_1, w_2)$ written in increasing powers of $w_2$
1	1,3,1
2	1,11,41,61,31,3
3	1,19,143,547,1132,1244,661,135,6
4	1,27,309,1961,7579,18441,28218,26354,14086,3817,414,10
5	1,35,539,4815,27694,107618,288453,534829,677921,571751,306251,96534,15742,1038,15
6	1,43,833,9621,73893,398535,1553872,4442120,9345547,14398537,16030128,12605006,6759506,485317,52357,2276,21
7	1,51,1191,16891,162688,1127448,5810931,22707547,67973178,156433962,276262234,371712868,376265551,281123407,150857707,55938623,13553613,1971415,149623,4529,28
8	1,59,1613,27137,314687,2669877,17169350,85552126,334853938,1037589342,2553803425,4990433843,7711656287,9352803755,8801483951,6324560617,3395386889,1322124110,358471282,63850156,6842838,381543,8368,36
9	1,67,2099,40871,554594,5573374,40333569,261410761,1268965511,4972794985,15828788075,41046957489,86738080903,149025190015,207199626684,231437473113,205577334315,143255713873,76929903871,31099715551,9174548032,1893084337,257272466,21031001,889793,14577,45

**Proof:**  $A_n$  has  $6n - 2$  nodes. There is only one matching with zero edges i.e the empty graph with  $6n - 2$  nodes. Therefore (i) follows. Now  $A_n$  has  $n-1$  cells. The first cell has 11 edges and the remaining  $(n-2)$  cells each have 8 edges. Thus  $\alpha_1 = 11 + 8(n-2) = 8n - 5$ .

There are  $2n + 4$  nodes of degree 2 and  $4n-6$  nodes of degree 3 in  $A_n$ . By using result (c) above, the expression follows easily for  $\alpha_2(A_n)$ .

By equating the coefficient of  $w_2^k$  in Theorem 2, we obtain the following result.

**Theorem 3:**  $A_n$  has a  $k$ -matching if and only if  $0 < k \leq (3n-1)$  In this case,

$$\begin{aligned} a_k(A_n) &= a_k(A_{n-1}) + 8a_{k-1}(A_{n-1}) + 17a_{k-2}(A_{n-1}) + 8a_{k-3}(A_{n-1}) - \\ & 3a_{k-2}(A_{n-2}) - 28a_{k-3}(A_{n-2}) - 84a_{k-4}(A_{n-2}) - 88a_{k-5}(A_{n-2}) - 28a_{k-6} \\ & (A_{n-2}) + 3a_{k-4}(A_{n-3}) + 32a_{k-5}(A_{n-3}) + 126a_{k-6}(A_{n-3}) + 228a_{k-7} \\ & (A_{n-3}) + 191a_{k-8}(A_{n-3}) + 56a_{k-9}(A_{n-3}) - a_{k-6}(A_{n-4}) - 12a_{k-7} \\ & (A_{n-4}) - 61a_{k-8}(A_{n-4}) - 172a_{k-9}(A_{n-4}) - 281a_{k-10}(A_{n-4}) - \\ & 224a_{k-11}(A_{n-4}) - 70a_{k-12}(A_{n-4}) + 3a_{k-10}(A_{n-5}) + 28a_{k-11} \\ & (A_{n-5}) + 102a_{k-12}(A_{n-5}) + 176a_{k-13}(A_{n-5}) + 151a_{k-14}(A_{n-5}) \\ & + 56a_{k-15}(A_{n-5}) - 3a_{k-14}(A_{n-6}) - 20a_{k-15}(A_{n-6}) - 52a_{k-16} \\ & (A_{n-6}) - 56a_{k-17}(A_{n-6}) - 28a_{k-18}(A_{n-6}) + a_{k-18}(A_{n-7}) + 4a_{k-19} \\ & (A_{n-7}) + 9a_{k-20}(A_{n-7}) + 8a_{k-21}(A_{n-7}) - a_{k-24}(A_{n-8}) (n \geq 9). \end{aligned}$$

By putting  $k = 3, 4, 5, 6, 7$  and  $8$  respectively in Theorem 3, we use generating functions to obtain the following result.

**Theorem 4:**

- (i)  $\alpha_3(A_n) = 175 + (1154/3)n - 304n^2 + (256/3)n^3$ . ( $n \geq 2$ ).
- (ii)  $\alpha_4(A_n) = 1079 - (7501/3)n + (6934/3)n^2 - (3008/3)n^3 + (512/3)n^4$  ( $n \geq 3$ ).
- (iii)  $\alpha_5(A_n) = -6755 + (242669/15)n - (49022/3)n^2 + 8656n^3 - (7168/3)n^4 + (4096/15)n^5$ . ( $n \geq 3$ ).
- (iv)  $\alpha_6(A_n) = 42798 - (314279/3)n + (5038516/45)n^2 - 66620n^3 + (208448/9)n^4 - (13312/3)n^5 + (16384/45)n^6$ . ( $n \geq 4$ )
- (v)  $\alpha_7(A_n) = -273818 + (71436107/105)n - (34011836/45)n^2 + (21830804/45)n^3 - (1741984/9)n^4 + (2150912/45)n^5 - (303104/45)n^6 + (131072/315)n^7$ . ( $n \geq 4$ ).
- (vi)  $\alpha_8(A_n) = 1766126 - (186256835/42)n + (3190961899/630)n^2 - (154254958/45)n^3 + (67447294/45)n^4 - (3888512/9)n^5 + (3595264/45)n^6 - (2718744/315)n^7 + (131072/315)n^8$ . ( $n \geq 5$ )

**Defect -d-matchings in  $A_n$ :** The following result is obtained from Theorem 1 by equating coefficients of the terms in  $w_1^d$ .

**Theorem 5:**  $A_n$  has a defect - d matching for  $0 \leq d \leq (3n - 1)$ . In this case,

$$\begin{aligned}
 N_d(A_n) = & N_{d-6}(A_{n-1}) + 8 N_{d-4}(A_{n-1}) + 17 N_{d-2}(A_{n-1}) + 8 \\
 & N_d(A_{n-1}) - 3 N_{d-8}(A_{n-2}) - \\
 & 28N_{d-6}(A_{n-2}) - 84N_{d-4}(A_{n-2}) - 88N_{d-2}(A_{n-2}) - 28N_d(A_{n-2}) \\
 & + 3N_{d-10}(A_{n-3}) + \\
 & 32N_{d-8}(A_{n-3}) + 126N_{d-6}(A_{n-3}) + 228N_{d-4}(A_{n-3}) + 191N_{d-2}(A_{n-3}) \\
 & + 56N_d(A_{n-3}) - \\
 & N_{d-12}(A_{n-4}) + 12N_{d-10}(A_{n-4}) - 61N_{d-8}(A_{n-4}) - 172N_{d-6}(A_{n-4}) \\
 & - 281N_{d-4}(A_{n-4}) - \\
 & 224N_{d-2}(A_{n-4}) - 70N_d(A_{n-4}) + 3N_{d-10}(A_{n-5}) + 28N_{d-8}(A_{n-5}) \\
 & + 102N_{d-6}(A_{n-5}) + \\
 & 176N_{d-4}(A_{n-5}) + 151N_{d-2}(A_{n-5}) + 56N_d(A_{n-5}) - 3N_{d-8}(A_{n-6}) \\
 & - 20N_{d-6}(A_{n-6}) - \\
 & 52N_{d-4}(A_{n-6}) - 56N_{d-2}(A_{n-6}) - 28N_d(A_{n-6}) + N_{d-6}(A_{n-7}) + \\
 & 4N_{d-4}(A_{n-7}) + \\
 & 9N_{d-2}(A_{n-7}) + 8N_d(A_{n-7}) - N_d(A_{n-8}). \quad (n \geq 9)
 \end{aligned}$$

**Lemma 2**

$$N_0(A_n) = 8N_0(A_{n-1}) - 28 N_0(A_{n-2}) + 56N_0(A_{n-3}) - 70N_0(A_{n-4}) + 56N_0(A_{n-5}) - 28N_0(A_{n-6}) + 8N_0(A_{n-7}) - N_0(A_{n-8}).$$

We then use the method of generating functions to get the following result.

**Theorem 6:**

$$N_0(A_n) = \frac{n(n+1)}{2} \quad (n \geq 1).$$

By putting  $n = 2$  in Lemma 2 , we get

$$\begin{aligned}
 N_2(A_n) = & 17N_0(A_{n-1}) + 8N_2(A_{n-1}) - 88N_0(A_{n-2}) - 28N_2(A_{n-2}) \\
 & + 191N_0(A_{n-3}) + 56N_2(A_{n-3}) - 224N_0(A_{n-4}) - 70N_2(A_{n-4}) + \\
 & 151N_0(A_{n-5}) + 56N_2(A_{n-5}) - 56N_0(A_{n-6}) - 28N_2(A_{n-6}) + \\
 & 9N_0(A_{n-7}) + 8N_2(A_{n-7}) - N_2(A_{n-8}). \quad (n \geq 9).
 \end{aligned}$$

We use Theorem 6 to substitute the values of  $N_0(A_{n-k})$  for  $k = 1, 2, \dots, 8$  to get

$$\begin{aligned}
 N_2(A_n) = & 8N_2(A_{n-1}) - 28N_2(A_{n-2}) + 56N_2(A_{n-3}) - 70N_2(A_{n-4}) \\
 & + 56N_2(A_{n-5}) - 28N_2(A_{n-6}) + 8N_2(A_{n-7}) - N_2(A_{n-8}). \quad (n \geq 9).
 \end{aligned}$$

We solve by the method of generating functions to get the following result.

**Theorem 7**

$$\begin{aligned}
 N_2(A_n) = & -216 + (5452/15)n - (89867/360)n^2 + (22459/240)n^3 \\
 & - (337/18)n^4 + (49/20)n^5 - \\
 & (53/360)n^6 + (1/240)n^7. \quad (n \geq 2).
 \end{aligned}$$

This procedure is repeated in turn for the values  $n = 4$  and  $6$ . In so doing we obtain the following result which gives the number of defect-4 and defect-6 matchings.

**Theorem 8:**

- (i)  $N_4(A_n) = -939 + (25826501/13860)n - (4985567/3150)n^2 + (687729289/907200)n^3 - (1181435/5184)n^4 + (16022679/34560)n^5 - (1009057/172800)n^6 + (99797/151200)n^7 - (979/24192)n^8 + (467/145152)n^9 - (67/518400)n^{10} + (1/316800)n^{11}$ . ( $n \geq 2$ ).
- (ii)  $N_6(A_n) = 28168 - (4479316873/90090)n + (1821886442977/50450400)n^2 - (3615817719847/259459200)n^3 + (134323583/44550)n^4 - (39042403529/119750400)n^5 + (12460517/21772800)n^6 + (426586513/87091200)n^7 - (23504843/38102400)n^8 + (1698391/21772800)n^9 - (139/43200)n^{10} + (40153/95800320)n^{11} - (269/29937600)n^{12} + (2071/3113510400)n^{13} - (17/871782912)n^{14} + (1/1779148800)n^{15}$ . ( $n \geq 2$ ).

**DISCUSSION**

This article has paved the way for further research in lattice type graphs. It is possible to get results on other coefficients but the calculations are tedious. It is interesting to note that all thirteen graphs mentioned in the Fig. 2 have the same recurrence for their matching polynomials. It is not simple to get a recurrence for the general lattice with  $m$  rows of hexagons with each row having  $n$  hexagons.

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