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MATCHINGS IN HEXAGONAL CACTI

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ABSTRACT. Explicit recurrences are derived for the matching polynomials of the basic types of hexagonal cacti, the linear cactus and the star cactus and also for an associated graph, called the hexagonal crown. Tables of the polynomials are given for each type of graph. Explicit formulae are then obtained for the number of defect-d matchings in the graphs, for various values of d. In particular, formulae are derived for the number of perfect matchings in all three types of graphs. Finally, results are given for the total number of matchings in the graphs.

KEY WORDS AND PHRASES. Cactus, chains, hexagon, linear cactus, star cactus, hexagonal crown, matching, matching polynomials, defect-d matching, perfect matching, generating function, recurrence relation.

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1. INTRODUCTION.

The graphs considered here will be finite and without loops or 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 contains d isolated nodes, then we call it a *defect-d matching* as did Berge ([1] and [2]) and Little [3]. Some general results on defect-d matchings have been given in [1], [2] and [3]. In the case where d=0, i.e. when the matchings has edges only, we call it a *perfect* or *complete matching*.

Let us associate with each node and edge of G the *weights* w_1 and w_2 respectively, and with each matching α in G, the weight

$$W(\alpha) = w_1^{\,r} w_2^{\,s} ,$$

where r and s are the number of nodes and edges respectively in α. Then the *matching polynomial* of a graph G with p nodes is

$$m(G) = \Sigma W(\alpha) = \Sigma a_k w_1^{\,p-2k} w_2^{\,k}, \tag{1.1}$$

where the summation is taken over all the matchings in G, and a_k is the number of matchings with k edges. It is clear that a_k will be the number of defect-(p-2k) matchings in G.

The general matching polynomial was introduced in Farrell [4]. Since then, it has been shown (See Gutman [5]) that several other well known polynomials in Theortical Physics are special matching polynomials. i.e. they can be obtained from m(G) by giving special values to w_1 and w_2. Gutman ([6] and [7]) has also established the matching polynomial as a useful device in Mathematical Chemistry. It should be pointed out however that Gutman's "matching polynomial" (previously called the acyclic polynomial) is a special form of m(G). This was established in Farrell [8].

The *cactus* is a connected graph in which no edge lies in more than one cycle. These graphs were introduced by Uhlenbeck and Ford [9] and Riddell [10], following a paper by Husimi [11]. Hence, they were originally called "Husimi trees". Some of these graphs were enumerated by Harary and Norman [12] and Harary and Uhlenbeck [13]. Some work on the enumeration of triangular cacti (every block is a triangle) can be found in Harary and Palmer ([14], pp. 70-73).

We define a *hexagonal cactus* to be a cactus in which every block is a hexagon. In addition to being interesting mathematical objects, some types of hexagonal cacti represent common chemical structures. Let H be a hexagon. We will call two nodes of H *opposite*, if they are separated by a path of length 3. Therefore H contains three pairs of opposite nodes. The hexagons which constitute a hexagonal cactus will be called *cells* of the cactus.

In this article, we will derive explicit recurrences for the matching polynomials of two types of hexagonal cacti, which represent the fundamental components of many types of hexagonal cacti. We will also derive similar results for an interesting associated graph, which we call a hexagonal crown. We will give tables of polynomials for all three types of graphs considered here. Following this, we will deduce explicit formulae for the number of defect-d matchings in these graphs, for various values of d. In particular, we will give formulae for the number of perfect matchings in the graphs. Finally, we give explicit formulae for the total number of matchings in each type of graph considered.

In the material which follows, we will sometimes write G for m(G), for brevity of notation. Also, we will denote the generating function for m(G) by G(t), where t is the indicator function. Let $a_1, a_2, \ldots, a_k$ be nodes of a graph G. We will denote by $G-\{a_1,a_2,\ldots,a_k\}$ the graph obtained from G by removing nodes $a_1,a_2,\ldots,a_k$. Finally, "cactus" would mean "hexagonal cactus" unless otherwise qualified.

2. THE BASIC THEOREMS.

The first two results given in this section have been proved in the introductory paper [4]. We repeat them here for completeness. The reader can consult [4] for detailed proofs, if necessary.

Let G be a graph and e an edge of G. By partitioning the matchings in G according to whether or not they contain the edge e, we obtain the following result.

THEOREM 1 (*The Fundamental Theorem*). Let G be a graph containing an edge ab. Let G' be the graph obtained from G by deleting ab and G'', the graph obtained from G by removing nodes a and b. Then

$$m(G) = m(G') + w_2 m(G'').$$

Given a graph G, we could apply Theorem 1 recursively to it, until we obtain graphs H_i for which $m(H_i)$ are known. This algorithm is called the *fundamental algorithm for matching polynomials*. We will refer to it simply as the *reduction process*. When applying Theorem 1, we will refer to the graph G' as the *reduced graph* and to the graph G'' as the *incorporated graph*.

The following theorem can be easily proved.

THEOREM 2 (*The Component Theorem*). Let G be a graph consisting of components H_i $(i = 1,2,\ldots,r)$. Then

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

3. SOME ASSOCIATED GENERAL RESULTS.

Let G be a graph with p nodes and q edges. Consider the expression for $m(G)$ given in Equation (1.1). a_0 is the number of matchings with no edges. There is only one such matching, viz. the empty graph with p nodes. Therefore $a_0 = 1$. a_1 is the number of matchings with 1 edge. Therefore $a_1 = q$, the number of edges in G. Consider the spanning subgraphs of G with two edges. These will consist of the matchings with two edges and the spanning subgraphs with a path of length 2 and $p-3$ isolated nodes. Let ε be the number of paths of length 2 in G. Then our discussion leads to following theorem.

THEOREM 3. Let G be a graph with q edges. Then in $m(G)$,

(i) $a_0 = 1$

(ii) $a_1 = q$

and (iii) $a_2 = \binom{q}{2} - \varepsilon$,

where ε is the number of paths of length 2 in G.

We define a *chain* to be a tree with nodes of valency 1 and 2 only. The chain with n nodes will be denoted by P_n. The *length* of P_n is the number of edges in P_n i.e. $n-1$.

COROLLARY 1.1. Let P_n be a chain with n nodes. Then

$$P_n = w_1 P_{n-1} + w_2 P_{n-2} , \quad \text{with} \quad P_0 = 1.$$

PROOF. Apply the reduction process to the graph P_n be deleting a terminal edge. The result then follows from Theorem 1.

□

Many of our results will be given in terms of matching polynomials of chains. We therefore give a table of values of $m(P_n)$, for $n = 1$, up to $n = 8$.

TABLE 1

Matching Polynomials of Chains

n	$m(P_n)$
1	w_1
2	$w_1^2+w_2$
3	$w_1^3+2w_1w_2$
4	$w_1^4+3w_1^2w_2+w_2^2$
5	$w_1^5+4w_1^3w_2+3w_1w_2^2$
6	$w_1^6+5w_1^4w_2+6w_1^2w_2^2+w_2^3$
7	$w_1^7+6w_1^5w_2+10w_1^3w_2^2+4w_1w_2^3$
8	$w_1^8+7w_1^6w_2+15w_1^4w_2^2+10w_1^2w_2^3+w_2^4$

By *attaching* a chain P_n to a graph G (both nonempty) we will mean that an end node of P_n is identified with a node of G, so that P_n becomes a path in the resulting graph.

LEMMA 1. Let G consist of a graph G_1 with the chain P_n attached to node x. Then

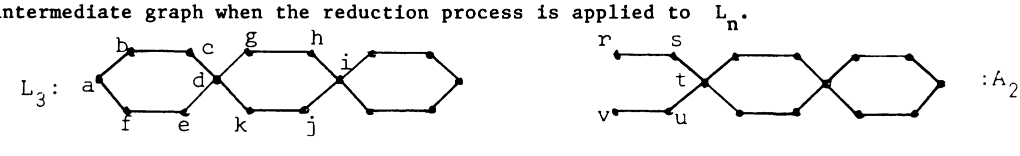
$$m(G) = p_{n-1}m(G_1) + w_2P_{n-2}m(G-\{x\}).$$

PROOF. Apply the reduction process to G by deleting the edge of P_n which is incident to node x. The reduced graph will consist of two components P_{n-1} and G_1. The incorporated grpah will contain two components, P_{n-2} and $G_1-\{x\}$. The result follows from Theorems 1 and 2.

□

4. MATCHING POLYNOMIALS OF LINEAR HEXAGONAL CACTI.

We define the *linear cactus* L_n to be the cactus consisting of n cells linked together in such a way that $n-2$ of them have exactly one pair of opposite nodes of valency 4 and exactly two (*terminal*) cells, each having a node of valency 2 opposite a node of valency 4. These nodes of valency 2 will be called the *terminal nodes* of L_n (see Figure 1 (i)). Clearly L_n contains $5n+1$ nodes and $6n$ edges. The graph obtained from L_n, by attaching two chains of length 2 to one of its terminal nodes, will be denoted by A_n (see Figure 1 (ii)). A_n occurs as an intermediate graph when the reduction process is applied to L_n.



(i) (ii)

Figure 1

LEMMA 2. $A_n = P_2^2L_n + 2w_1w_2P_2A_{n-1}$.

PROOF. Apply the reduction process to the graph A_n by deleting edge st (see Figure 1 (ii)). The reduced graph G' will contain two components P_2 and the graph A_n with P_3 attached to it. The incorporated graph will contain three components, an isolated node, P_2 and A_{n-1}. Therefore

$$A_n = G' + w_1 w_2 P_2 A_{n-1} .$$

Apply the reduction process to G by deleting edge tu. This yields

$$G' = P_2^2 L_n + w_1 w_2 P_2 A_{n-1} .$$

The result follows by substituting for G' in the equation above.

□

Let us apply the reduction process to the graph L_n by deleting edge cd (see Figure 1 (i)). The reduced graph G' will consist of L_{n-1} with P_6 attached to it. The incorporated graph will contain two components, P_4 and A_{n-2}. Therefore

$$L_n = G' + w_2 P_4 A_{n-2}. \tag{4.1}$$

Using Lemma 1, we get

$$G' = P_5 L_{n-1} + w_2 P_4 A_{n-2} .$$

Hence from Equation (4.1),

$$L_n = P_5 L_{n-1} + 2w_2 P_4 A_{n-2} . \tag{4.2}$$

From Lemma 2, we get

$$\Rightarrow \quad A_{n-2} = P_2^2 L_{n-2} + 2w_1 w_2 P_2 A_{n-3} . \tag{4.3}$$

$$\Rightarrow \quad 2w_2 P_4 A_{n-2} = 2w_2 P_4 (P^2 L_{n-2} + 2w_1 w_2 P_2 A_{n-3}) .$$

By substituting the expression for $2w_2 P_4 A_{n-2}$ obtained from Equation (4.2) we obtain the following explicit recurrence for L_n.

$$L_n = (P_5 + 2w_1 w_2 P_2) L_{n-1} + (2w_2 P_2^2 P_4 - 2w_1 w_2 P_2 P_5) L_{n-2}$$

Hence by using the expressions for P_2 and P_5 obtained from Table 1 and then simplifying, we obtain the following theorem.

THEOREM 4. $L_n = (w_1^5 + 6w_1^3 + 5w_1^2 w_2^2) L_{n-1} + (2w_1^4 w_2^3 + 4w_1^2 w_2^4 + 2w_2^5) L_{n-2}$ $(n>1)$, with $L_0 = w_1$ (by convention) and $L_1 = w_1^6 + 6w_1^4 w_2 + 9w_1^2 w_2^2 + 2w_2^3$.

Let us put $\underline{\alpha = w_1^5 + 6w_1^3 w_2 + 5w_1 w_2^2}$ and $\underline{\beta = 2w_1^4 w_2^3 + 4w_1^2 w_2^2 + 2w_2^5}$. Then the recurrence given in Theorem 4 becomes

$$L_n = \alpha\, L_{n-1} + \beta\, L_{n-2}. \tag{4.4}$$

By multiplying both sides of this equation by t^n, and summing from $n = 2$ to ∞, we obtain the following generating function $L(t)$ for $m(L_n)$.

COROLLARY 4.1. $L(t) = \dfrac{L_0 + (L_1 - \alpha L_0)t}{1 - \alpha t - \beta t^2}$, where L_0 and L_1 are as given in Theorem 4.

The following table gives values of $m(L_n)$ for $n = 1$, up to $n = 6$.

TABLE 2

Matching Polynomials of Linear Hexagonal Cacti

n	$m(L_n)$
1	$w_1^6 + 6w_1^4w_2 + 9w_1^2w_2^2 + 2w_2^3$
2	$w_1^{11} + 12w_1^9w_2 + 50w_1^7w_2^2 + 88w_1^5w_2^3 + 61w_1^3w_2^4 + 12w_1w_2^5$
3	$w_1^{16} + 18w_1^{14}w_2 + 127w_1^{12}w_2^2 + 450w_1^{10}w_2^3 + 855w_1^8w_2^4 + 862w_1^6w_2^5 + 429w_1^4w_2^6 + 86w_1^2w_2^7 + 4w_2^8$
4	$w_1^{21} + 24w_1^{19}w_2 + 240w_1^{17}w_2^2 + 1304w_1^{15}w_2^3 + 4218w_1^{13}w_2^4 + 8392w_1^{11}w_2^5 + 10276w_1^9w_2^6 + 7544w_1^7w_2^7 + 3109w_1^5w_2^8 + 624w_1^3w_2^9 + 44w_1w_2^{10}$
5	$w_1^{26} + 30w_1^{24}w_2 + 389w_1^{22}w_2^2 + 2866w_1^{20}w_2^3 + 13282w_1^{18}w_2^4 + 40548w_1^{16}w_2^5 + 83162w_1^{14}w_2^6 + 114924w_1^{12}w_2^7 + 105797w_1^{10}w_2^8 + 63014w_1^8w_2^9 + 22945w_1^6w_2^{10} + 4594w_1^4w_2^{11} + 408w_1^2w_2^{12} + 8w_2^{13}$
6	$w_1^{31} + 36w_1^{29}w_2 + 574w_1^{27}w_2^2 + 5352w_1^{25}w_2^3 + 32475w_1^{23}w_2^4 + 135148w_1^{21}w_2^5 + 396476w_1^{19}w_2^6 + 830768w_1^{17}w_2^7 + 1247415w_1^{15}w_2^8 + 1334972w_1^{13}w_2^9 + 1002990w_1^{11}w_2^{10} + 514280w_1^9w_2^{11} + 171469w_1^7w_2^{12} + 34228w_1^5w_2^{13} + 3512w_1^3w_2^{14} + 128w_1w_2^{15}$

We will obtain some results for the graph A_n. These will be useful in the material which follows.

From Lemma 1, we have

$$P_2^2L_n = A_n - 2w_1w_2P_2A_{n-1}. \tag{4.5}$$

Multiplying Equation (4.2) by P_2^2, yields

$$P_2^2L_n = P_2^2(P_5L_{n-1}+2w_2P_4A_{n-2}).$$

By substituting for $P_2^2L_n$ and $P_2^2L_{n-1}$, using Equation (4.5), we get the following recurrence for A_n.

$$A_n = (2w_1w_2P_2+P_5)A_{n-1} + (2w_2P_2^2P_4-2w_1w_2P_2P_5)A_{n-2}$$

Hence by comparing with Equation (4.4) and Corollary 4.1, we obtain the following lemma.

LEMMA 5.

(i) $A_n = \alpha A_{n-1} + \beta A_{n-2}$ $(n>2)$,

with $A_1 = w_1^{10}+10w_1^8w_2+32w_1^6w_2^2+40w_1^4w_2^3+19w_1^2w_2^4+2w_2^5$.

(ii) $A(t) = \mu(1-\alpha t-\beta t^2)^{-1}$;

where $\mu = \alpha + (A_1-\alpha^2)t$.

(N.B. We take A_0 to be α).

5. MATCHING POLYNOMIALS OF HEXAGONAL STAR CACTI.

We define the *star cactus* S_n to be the cactus consisting of n cells attached to a single node. It is clear that S_n contains 5n+1 nodes and 6n edges. S_4 is shown below in Figure 2.

S_4:

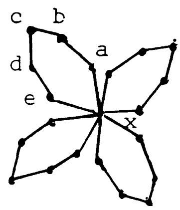


Figure 2

Let us apply the reduction process to S_n by deleting the edge ab (see Figure 2). The reduced graph G' will consist of S_{n-1} with P_5 attached to it. The incorporated graph will contain n components, P_4 and n-1 copies of P_5. Therefore

$$S_n = G' + w_2P_4P_5^{n-1} . \tag{5.1}$$

By applying Lemma 1 to the graph G' , we get

$$G' = P_5S_{n-1} + w_2P_4P_5^{n-1} .$$

Hence by substituting for G' in Equation (5.1), we get the recurrence for $m(S_n)$, given in the following lemma.

LEMMA 6. $S_n = P_5S_{n-1} + 2w_2P_4P_5^{n-1}$ $(n>1)$,

with $S_1 = L_1$.

We can use Lemma 6 in order to obtain an explicit formula for $m(S_n)$. However, we will obtain the result by using a simple combinatorial argument.

THEOREM 5. $S_n = w_1P_5^n + 2nw_2P_4P_5^{n-1}$ $(n>0)$.

PROOF. Partition the matchings in the graph S_n, into two classes (i) those in which node x (see Figure 3) is isolated and (ii) those in which it is not. The matchings in (i) are matchings in the graph $S_n-\{x\}$. Therefore the contribution of these matchings to $m(S_n)$ is $w_1P_5^n$. If node x is not isolated, then it is joined to an edge. There are 2n edges incident to node x. Hence an edge can be chosen in 2n ways. Once an edge is chosen, the 2n edges adjacent to it cannot be used in any matching. Therefore the contribution of the matchings in class (ii) is

$2nP_nP_5^{n-1}$. Hence the result follows. □

The following table gives values of $m(S_n)$ for $n=1$, up to $n=7$.

TABLE 3

Matching Polynomials of Hexagonal Star Cacti

n	$m(S_n)$
1	$w_1^6 + 6w_1^4w_2 + 9w_1^2w_2^2 + 2w_2^3$
2	$w_1^{11} + 12w_1^9w_2 + 50w_1^7w_2^2 + 88w_1^5w_2^3 + 61w_1^3w_2^4 + 12w_1w_2^5$
3	$w_1^{16} + 18w_1^{14}w_2 + 123w_1^{12}w_2^2 + 418w_1^{10}w_2^3 + 759w_1^8w_2^4 + 726w_1^6w_2^5 + 333w_1^4w_2^6 + 54w_1^2w_2^7$
4	$w_1^{21} + 24w_1^{19}w_2 + 228w_1^{17}w_2^2 + 1152w_1^{15}w_2^3 + 3438w_1^{13}w_2^4 + 6288w_1^{11}w_2^5 + 7028w_1^9w_2^6 + 4608w_1^7w_2^7 + 1593w_1^5w_2^8 + 216w_1^3w_2^9$
5	$w_1^{26} + 30w_1^{24}w_2 + 365w_1^{22}w_2^2 + 2450w_1^{20}w_2^3 + 10210w_1^{18}w_2^4 + 27884w_1^{16}w_2^5 + 51010w_1^{14}w_2^6 + 62500w_1^{12}w_2^7 + 50205w_1^{10}w_2^8 + 25110w_1^8w_2^9 + 6993w_1^6w_2^{10} + 810w_1^4w_2^{11}$
6	$w_1^{31} + 36w_1^{29}w_2 + 534w_1^{27}w_2^2 + 4472w_1^{25}w_2^3 + 23955w_1^{23}w_2^4 + 87324w_1^{21}w_2^5 + 223684w_1^{19}w_2^6 + 408336w_1^{17}w_2^7 + 531543w_1^{15}w_2^8 + 487260w_1^{13}w_2^9 + 305478w_1^{11}w_2^{10} + 123768w_1^9w_2^{11} + 28917w_1^7w_2^{12}$
7	$w_1^{36} + 42w_1^{34}w_2 + 735w_1^{32}w_2^2 + 7378w_1^{30}w_2^3 + 48321w_1^{28}w_2^4 + 220626w_1^{26}w_2^5 + 728903w_1^{24}w_2^6 + 1778970w_1^{22}w_2^7 + 3238347w_1^{20}w_2^8 + 4399934w_1^{18}w_2^9 + 4426821w_1^{16}w_2^{10} + 3238326w_1^{14}w_2^{11} + 166035w_1^{12}w_2^{12} + 568134w_1^{10}w_2^{13} + 114453w_1^8w_2^{14} + 10206w_1^6w_2^{15}$

6. MATCHING POLYNOMIALS OF HEXAGONAL CROWNS.

We define the hexagonal crown C_n, to be the graph obtained by identifying the two terminal nodes of L_n. We take C_1 to be the graph shown below in Figure 3 (ii). Clearly C_n contains $5n$ nodes and $6n$ edges. C_5 is shown below in Figure 3(i).

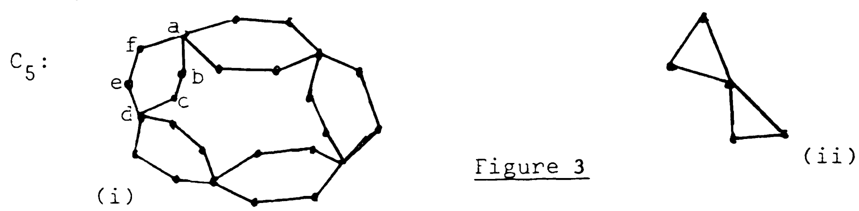


Figure 3

Let us apply the reduction process to C_n by deleting edge ab (see Figure 3). Let the reduced graph be G_1' and the incorporated graph G''. Apply the reduction process to G_1' by deleting edge af.; the reduced graph will be A_{n-1} and the incorporated graph will be G''. Therefore we get

$$C_n = A_{n-1} + 2w_2G'' . \tag{6.1}$$

Let us define the graph B_n to be the graph obtained from L_n by attaching two chains of length 2 to <u>each</u> of its terminal nodes. Then G'' is the graph obtained from B_{n-2} by removing one of its nodes of valency 1. Let x be the associated terminal node. Apply the reduction process to G'' by deleting the edge incident with x and containing a node of valency 1. The reduced graph will consist of a nontrivial component G_2' and an isolated node. The incorporated graph will contain two components, P_2 and B_{n-3}. Therefore we get

$$G'' = w_1G_2' + w_2P_2B_{n-3} . \tag{6.2}$$

Apply the reduction process to G_2' by deleting the edge of the chain attached to node x, which is incident to x. The reduced graph will contain two components, A_{n-2} and P_2. The incorporated graph will contain two components, B_{n-3} and an isolated node. Therefore

$$G_1' = P_2A_{n-2} + w_1w_2B_{n-3} . \tag{6.3}$$

Hence by substituting for G'' in Equation (6.1) using Equations (6.2) and (6.3), we get

$$C_n = A_{n-1} + 2w_1w_2P_2A_{n-2} + 2w_2(w_1^2w_2+w_2P_2)B_{n-3} . \tag{6.4}$$

LEMMA 7. (i) $B_n = P_2^2A_n + 2w_1w_2P_2B_{n-1}$ $(n>1)$

and therefore

$$\text{(ii)}\quad B(t) = P_2^2A(t)\ [1-2w_1w_2P_2t]^{-1},$$

when we take $B_0 = P_2^2\alpha$.

PROOF. Apply the reduction process to B_n by deleting one of the edges of an attached chain, which is incident to a terminal node x of L_n. The reduced graph will contain two components. P_2 and a non-trivial component G'. The incorporated graph will contain three components P_1, P_2 and B_{n-1}. Therefore

$$B_n = P_2G' + w_1w_2P_2B_{n-1} \tag{6.5}$$

By using Equation (6.3) with n replacing n-2, we get

$$G' = P_2A_n + w_1w_2B_{n-1} .$$

Hence (i) follows by substituting for G' in (6.5). (ii) can be established using standard techniques.

□

The following lemma can be obtained by multiplying Equation (6.4) by t^n, summing from $n = 3$ to ∞, then using (ii) of Lemma 7. The generating function $C(t)$ for $m(C_n)$ gives correct coefficients of t^n for $n > 2$.

LEMMA 8.

$$C(t) = \frac{\mu(\gamma\delta+\varepsilon)}{\gamma(1-\alpha t-\beta t^2)} \quad ,$$

where

$$\gamma = 1-2w_1w_2P_2t, \quad \delta = 1+2w_1w_2P_2t^2 \quad \text{and}$$

$$\varepsilon = 2w_2(w_1^2w_2+w_2P_2) \quad .$$

The following theorem is immediate from Lemma 8.

THEOREM 6.

$$C_n = (w_1^5+8w_1^3w_2+7w_1w_2^2)C_{n-1} - (2w_1^8w_2+14w_1^6w_2^2+20w_1^4w_2^3+6w_1^2w^4-2w_2^5)C_{n-2}$$
$$- 4w_1w_2^4(w_1^6+3w_1^4w_2+3w_1^2w_2^2+w_2^3)C_{n-3} \quad (n>3),$$

with C_1, C_2 and C_3 as given below in Table 4.

The following table gives values of $m(C_n)$ for $n = 1$, up to $n = 6$.

TABLE 4

Matching Polynomials of Hexagonal Crowns

n	$m(C_n)$
1	$w_1^5+6w_1^3w_2+5w_1w_2^2$
2	$w_1^{10}+12w_1^8w_2+46w_1^6w_2^2+64w_1^4w_2^3+33w_1^2w_2^4+4w_2^5$
3	$w_1^{15}+18w_1^{13}w_2+123w_1^{11}w_2^2+402w_1^9w_2^3+663w_1^7w_2^4+558w_1^5w_2^5$ $+221w_1^3w_2^6+30w_1w_2^7$
4	$w_1^{20}+24w_1^{18}w_2+236w_1^{16}w_2^2+1232w_1^{14}w_2^3+3718w_1^{12}w_2^4+6688w_1^{10}w_2^5$ $+7220w_1^8w_2^6+4560w_1^6w_2^7+1553w_1^4w_2^8+232w_1^2w_2^9+8w_2^{10}$
5	$w_1^{25}+30w_1^{23}w_2+385w_1^{21}w_2^2+2770w_1^{19}w_2^3+12330w_1^{17}w_2^4+35476w_1^{15}w_2^5$ $+67270w_1^{13}w_2^6+84500w_1^{11}w_2^7+69585w_1^9w_2^8+36350w_1^7w_2^9+11225w_1^5w_2^{10}$ $+1770w_1^3w_2^{11}+100w_1w_2^{12}$
6	$w_1^{30}+36w_1^{28}w_2+570w_1^{26}w_2^2+5232w_1^{24}w_2^3+30927w_1^{22}w_2^4+123876w_1^{20}w_2^5$ $345232w_1^{18}w_2^6+678336w_1^{16}w_2^7+943647w_1^{14}w_2^8+924988w_1^{12}w_2^9$ $+628626w_1^{10}w_2^{10}+286656w_1^8w_2^{11}+82641w_1^6w_2^{12}+13500w_1^4w_2^{13}$ $+996w_1^2w_2^{14}+16w_2^{15}$

7. DEFECT-d MATCHINGS IN LINEAR HEXAGONAL CACTI.

We will denote the number of defect-d matchings in a graph G by $N_d(G)$. Therefore the number of perfect matchings will be $N_0(G)$. The total number of matchings in G will be denoted by $N_T(G)$. It is clear that $N_d(G)$ is the coefficient of the term in w_1^d in $m(G)$, and that $N_0(G)$ is the coefficient of the term in w_1^0. Also $N_T(G)$ is obtained from $m(G)$ by putting $w_1 = w_2 = 1$.

The following theorem is immediate from Theorem 4, by equating coefficients of the terms in $w_1 d$. Notice that $m(G)$ contains a term in w_1^d if and only if d and p (the number of nodes in G) have the same parity, since the edges in a matching are incident to an even number of nodes.

THEOREM 7. $L_n (n>1)$ has a defect-d matching if and only if d and n have opposite parities and $0 \leqq d \leqq 5n+1$, if n is odd, or $1 \leqq d \leqq 5n+1$, if n is even. In this case,

$$N_d(L_n) = N_{d-5}(L_{n-1})+6N_{d-3}(L_{n-1})+5N_{d-1}(L_{n-1})+2N_{d-4}(L_{n-2})+4N_{d-2}(L_{n-2})+2N_d(L_{n-2}) ,$$

with the initial values of $N_d(L_n)$ as given above in Table 2.

The following corollary of Theorem 3 gives explicit formulae for the first three coefficients of $m(L_n)$.

COROLLARY 3.1. In $m(L_n)$,

$$\text{(i)} \quad N_{5n+1}(L_n) = 1$$

$$\text{(ii)} \quad N_{5n-1}(L_n) = 6n$$

$$\text{and (iii)} \quad N_{5n-3}(L_n) = 18n^2-13n+4 .$$

PROOF. Since L_n has $5n+1$ nodes and $6n$ edges, (i) and (ii) follow immediately from Theorem 3. L_n has $n-1$ nodes of valency 4 and the remaining $4n+2$ have valency 2. Therefore

$$\varepsilon = (n-1) \binom{4}{2} + 4n+2 = 10n-4 .$$

$$\Rightarrow N_{5n-3}(L_n) = \binom{6n}{2} - (10n-4) .$$

The result follows after simplifications.

□

Theorem 7 is a useful result, because it can be used to obtain explicit formulae for all the coefficients of $m(L_n)$. We will illustrate this by finding formulae for the fourth and fifth coefficients of $m(L_n)$.

Put $d = 5n-5$ in Theorem 7. This yields

$$\begin{aligned} N_{5n-5}(L_n) = {} & N_{5n-10}(L_{n-1})-6N_{5n-8}(L_{n-1})+5N_{5n-6}(L_{n-1}) \\ & + 2N_{5n-9}(L_{n-2})+4N_{5n-7}(L_{n-2})+2N_{5n-5}(L_{n-2}) \end{aligned} \tag{7.1}$$

Notice that $N_{5n-10}(L_{n-1})$, $N_{5n-8}(L_{n-1})$ and $N_{5n-6}(L_{n-1})$ are the fourth, third and second coefficients of $m(L_{n-2})$ and that

$$N_{5n-7}(L_{n-2}) = N_{5n-5}(L_{n-2}) = 0 .$$

Therefore by using Corollary 3.1, we get

$$N_{5n-8}(L_{n-1}) = 18(n-1)^2-13(n-1)+4, \quad N_{5n-6}(L_{n-1}) = 6(n-1)$$

and $\quad N_{5n-9}(l_{n-2}) = 1$.

By substituting these values in Equation (7.1), we obtain the following lemma which give a recurrence for the fourth coefficient of $m(L_n)$.

LEMMA.

$$N_{5n-5}(L_n) = N_{5n-10}(L_{n-1})+108n^2-264n+182 \quad (n>2),$$

with $N_0(L_1) = 2$.

By using standard techniques we establish the following theorem.

THEOREM 8.

$$N_{5n-5}(L_n) = 2(18n^3-39n^2+34n-12) \quad (n>0)$$

Put $d = 5n-7$ in Theorem 7. This yields

$$N_{5n-7}(L_n) = N_{5n-12}(L_{n-1})+6N_{5n-10}(L_{n-1})+5N_{5n-8}(L_{n-1})$$

$$+ 2N_{5n-11}(L_{n-2})+4N_{5n-9}(L_{n-2})+2N_{5n-7}(L_{n-2}) \tag{7.2}$$

Using Theorem 8, we get

$$N_{5n-10}(L_{n-1}) = 2\ [18(n-1)^3-39(n-1)^2+34(n-1)+12] .$$

using Corollary 3.1, we get

$$N_{5n-8}(L_{n-1}) = 18(n-1)^2-13(n-1)+4, \quad N_{5n-11}(L_{n-2}) = 6(n-2)$$

and $\quad N_{5n-9}(L_{n-2}) = 1$.

It is clear that $N_{5n-7}(L_{n-2}) = 0$. By substituting these values in Equation (7.2) and then simplifying, we obtain the following lemma.

LEMMA 10.

$$N_{5n-7}(L_n) = N_{5n-12}(L_{n-1}) + (261n^3-1026n^2+1759n-1081) \quad (n>2),$$

with $N_3(L_2) = 61$.

By solving the above recurrence, we obtain the following theorem which gives an explicit formula for the fifth coefficient of $m(L_n)$.

THEOREM 9.

$$N_{5n-7}(L_n) = \frac{1}{2}\ (108n^4-468n^3+841n^2-745n+264) \quad (n>1) .$$

The following theorem gives an explicit formula for the number of perfect matchings in L_n.

THEOREM 10. L_n has a perfect matching if and only if n is odd, and in this case,

$$N_0(L_n) = 2^{(n+1)/2} .$$

PROOF. Suppose that n is odd. Then from Theorem 7, $d = 0$. Put $d = 0$ in Theorem 7. This yields

$$N_0(L_n) = 2\,N_0(L_{n-2})\ , \quad \text{with} \quad N_0(L_1) = 2.$$

$$= 2^2 N_0(L_{n-4})$$

$$\vdots$$

$$= 2^{(n-1)/2} N_0(L_1) = 2^{(n+1)/2}\ .$$

Conversely, suppose that L_n has a perfect matching. Then it must have an even number of nodes. $\Rightarrow$ $5n+1$ is even. $\Rightarrow$ n is odd.

□

We will use Theorem 7 in order to derive explicit expressions for the number of defect-d matchings in L_n, for $d = 1$ and $d = 2$.

LEMMA 11.

$$N_1(L_n) = 2N_1(L_{n-2}) + 5(2^{n/2}) \quad (\text{n-even})$$

with $N_1(L_0) = 1$

PROOF. Put $d = 1$ in Theorem 7. This yields

$$N_1(L_n) = 5N_0(L_{n-1}) + 2N_1(L_{n-1})\ .$$

The result then follows from Theorem 10.

□

The following theorem gives an explicit formula for the number of defect-1 matchings in L_n (n-even).

THEOREM 11.

$$N_1(L_n) = (5n+2)2^{(n-2)/2} \quad (\text{n-even})\ .$$

PROOF. From Lemma 11,

$$N_1(L_n) = 2N_1(L_{n-2}) + \delta_n\ , \text{ where } \delta_n = 5(2^{n/2}).$$

$$\Rightarrow N_1(L_n) = \delta_n + 2\delta_{n-2} + 2^2 N_1(L_{n-4})\ .$$

$$\vdots$$

$$= \sum_{k=0}^{n-4} 2^{k/2}\delta_{n-k} + 2^{(n-2)/2} N_1(L_2) \quad (\text{k-even})$$

$$= 5.2^{n/2}\left(\frac{n-2}{2}\right) + 6.2^{n/2}\ .$$

The result follows after simplifications.

□

LEMMA 12. $N_2(L_n) = 2N_2(L_{n-2}) + (25n-7)2^{(n-3)/2}$ (n-odd),

with $N_2(L_1) = 9$.

PROOF. Put $d = 2$ in Theorem 7. This yields

$$N_2(L_n) = 5N_1(L_n) + N_0(L_{n-2}) + 2N_2(L_{n-2}) \quad (\text{n-odd})$$

$$= 5[5(n-1)+2]2^{(n-3)/2} + 4(2^{(n-1)/2}) + 2N_2(L_{n-2})\ ,$$

using Theorems 10 and 11. The result follows after simplifications.

□

By solving the recurrence given in Lemma 12, using standard techniques (e.g. see Proof of Theorem 11), we obtain the following theorem, which gives an explicit formula for the number of defect-2 matchings in L_n(n-odd).

THEOREM 12.

$$N_2(L_n) = (25n^2+36n+11)2^{(n-7)/2} \quad \text{(n-odd)} .$$

By putting $w_1 = w_2 = 1$ in Corollary 4.1, we obtain the following generating function $N_T L(t)$ for $N_T(L_n)$.

$$N_T L(t) = \frac{1+6t}{1-12t-8t^2} .$$

Now $\dfrac{1+6t}{1-12t-8t^2} = \dfrac{A}{t-a} + \dfrac{B}{t-b}$, where a and b are the roots of the equation $t^2 + \frac{3t}{2} - \frac{1}{8} = 0$.

$$\therefore \quad N_T L(t) = \frac{A/a}{1-t/_a} + \frac{-B/b}{1-t/_b} .$$

By equating coefficients of t^n, we get

$$N_T(L_n) = -A(1/a)^{n+1} - B(1/b)^{n+1} .$$

By finding A, B, a and b from the relation above, we obtain the following theorem which gives an explicit formula for the total number of matchings in L_n.

THEOREM 13.

$$N_T(L_n) = c(6-2\sqrt{11})^{n+1} + \bar{c}(6+2\sqrt{11})^{n+1} \quad (n>0) ,$$

where $c = \dfrac{7+3\sqrt{11}}{8\sqrt{11}}$ and $\bar{c}$ is the surd conjugate of c.

8. DEFECT-d MATCHINGS IN STAR CACTI.

The following corollary of Theorem 3 gives simplified formulae for the first three coefficients of $m(S_n)$.

COROLLARY 3.2. In $m(S_n)$,

(i) $N_{5n+1}(S_n) = 1$

(ii) $N_{5n-1}(S_n) = 6n$

and (iii) $N_{5n-3}(S_n) = n(16n-7)$.

PROOF. (i) and (ii) are immediate from the theorem. S_n has one node of valency $2n$ and $5n$ nodes of valency 2. It follows that

$$\varepsilon = \binom{2n}{2} + 5n = 2n^2+4n .$$

$$\Rightarrow N_{5n-3}(S_n) = \binom{6n}{2} - (2n^2+4n) .$$

The desired result is obtained after simplifications.

□

The following result is added for completeness. It can be easily established.

LEMMA 13. $N_0(S_n) = 0 , \ \forall\, n > 0.$

The following theorem gives an explicit formula for the total number of matchings in S_n.

THEOREM 14. $N_T(S_n) = 2(4+5n)8^{n-1}$.

PROOF. Put $w_1 = w_2 = 1$ in Theorem 5. This yields

$$N_T(S_n) = 8^n + 2n.5(8^{n-1}) .$$

This reduces to the desired result.

□

9. DEFECT-d MATCHINGS IN HEXAGONAL CROWNS.

The following theorem can be obtained from Theorem 6 by equating coefficients of the terms in w_1^d.

THEOREM 15. $C_n(n>4)$ has a defect-d matching if and only if n and d have the same parity and $0 \leqq d \leqq 5n$ if n is even or $1 \leqq d \leqq 5n$ if n is odd. In this case,

$$\begin{aligned} N_d(C_n) &= N_{d-5}(C_{n-1}) + 8N_{d-3}(C_{n-1}) + 7N_{d-1}(C_{n-1}) \\ &\quad - 2N_{d-8}(C_{n-2}) - 14N_{d-6}(C_{n-2}) - 20N_{d-4}(C_{n-2}) \\ &\quad - 6N_{d-2}(C_{n-2}) + 2N_d(C_{n-2}) - 4N_{d-7}(C_{n-3}) \\ &\quad - 12N_{d-5}(C_{n-3}) - 12N_{d-3}(C_{n-3}) - 4N_{d-1}(C_{n-3}) \quad (n>4), \end{aligned}$$

with the initial values of $N_d(C_n)$ as given in Table 4.

COROLLARY 3.3. In $m\ (C_n)$,

$$\text{(i)}\quad N_{5n}(C_n) = 1$$

$$\text{(ii)}\quad N_{5n-2}(C_n) = 6n$$

$$\text{and}\quad \text{(iii)}\quad N_{5n-4}(C_n) = n(18n-13) \quad (n>1).$$

PROOF. (i) and (ii) follow immediately from the theorem. C_n has n nodes of valency 4 and $4n$ nodes of valency 2. Therefore

$$\varepsilon = n\binom{4}{2} + 4n = 10n .$$

$$\Rightarrow N_{5n-4}(C_n) = \binom{6n}{2} - 10n .$$

The result therefore follows.

□

We will use Theorem 15 and Corollary 3.3 in order to obtain explicit formulae for the fourth and fifth coefficients of $m(C_n)$.

Let us put $d = 5n - 6$ in Theorem 15. This yields

$$\begin{aligned} N_{5n-6}(C_n) &= N_{5n-11}(C_{n-1}) + 8N_{5n-9}(C_{n-1}) + 7N_{5n-7}(C_{n-1}) \\ &\quad - 2N_{5n-14}(C_{n-2}) - 14N_{5n-12}(C_{n-2}) - 20N_{5n-10}(C_{n-2}) \\ &\quad - 6N_{5n-8}(C_{n-2}) + 2N_{5n-6}(C_{n-2}) - 4N_{5n-13}(C_{n-3}) \\ &\quad - 12N_{5n-11}(C_{n-3}) - 12N_{5n-9}(C_{n-3}) - 4N_{5n-7}(C_{n-3}) \end{aligned} \tag{9.1}$$

It is clear that $N_{5n-7}(C_{n-1})$ and $N_{5n-9}(C_{n-1})$ are the second and third coefficients respectively of $m(C_{n-1})$. $N_{5n-10}(C_{n-2})$, $N_{5n-12}(C_{n-2})$ and $N_{5n-14}(C_{n-2})$ are the first, second and third coefficients respectively of $m(C_{n-2})$. Also $N_{5n-8}(C_{n-2}) = N_{5n-6}(C_{n-2}) = 0$. It can be easily seen that

$$N_{5n-13}(C_{n-3}) = N_{5n-11}(C_{n-3}) = N_{5n-9}(C_{n-3}) = N_{5n-7}(C_{n-3}) = 0 \ .$$

From Corollary 3.3, we have

$$N_{5n-7}(C_{n-1}) = 6(n-1)$$

$$N_{5n-9}(C_{n-1}) = 18(n-1)^2-13(n-1)$$

$$N_{5n-10}(C_{n-2}) = 1$$

$$N_{5n-12}(C_{n-2}) = 6(n-2)$$

$$\text{and} \quad N_{5n-14}(C_{n-2}) = 18(n-2)^2-13(n-2) \ .$$

By substituting these values into Equation (9.1), and then simplifying, we obtain the following lemma.

LEMMA 13. $N_{5n-6}(C_n) = N_{5n-11}(C_{n-1}) + 2(54n^2-132n+79) \quad (n>2)$

with $N_4(C_2) = 64$.

The recurrence given in the above lemma can be solved by standard techniques. The solution is given in the following theorem.

THEOREM 16. $N_{5n-6}(C_n) = 2n(18n^2-39n+22) \quad (n>0)$.

A similar analysis can be done by putting $d = 5n-8$ in Theorem 15. This would yield an explicit formula and a recurrence for the fifth coefficient of $m(C_n)$. We will omit the proofs, since they would be quite similar to those of Lemma 13 and Theorem 16.

LEMMA 14. $N_{5n-8}(C_n) = N_{5n-13}(C_{n-1}) + (216n^3-1026n^2+1615n-809) \quad (n>3)$,

with $N_7(C_3) = 663$.

The solution of the recurrence given in the above lemma, is given in the following theorem.

THEOREM 17. $N_{5n-8}(C_n) = \frac{n}{2}(108n^3-468n^2+697n-353) \quad (n>1)$.

The following theorem gives an explicit formula for the number of perfect matchings in C_n.

THEOREM 18. $N_0(C_n) = 2^{(n+2)/2} \quad (n\text{-even})$.

PROOF. Put $d = 0$ in Theorem 15. This yields

$$\begin{aligned} N_0(C_n) &= 2N_0(C_{n-2}) \quad (n\text{-even}) \\ &= 2^2 N_0(C_{n-4}) \\ &\vdots \\ &= 2^{n-2} N_0(C_2). \end{aligned}$$

Hence the result follows. $\square$

The following lemma is analogous to Lemma 11. It can be established by putting $d = 1$ in Theorem 15 and then substituting for $N_0(C_{n-1})$ and $N_0(C_{n-3})$ using Theorem 18.

LEMMA 15. $N_1(C_n) = 2N_1(C_{n-2}) + 5.2^{(n+1)/2}$ (n-odd and n>1), with $N_1(C_1) = 5$.

An explicit formula for the number of defect-1 matchings in C_n can now be obtained by solving the above recurrence for $N_1(C_n)$. A solution constructed along the lines of the proof of Theorem 11, yields the following result.

THEOREM 19. $N_1(C_n) = (5n)2^{(n-1)/2}$ (n-odd) .

Put $d = 2$ in Theorem 15. This yields

$$\begin{aligned} N_2(C_n) &= 7N_1(C_{n-1}) - 6N_0(C_{n-2}) + 2N_2(C_{n-2}) - 4N_1(C_{n-3}) \\ &= 7.5(n-1)2^{(n-2)/2} - 6.2^{n/2} + 2N_2(C_{n-2}) - 4.5(n-3)2^{(n-4)/2} . \end{aligned}$$

On simplification, we obtain the following lemma.

LEMMA 16. $N_2(C_n) = 2N_2(C_{n-2}) + (25n-17)2^{(n-2)/2}$ (n-even), with $N_2(C_0) = 0$.

By solving the above recurrence using standard techniques, we obtain the following theorem which gives an explicit formula for the number of defect-2 matchings in C_n(n-even).

THEOREM 20. $N_2(C_n) = n(25n+16)2^{(n-6)/2}$(n-even).

The following lemma gives a recurrence for the total number of matchings in C_n. It can be obtained from Theorem 6 by putting $w_1 = w_2 = 1$.

LEMMA 17. $N_T(C_n) = 16N_T(C_{n-1}) - 40N_T(C_{n-2}) - 32N_T(C_{n-3})$ (n>4), with $N_T(C_1) = 18$, $N_T(C_2) = 160$, $N_T(C_3) = 2016$ and $N_T(C_4) = 25472$.

By multiplying the above recurrence by t^n, summing from $n = 0$ to ∞, and then simplifying, using the boundary conditions, we obtain (with $N_T(C_0)=0$),

$$\begin{aligned} N_TC(t) &= \frac{18t-128t^2+176t^3+192t^4}{1-16t+40t^2+32t^3} . \\ &= 6t-2 + \frac{2(1-6t)}{1-12t-8t^2} \end{aligned}$$

Hence we obtain the following lemma, which gives a generating function $N_TC(t)$ for $m(C_n)$. (It gives correct coefficients of t^n, for n>1).

LEMMA 18.

$$N_TC(t) = \frac{2(1-6t)}{1-12t-8t^2} .$$

Hence by using the standard technique illustrated above in establishing Theorem 13, we obtain the following theorem which gives an explicit formula for the total number of matchings in a hexagonal crown.

THEOREM 21. $N_T(C_n) = c(6+2\sqrt{11})^{n+1} + \bar{c}(6-2\sqrt{11})^{n+1}$ (n>1), where $c = \frac{\sqrt{11}-3}{4}$.

10. DISCUSSION.

Our article gives a comprehensive account about matchings in the linear and star cacti, and in the hexagonal crown. As far as other hexagonal cacti are concerned, we have given results which, together with the theorems given in Sections 2 and 3, can be used to obtain their matching polynomials. It would be virtually impossible to give results from which the matching polynomial any arbitrary hexagonal cactus could be obtained by mere substitution.

Most of our results on defect-d matchings (d>0) can be extended. We have indeed extended some of these results, but have not given them here, since no new techniques are involved. Also, they would have made the article unacceptably long.

REFERENCES

1. BERGE, C. Sur le Couplage Maximum d'un Graphe, C.R. Acad. Sci., Paris, 247(1958), 258-259.
2. BERGE, C. "Graphs and Hypergraphs", North-Holland, Amsterdam, 1973.
3. LITTLE, C.H.C., GRANT, D.D. and HOLTON, D.A. On Defect-d Matchings in Graphs, Discrete Math. 13(1975), 41-54.
4. FARRELL, E.J. Introduction to Matching Polynomials, J. Comb. Theory B 27(1979), 75-86.
5. GUTMAN, I. The Matching Polynomial, Match. No. 6(1979), 75-91.
6. GUTMAN, I. The Energy of a Graph, Bericht. Nr. 103, Mathematisch-Statistiche Sektion in Forschungszentrum Graz (1978).
7. GUTMAN, I. On the Topological Resonance Energy of Heteroconjugated Molecules, Croatica Chemica Acta 54(1953), 134-141.
8. FARRELL, E.J. The Matching Polynomial and its Relation to the Acyclic Polynomial of a Graph, ARS Combinatoria 9(1980), 221-228.
9. UHLENBECK, G.E. and FORD, G.W. "Lectures in Statistical Mechanics", Amer. Math. Soc., Providence, Rhode Island, 1963.
10. RIDDELL, R.J. Contributions to the Theory of Condensation, Dissertation, Univ. of Michigan, Ann Arbor, 1951.
11. HUSIMI, K. Note on Mayer's Theory of Cluster Integrals, J. Chem. Phys. 18(1975), 682-684.
12. HARARY, F. and NORMAN, R.Z. The Dissimilarity Characteristic of Husimi Trees, Ann. of Math. 58(1953), 134-141.
13. HARARY, F. and UHLENBECK, G.E. On the Number of Husimi Trees, Proc. Nat. Acad. Sci. 39(1953), 315-322.
14. HARARY, F. and PALMER, E.M. "Graphical Enumeration", Academic Press, New York, and London, 1973.