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MATCHINGS IN LONG BENZENE CHAINS

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Abstract

An explicit recurrence relation is derived for the matching polynomial of the long hexagonal (benzene) chain. From this several formulae are derived for the number of various kinds of matchings in the chain.

Keywords and Phrases

matching	recurrence relation
matching polynomial	generating function
defect-d matching	reduction process
k-matching	benzene chain
long benzene chains	

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1. *Introduction*

The graphs considered here will be finite and will contain no loops nor multiple edges. Let G be such a graph. A *matching* in G is a spanning subgraph of G whose components are nodes and edges only. If the matching has d nodes, it is called a *defect-d* matching. If it has k edges, it is called a *k-matching*. Clearly a k-matching is also a defect - (p-2k) matching, where p is the number of nodes in G. The *matching polynomial* of G - denoted by m(G), is the following

$$m(G) = \sum_{n=0}^{[p/2]} a_k w_1^{p-2k} w_2^{k},$$

where a_k is the number of k-matching in G, and w_1 and w_2 are indeterminates associated with each node and edge respectively in G. For the basic properties of m(G), we refer the reader to Farrell [1], and Godsil and Gutman [3].

There are many interesting forms of m(G), when special values are assigned to w_1 and w_2. Some of these polynomials already existed in the Chemical and Physical literatures. An account of these can be found in Gutman [8] and Godsil and Gutman [4]. Recent applications of m(G) in Chemistry can be found in Gutman [5,6,7].

We define the *hexagonal* or *benzene chain* to be the graph formed by attaching a finite number n of regular hexagons together in a linear manner, in such a way, that adjacent hexagons have exactly one edge in common. This graph is also called a hexagonal animal (see Harary [9]). We call it the benzene chain A_n. Matchings in A_n were discussed in Farrell & Wahid [2]. The *long benzene chain* L_n is the graph formed by identifying the two *terminal edges* (See edges ab and xy in Figure 1(i) below) of A_n. A_4 and L_4 are shown below in Figure 1. It is clear that L_n has 4n nodes and 5n edges. L_n is a special case of a rotagraph (See [10]). Its chemical name is rotapolyacene.

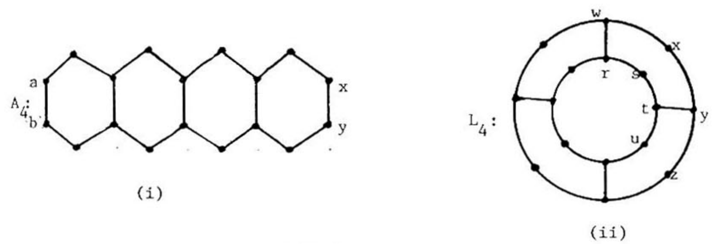

Figure 1

In this paper we will derive an explicit recurrence for L_n. This will be used to obtain explicit formulae for the numbers of various kinds of matchings in L_n. L_n will be written for $m(L_n)$, when it would lead to no confusion, and especially in recurrence relations. We will denote the generating function of m(G) with indicator function t, by G(t). The number of defect-d matchings in G will be denoted by $N_d(G)$ and the number of k-matchings, by $\gamma_k(G)$. Their generating functions will be denoted by $N_d\ G(t)$ and $\gamma_k G(t)$ respectively. The notation $(N_{d_1} + N_{d_2} \dots + N_{d_r})L_n$ would mean $N_{d_1}(L_n) + N_{d_2}(L_n) + \dots + N_{d_r}(L_n)$. Clearly from our definitions we must have 1. $N_d(G) = 0$, for $d < 0$

and 2. $\gamma_k(G) = 0$, for $k < 0$.

Also, $a_k = a_k(G) = \gamma_k(G)$.

2. *Preliminary Results*

The following theorem, called the fundamental theorem for matching polynomials was proved in [1].

Theorem 1

Let G be a graph containing an edge xy. Let G' be the graph obtained from G by deleting xy and G" the graph G-{x,y}. Then

$$m(G) = m(G') + w_2\, m(G'')$$

The algorithm implied by this theorem will be called the *reduction process*. In order to effectively carry out the reduction process, we need the Component Theorem, also given in [3].

Theorem 2 (The Component Theorem)

Let G be a graph with r components H_i (i = 1,2, ..., r). Then

$$m(G) = \prod_{i=1}^{r} m(H_i) .$$

The following result can be easily proved. It was also given in [2].

Theorem 3

Let G be a graph with p nodes and q edges. Then in m(G),

$$\text{(i) } a_0 = 1, \quad \text{(ii) } a_1 = q \text{ and (iii) } a_2 = \binom{q}{2} - \sum_{i=1}^{p} \binom{v_i}{2} ,$$

where v_i is the valency of node i.

Theorems 1, 2 and 3 will be used in the material which follows. Notice that in applications of the reduction process, the graphs G' and G" will be called the *reduced graph* and the *incorporated graph* respectively.

3. *Matching Polynomials of Long Benzene Chains*

When applying the reduction process to L_n, we will obtain graphs which comprise of the benzene chain A_{n-1} with edges attached to its terminal nodes in various ways. These graphs are shown below in Figure 2.

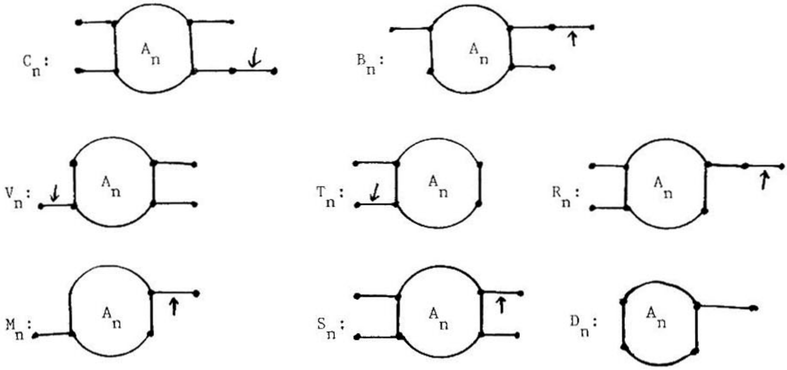

Figure 2

Let us apply the reduction process to L_n (see Figure 1(ii)) in the following manner. Delete edge ty. In the reduced graph delete tu. In the subsequent reduced and incorporated graphs delete xy. In the next reduced graph, delete st. This yields the following lemma.

Lemma 1

$$L_n = w_1 C_{n-2} + w_2 B_{n-2} + 2w_2 R_{n-2} + w_2^2 M_{n-2} + w_2 S_{n-2} \quad (n>1) .$$

By appropriate applications of the reduction process to the graphs in Figure 2, using the indicated edges, we obtain the following lemma.

Lemma 2

For all $n > 0$

(i) $C_n = w_1 S_n + w_2 V_n$

(ii) $B_n = w_1 V_n + w_2 M_n$

(iii) $R_n = w_1 V_n + w_2 T_n$

(iv) $D_n = (w_1^3 + 2w_1 w_2) T_{n-1} + w_1 w_2^2 A_{n-1} + (2w_1^2 w_2 + w_2^2) D_{n-1}$

(v) $M_n = w_1 D_n + w_2 B_{n-1}$

(vi) $S_n = w_1 V_n + (w_1^2 w_2 + w_2^2) S_{n-1} + w_1 w_2^2 V_{n-1}$

(vii) $V_n = w_1 T_n + w_2 C_n$

(viii) $T_n = w_1 D_n + w_1 w_2^2 D_{n-1} + (w_1^2 w_2 + w_2^2) T_{n-1}$.

These lemmas can be used to obtain the following result.

Lemma 3

$$L_n = (w_1^2 + w_2) S_{n-2} + 4w_1 w_2 V_{n-2} + 2w_2^2 M_{n-2} + 2w_2^2 T_{n-2} \quad (n>1).$$

By obtaining the associated relations between the generating functions and by extremely tedious algebraic manipulations, we obtain the following result for the generating function for L_n.

Theorem 4

$$\begin{aligned} L_n = {} & (w_1^4 + 8w_1^2 w_2 + 8w_2^2) L_{n-1} - (3w_1^6 w_2 + 23w_1^4 w_2^2 + 47w_1^2 w_2^3 + 28w_2^4) L_{n-2} \\ & + (2w_1^8 w_2^2 + 23w_1^6 w_2^3 + 84w_1^4 w_2^4 + 116w_1^2 w_2^5 + 56w_2^6) L_{n-3} \\ & - (6w_1^8 w_2^4 + 48w_1^6 w_2^5 + 130w_1^4 w_2^6 + 155w_1^2 w_2^7 + 70w_2^8) L_{n-4} \\ & + (6w_1^8 w_2^6 + 40w_1^6 w_2^7 + 101w_1^4 w_2^8 + 120w_1^2 w_2^9 + 56w_2^{10}) L_{n-5} \\ & - (2w_1^8 w_2^8 + 13w_1^6 w_2^9 + 39w_1^4 w_2^{10} + 53w_1^2 w_2^{11} + 28w_2^{12}) L_{n-6} \\ & + (w_1^6 w_2^{11} + 6w_1^4 w_2^{12} + 12w_1^2 w_2^{13} + 8w_2^{14}) L_{n-7} \\ & - (w_1^2 w_2^{15} + w_2^{16}) L_{n-8} \quad (n>7), \end{aligned}$$

with $L_0 = 4$ (by convention) and the other initial values of L_n as given below in Table 1.

We note that there are many ways of applying the reduction process to L_n and its associated graphs. Perhaps a simpler recurrence could be obtained for L_n by applying the reduction process in a different manner.

The following Table gives the coefficients of $m(L_n)$ for n = 1 up to n = 8. The first coefficient is omitted, since it is always 1.

Table 1

Matching Polynomials of Long Benzene Chains

n	$M(L_n)$									
1	5	4								
2	10	29	24	4						
3	15	81	191	189	63	4				
4	20	158	628	1325	1440	724	128	4		
5	25	260	1460	4810	9470	10895	6875	2085	225	4
6	30	387	2812	12669	36738	68993	82476	60207		
	24846	5013	360	4						
7	35	539	4809	27552	106204	280721	509395			
	625989	505967	255794	74298	10633	539	4			
8	40	716	7576	52734	254328	872132	2148456			
	3798173	4765888	4153792	2427744	900228	193536				
	20560	768	4							

4. *Defect-d Matchings in Long Benzene Chains*

The following result is obtained from Theorem 4, by equating coefficients of w_1^d. (N.B. In the theorem we write N_d as an operator for simplification of the notation).

Theorem 5

L has a defect-d matching if and only if d is even and $0 \leq d \leq 4n$. In this case,

$$\begin{aligned} N_d(L_n) = {} & (N_{d-4} + 8N_{d-2} + 8N_d)\, L_{n-1} \\ & - (3N_{d-6} + 23N_{d-4} + 47N_{d-2} + 28N_d)\, L_{n-2} \\ & + (2N_{d-8} + 23N_{d-6} + 84N_{d-4} + 116N_{d-2} + 56N_d)\, L_{n-3} \\ & - (6N_{d-8} + 48N_{d-6} + 130N_{d-4} + 155N_{d-2} + 70N_d)\, L_{n-4} \\ & + (6N_{d-8} + 40N_{d-6} + 110N_{d-4} + 120N_{d-2} + 56N_d)\, L_{n-5} \\ & - (2N_{d-8} + 13N_{d-6} + 39N_{d-4} + 53N_{d-2} + 28N_d)\, L_{n-6} \\ & + (N_{d-6} + 6N_{d-4} + 12N_{d-2} + 8N_d)\, L_{n-7} \\ & - (N_{d-2} + N_d)\, L_{n-8} \quad (n>7), \end{aligned}$$

with the initial values as obtained from Table 1.

This theorem can be used to obtain recurrences and explicit formulae for the numbers of defect-d matchings in L_n for any specified value of d. The following theorem is inserted for completeness. It can be easily proved.

Theorem 6

$N_0(L_n) = 4$, for all values of $n > 0$.

By putting $d = 2$ in Theorem 5 and using Theorem 6 we obtain the following result about the number of matchings in L_n, consisting of two nodes and $2n - 1$ edges.

Theorem 7

(i) $N_2(L_n) = 8N_2(L_{n-1}) - 28N_2(L_{n-2}) + 56N_2(L_{n-3}) - 70N_2(L_{n-4})$

$$+ 56N_2(L_{n-5}) - 28N_2(L_{n-6}) + 8N_2(L_{n-7}) - N_2(L_{n-8}) \quad (n>7) .$$

with the initial values as obtained from Table 1.

(ii) $N_2L(t) = (5t + 4t^2 - 3t^3)(1 - t)^{-4}$.

Therefore

$$N_2(L_n) = n^3 + 4n^2 .$$

By putting d = 4 in Theorem 5, and using Theorems 6 and 7, we obtain the following implicit recurrence .

$$N_4(L_n) = (8N_2 + 8N_4) L_{n-1} - (47N_2 + 28N_4) L_{n-2} + (116N_2 + 56N_4) L_{n-3}$$

$$- (155N_2 + 70N_4) L_{n-4} + (120N_2 + 56N_4) L_{n-5} - (53N_2 + 28N_4) L_{n-6}$$

$$+ (12N_2 + 8N_4) L_{n-7} - (N_2 + N_4) L_{n-8} + 36 .$$

By finding the implied relation between $N_4L(t)$ and $N_2L(t)$ and then using Theorem 7(ii), an explicit generating function $N_4L(t)$ can be obtained. From this, an explicit recurrence and an explicit formulae for $N_4(L_n)$ can be obtained.

These results can be extended for higher values of d. However the algebraic manipulations involved will become more and more tedious and forbidding.

5. *K-matching in Long Benzene Chains*

The following result is obtained by equating the coefficients of ${w_2}^k$ in Theorem 4.

Theorem 8

L_n has a k-matching if and only if $0 \le k \le 2n$. In this case,

$$\gamma_k(L_n) = (\gamma_k + 8\gamma_{k-1} + 8\gamma_{k-2})\, L_{n-1}$$

$$- (3\gamma_{k-1} + 23\gamma_{k-2} + 47\gamma_{k-3} + 28\gamma_{k-4})\, L_{n-2}$$

$$+ (2\gamma_{k-2} + 23\gamma_{k-3} + 84\gamma_{k-4} + 116\gamma_{k-5} + 56\gamma_{k-6})\, L_{n-3}$$

$$- (6\gamma_{k-4} + 48\gamma_{k-5} + 130\gamma_{k-6} + 155\gamma_{k-7} + 70\gamma_{k-8})\, L_{n-4}$$

$$+ (6\gamma_{k-6} + 40\gamma_{k-7} + 101\gamma_{k-8} + 120\gamma_{k-9} + 56\gamma_{k-10})\, L_{n-5}$$

$$- (2\gamma_{k-8} + 13\gamma_{k-9} + 39\gamma_{k-10} + 53\gamma_{k-11} + 28\gamma_{k-12})\, L_{n-6}$$

$$+ (\gamma_{k-11} + 6\gamma_{k-12} + 12\gamma_{k-13} + 8\gamma_{k-14})\, L_{n-7}$$

$$- (\gamma_{k-15} + \gamma_{k-16})\, L_{n-8} \quad (n>7),$$

with the initial values of γ_n as given in Table 1.

The following corollary is immediate from Theorem 3.

Corollary 3.1.1

$$\gamma_0(L_n) = 1,$$

$$\gamma_1(L_n) = 5n$$

and $$\gamma_2(L_n) = \tfrac{1}{2}(25n^2 - 21n) \quad (n > 1).$$

By putting k = 3 in Theorem 8, and using Corollary 3.1.1, we obtain the following result.

Theorem 9

$$\gamma_3(L_n) = \gamma_3(L_{n-1}) + \tfrac{1}{2}(125n^2 - 335n + 214) \quad (n > 2) .$$

Hence

$$\gamma_3(L_n) = \frac{1}{6}(125n^3 - 315n^2 + 202n) \quad (n > 1) .$$

The calculation of $\gamma_4(L_n)$ is a bit more tedious. Theorems 8 and 9 and also Corollary 3.1. must be used. The analogous result is the following.

Theorem 10

$$\gamma_4(L_n) = \gamma_4(L_{n-1}) + \frac{1}{6}(625n^3 - 3300n^2 + 5669n - 3060) \quad (n > 2) .$$

Hence

$$\gamma_4(L_n) = \frac{1}{24}(625n^4 - 3150n^3 + 5363n^2 - 3102n) \quad (n > 2) .$$

6. *Discussion*

We have given a comprehensive account about the various types of matchings in the long benzene chain L_n. No doubt, our technique can be used to obtain results about matchings in other long chains. However each such chain will involve a great amount of algebraic manipulations. There seems to be no easy way to shift from the results for one kind of chain to the results for another.

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