

CIRCUIT POLYNOMIALS, CHARACTERISTIC POLYNOMIALS AND μ -POLYNOMIALS
OF SOME
POLYGONAL CHAINS

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Abstract

Recurrences are obtained for the circuit polynomials of linear polygonal chains, when the polygon is a triangle, a rectangle and pentagon. In the cases of the triangle and the rectangle, explicit recurrences are given. Parallel results are then deduced for the characteristic polynomials of these graphs. The μ -polynomials of these graphs are discussed and some partial results given.

Keywords and Phrases

circuit polynomial	recurrence relation
characteristic polynomial	polygonal chain
μ -polynomial	matching polynomial

1. INTRODUCTION

The graphs considered here will be finite and will contain no loops nor multiple edges. Let G be such a graph. A *cycle* or *circuit cover* of G is a spanning subgraph of G whose components are all cycles, edges or isolated nodes. We will consider a node and an edge to be a cycle with one and two nodes respectively. A cycle with more than two nodes will be called a *proper cycle*. If the cycle cover has no proper cycles, then it is a *matching*.

Let us associate with every cycle α in G , an indeterminate or weight w_α , and with each cycle cover C , the weight

$$w(C) = \prod_{\alpha} w_{\alpha},$$

where the product is taken over all the components in C . Then the *circuit polynomial* of G is

$$C(G; \underline{w}) = \sum w(C),$$

where the summation is taken over all the cycle covers of G and \underline{w} is a vector of indeterminates. In this paper, we will assign to each cycle α with n nodes, the weight w_n . Therefore we will have $\underline{w} = (w_1, w_2, w_3, \dots, w_p)$, where p is the number of nodes in G .

The polynomial $C(G; \underline{w})$ was introduced in the paper [1] Its basic properties and its connection with the characteristic polynomial of graph have been given in Farrell [2]. Its connection with the μ -polynomial is given in Farrell and Gutman [5].

We define a linear *polygonal chain* G_n to be the graph obtained by the edge concatenation of n (a finite number) congruent k -gons (*cells*). We take G_0 to be an edge. These graphs belong to a family of graphs called *animals*. There are many interesting problems associated with animals, the most famous of these being cell-growth problems. An account of these problems can be found in Harary ([10], pp. 33-38) and also in Harary and Palmer ([11], pp. 234-237).

It is clear that the coefficient of the monomial $w_1^{r_1} w_2^{r_2} \dots w_n^{r_n}$ in $C(G; \underline{w})$ will be the number of ways of decomposing G into r_1 nodes, r_2 edges, r_3 triangles etc. Thus $C(G; \underline{w})$ will contain a wealth of information, not only about the kinds of cycle decompositions that G has, but also on their numbers. Since the characteristic polynomial of a graph is a specially weighted circuit polynomial, it follows that the characteristic polynomials of the polygonal chains can be deduced from $C(G; \underline{w})$. Some of these chains represent chemical structures and the characteristic polynomial has been used (see Gutman [5]) to investigate properties of chemical structures. The μ -polynomial has been used in investigations of topological properties of conjugated molecules [7-9, 12-15]. Thus our results might be useful to researchers in Physical Chemistry.

We will derive explicit recurrences for the circuit polynomials of the triangular and rectangular chains. We will also derive two recurrences which can be used to obtain explicit formulae for pentagonal chains. Parallel results will be deduced for characteristic polynomials of triangular, rectangular and pentagonal chains. Finally, some results on the μ -polynomials of these graphs will then be given.

Let G be a graph and x a node in G . We will denote by $G-x$, the graph obtained from G , by removing node x . In general, if it is a subgraph of G , $G-H$ will be the graph obtained from G by removing the nodes of H . If xy is an edge in G , then $G-xy$ will be the graph obtained from G by deleting the edge xy . Let

B be a non-empty graph. We *attach* B to G by identifying a node of B with a node of G, so as to form a new graph in which B and G are subgraphs with one node in common.

In the material which follows, we will often write $C(G)$ for $C(G; \underline{w})$. Also, in recurrences, we will write G for $C(G; \underline{W})$, when it would lead to no confusion. This will greatly simplify the presentation of the formulae given.

2. PRELIMINARY RESULTS

The following lemma is taken from [2]. It is called the fundamental theorem for circuit polynomials. Its proof is quite straightforward.

Lemma 1

Let G be a graph containing an edge xy . Let G' be the graph $G - xy$, G'' the graph $G - x - y$ and G^* , the graph obtained from G by requiring xy to be part of a proper cycle in every cycle cover of G . Then

$$C(G; \underline{w}) = C(G'; \underline{w}) + w_{xy} C(G''; \underline{w}) + C(G^*; \underline{w}).$$

The graph G^* will be called a *restricted graph*. Notice that if xy cannot be part of a proper cycle, then $C(G^*; \underline{w}) = 0$. The algorithm implied by this lemma will be called the *reduction process*. The following lemma will be useful in applications of the reduction process. It is also given in [2].

Lemma 2

Let G be a graph consisting of components G_1, G_2, \dots, G_k . Then

$$C(G; \underline{w}) = \prod_{i=1}^k C(G_i; \underline{w}).$$

By a *cadena*, we will mean a tree with nodes of valencies 1 and 2 only. The chain with n nodes will be denoted by P_n .

Since P_n has no proper cycles, every cycle cover will be a matching. It follows that the circuit polynomial of P_n coincides with its matching polynomial (see Farrell [3]) $m(P_n; \underline{w})$. In [3] an explicit formula is given for $m(P_n; \underline{w})$. A table of values of the polynomials $m(P_n; \underline{w})$ is also given. We will use this table whenever specific values of $C(P_n; \underline{w})$ ($= m(P_n; \underline{w})$) are required.

The following theorem is crucial to our main results.

Theorem 1

Let G be a graph and xy an edge in G . Let P_k be a chain with $k (>3)$ nodes. Let H be the graph obtained from G by identifying the endnodes of P_k with nodes x and y of G . Then, if P_j is a path with j nodes in G and with endnodes x and y , the circuit polynomial of H is given by

$$C(H; \underline{w}) = C(G; \underline{w}) C(P_{k-2}; \underline{w}) + w_2 C(P_{k-3}; \underline{w}) [C(G-x; \underline{w}) + C(G-y; \underline{w})] + w_2^2 C(P_{k-4}; \underline{w}) C(G-x-y; \underline{w}) + \sum_{P_j} w_{k+j-2} C(G-P_j; \underline{w}),$$

where the summation is taken over all paths P_j in G , with x and y as endnodes.

Proof

Let us apply the reduction process to H using the edge zx of P_k which is incident to node x . Then G' will be the graph G with P_{k-1} attached to it (at node y). G'' will be the graph $G-x$ with P_{k-2} attached to it (at node y). G^* will be the graph in which every cover contains zx as part of a proper cycle. Now the only proper cycles that contain zx will be those comprising of the path P_k together with a path P_j in G with x and y as endnodes. Such a cycle has $k+j-2$ nodes, and therefore will be assigned the weight w_{k+j-2} . The rest of the cover if it will be a cover of the graph $G-P_j$. In fact every cover of $G-P_j$ can be combined with the cycle with $k+j-2$ nodes, to form a cover of H . Therefore the

contribution to $C(H; \underline{w})$ of all these covers is

$$C(G^*; \underline{w}) = \sum_{P_j} w_{k+j-2} C(G-P_j; \underline{w}) . \quad (1)$$

Let us apply the reduction process to G' by deleting the edge vy of P_n incident to node y . Then the edge-deleted graph will consist of the components P_{k-2} and G . The graph $G'-v-y$ will consist of two components P_{k-3} and $G-y$. The restricted graph will not contribute since vy cannot be part of a proper cycle. We therefore have

$$C(G'; \underline{w}) = C(P_{k-2}; \underline{w})C(G; \underline{w}) + w_2 C(P_{k-3}; \underline{w})C(G-y; \underline{w}) .$$

Apply the reduction process to G'' by deleting the edge vy . $G''-vy$ will consist of the components $G-x$ and P_{k-3} . $G''-v-y$ will consist of the components P_{k-4} and $G-x-y$. Therefore we have

$$C(G''; \underline{w}) = C(P_{k-3}; \underline{w})C(G-x; \underline{w}) + w_2 C(P_{k-4}; \underline{w})C(G-x-y; \underline{w}) .$$

The result follows by adding the contributions in accordance with Lemma 1. □

The following relation between $C(G; \underline{w})$ and the characteristic polynomial of G , denoted by $\phi(G; x)$ is taken from [2].

Lemma 2

$$\phi(G; x) = C(G; (x, -1, -2, -2, \dots, -2)) ,$$

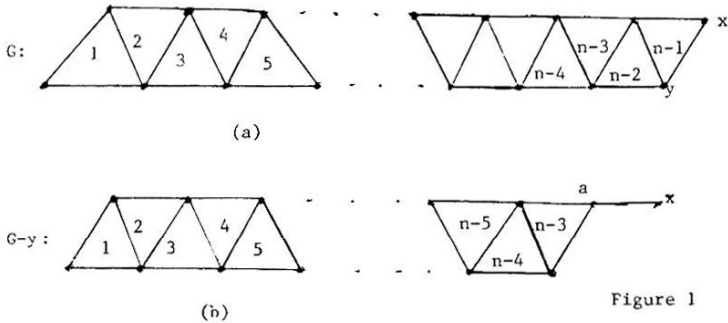
i.e. $\phi(G; x)$ is obtained from $C(G; \underline{w})$ by putting $w_1 = x, w_2 = -1$ and $w_r = -2$ for $r > 2$.

3. CIRCUIT POLYNOMIALS AND CHARACTERISTIC POLYNOMIALS OF TRIANGULAR CHAINS

We will denote the triangular chain comprising of n triangles, by T_n . The two nodes of valency 2 in T_n will be called *terminal nodes*. Edges incident to the terminal nodes will be called *terminal edges* and the two triangles containing

terminal edges will be called *terminal cells*. Generally, the terminal cells of a polygonal chain will be its initial and final cells.

We can "apply" Theorem 1 to T_n by taking the graph G to be T_{n-1} , $k=3$ and xy a terminal edge. (See Figure 1 (a) below). However we must put $P_{k-4} = 0$. The graph $G-y$ is shown below in Figure 1 (b).



The graph $G-x$ will be T_{n-2} . Let us apply the reduction process to the graph $G-y$ by deleting edge xa . This yields

$$G-y = w_1 T_{n-3} + w_2 T_{n-4}.$$

It can be seen from Figure 1 (a) that the paths P_j in G having x and y as endnodes are those for which $j = 2, 3, 4, \dots, (n+1)$. In this case, P_2 will be edge xy itself. P_{n+1} will contain all the nodes of G . Also the removal of P_2 from G yields T_{n-3} . The removal of P_3 leaves T_{n-4} etc. In general, the graph $G-P_j$ ($2 \leq j \leq n-2$) will be T_{n-j-1} . $G-P_{n-1}$ will be an edge, $G-P_n$ will be a node and $G-P_{n+1}$ the empty graph. For compactness of the results, we will denote these graph by T_0 , T_{-1} and T_{-2} respectively. Hence

Equation (1) becomes

$$G^* = \sum_{j=2}^{n+1} w_{3+j-2} T_{n-j-1} = \sum_{r=1}^{n+2} w_r T_{n-r}$$

Hence we obtain the following theorem.

Theorem 2

$$C(T_n; \underline{w}) = \sum_{r=1}^{n+2} w_r C(T_{n-r}; \underline{w}) + w_2 \sum_{r=1}^2 w_r C(T_{n-r-2}; \underline{w}) \quad (n > 0).$$

The following table gives values of $C(T_n; \underline{w})$ for $n=1, 2, 3$ and 4 .

Table 1

Circuit Polynomials of Triangular Chains

n	$C(T_n; \underline{w})$
1	$w_1^3 + 3w_1 w_2 + w_3$
2	$w_1^4 + 5w_1^2 w_2 + 2w_1 w_3 + 2w_2^2 + w_4$
3	$w_1^5 + 7w_1^3 w_2 + 3w_1^2 w_3 + 7w_1 w_2^2 + 2w_1 w_4 + 2w_2 w_3 + w_5$
4	$w_1^6 + 9w_1^4 w_2 + 4w_1^3 w_3 + 16w_1^2 w_2^2 + 3w_1^2 w_4 + 8w_1 w_2 w_3 + 2w_1 w_5 + 3w_2^3 + 2w_2 w_4 + w_3^2 + w_6$
5	$w_1^7 + 11w_1^5 w_2 + 5w_1^4 w_3 + 29w_1^3 w_2^2 + 4w_1^3 w_4 + 18w_1^2 w_2 w_3 + 3w_1^2 w_5 + 15w_1 w_2^3 + 8w_1 w_2 w_4 + 3w_1 w_3^2 + 2w_1 w_6 + 5w_2^2 w_3 + 2w_2 w_5 + 2w_3 w_4 + w_7$

Parallel results for the **characteristic equation** of T_n is immediate from Theorem 2 using Lemma 2. It is given in the following corollary.

Corollary 2.1

$$\phi(T_n; x) = x \phi(T_{n-1}; x) - \phi(T_{n-2}; x) - x \phi(T_{n-3}; x) + \phi(T_{n-4}; x) - 2 \sum_{r=3}^{n+2} \phi(T_{n-r}; x) \quad (n > 0),$$

where $\phi(T_0; x) = x^2 - 1$, $\phi(T_{-1}; x) = x$, $\phi(T_{-2}; x) = 1$ and $\phi(T_{-k}; x) = 0$, for $k > 2$.

The following table gives the values of $\phi(T_n; x)$ for $n=1, 2, 3, 4$, and 5 .

Table 2

Characteristic Polynomials of Triangular Chains

n	$\psi (T_n ; x)$
1	$x^3 - 3x - 2$
2	$x^4 - 5x^2 - 4x$
3	$x^5 - 7x^3 - 6x^2 + 3x + 2$
4	$x^6 - 9x^4 - 8x^3 + 10x^2 + 12x + 3$
5	$x^7 - 11x^5 - 10x^4 + 21x^3 + 30x^2 + 9x$

4 CIRCUIT POLYNOMIALS AND CHARACTERISTIC POLYNOMIALS OF RECTANGULAR CHAINS

Results for the circuit polynomial and characteristic polynomial of rectangular chains (also called *short ladders*) are given in Farrell [4]. The results obtained in this paper will be a significant improvement on those given in 4.

We will denote the rectangular chain with n cells by S_n . Theorem 1 can be applied to S_n by taking G to be S_{n-1} , $k=4$ and xy a terminal edge (an edge joining two nodes of valency 2) of S_{n-1} . In this case, G-x and G-y will be isomorphic graphs and will consist of S_{n-2} with an edge attached to one of its terminal nodes (nodes of valency 2). G-x-y will be the graph S_{n-2} .

Let us apply the reduction process to the graph G-x by deleting the attached edge. Then, with R_{n-2} written for G-x, we get

$$R_{n-2} = w_1 S_{n-2} + w_2 R_{n-3} .$$

$$\therefore R_{n-2} - w_2 R_{n-3} = w_1 S_{n-2} .$$

Similarly,

$$w_2 R_{n-3} - w_2^2 R_{n-4} = w_1 w_2 S_{n-3}$$

$$\begin{aligned} w_2^2 R_{n-4} - w_2^3 R_{n-5} &= w_1 w_2^2 S_{n-4} \\ \vdots \\ w_2^{n-4} R_2 - w_2^{n-3} R_1 &= w_1 w_2^{n-4} S_2 . \end{aligned}$$

By adding these equations and simplifying, we get

$$R_{n-2} - w_2^{n-3} R_1 = w_1 \sum_{r=0}^{n-4} w_2^r S_{n-2-r} . \quad (2)$$

The reduction process can now be applied to the graph R_1 to yield

$$R_1 = w_1 S_1 + w_2 P_3 .$$

But $P_3 = w_1 P_2 + w_1 w_2 = w_1 S_0 + w_1 w_2 .$

Hence $R_1 = w_1 S_1 + w_1 S_0 + w_1 w_2 .$

By substituting this expression for R_1 into Equation (2) and simplifying, we get

$$R_{n-2} = w_1 \sum_{r=0}^{n-1} w_2^r S_{n-2-r} ,$$

where we take

$$S_{-1} = 1 \text{ and } S_{-k} = 0 , \text{ for } k > 1 .$$

We will now consider the summation term of the theorem. In this case the paths P_j will all have even numbers of nodes. We will have $j = 2, 4, 6, \dots, 2n$. P_2 will be the edge xy when P_2 is removed the remaining graph $G - P_2$ will be S_{n-2} . Similarly $G - P_4$ will be S_{n-3} etc. $G - P_{2n-2}$ will be the edge S_0 and $G - P_{2n}$, the empty graph, which in this case, can be denoted by S_{-1} . Hence Equation (1) becomes

$$C^* = \sum_{j=2}^{2n} w_{j+2} S_{n-j} - 1 = \sum_{r=1}^n w_2^{r+1} S_{n-r-1} .$$

Hence by substituting into Theorem 1, we get the following result after simplifications.

Theorem 3

$$\begin{aligned} C(S_n; \underline{w}) &= (w_1^2 + w_2) C(S_{n-1}; \underline{w}) + (2w_1^2 w_2 + w_2^2 + w_4) C(S_{n-2}; \underline{w}) + \sum_{r=2}^n (2w_1^2 w_2^r + w_2^{r+1}) \\ &C(S_{n-r-1}; \underline{w}) \quad (n > 0) \end{aligned}$$

where we define

$$C(S_0; \underline{w}) = w_1^2 + w_2, \quad C(S_{-1}; \underline{w}) = 1 \quad \text{and} \quad C(S_{-k}; \underline{w}) = 0, \quad \text{for } k > 1.$$

In the following table, we give values of $C(S_n; \underline{w})$ for $n = 1, 2, 3, 4$ and 5 .

Table 3

Circuit Polynomials of Rectangular Chains

n	$C(S_n; \underline{w})$
1	$w_1^4 + 4w_1^2 w_2 + 2w_2^2 + w_4$
2	$w_1^6 + 7w_1^4 w_2 + 11w_1^2 w_2^2 + 2w_1^2 w_4 + 3w_2^3 + 2w_2 w_4 + w_6$
3	$w_1^8 + 10w_1^6 w_2 + 29w_1^4 w_2^2 + 3w_1^4 w_4 + 26w_1^2 w_2^3 + 10w_1^2 w_2 w_4 + 2w_1^2 w_6 + 5w_2^4 + 5w_2^2 w_4 + 2w_2 w_6 + w_4^2 + w_8$
4	$w_1^{10} + 13w_1^8 w_2 + 56w_1^6 w_2^2 + 94w_1^4 w_2^3 + 4w_1^6 w_4 + 24w_1^4 w_2 w_4 + 3w_1^4 w_6 + 56w_1^2 w_2^4 + 34w_1^2 w_2^2 w_4$ $+ 10w_1^2 w_2 w_6 + 3w_1^2 w_4^2 + 2w_1^2 w_8 + 8w_2^5 + 10w_2^3 w_4 + 5w_2^2 w_6 + 3w_2 w_4^2 + 2w_2 w_8 + 2w_4 w_6 + w_{10}$
5	$w_1^{12} + 16w_1^{10} w_2 + 92w_1^8 w_2^2 + 23w_1^6 w_2^3 + 5w_1^8 w_4 + 44w_1^6 w_2 w_4 + 4w_1^6 w_6 + 263w_1^4 w_2^4 + 114w_1^4 w_2^2 w_4$ $+ 24w_1^4 w_2 w_6 + 6w_1^4 w_4^2 + 3w_1^4 w_8 + 114w_1^2 w_2^5 + 96w_1^2 w_2^3 w_4 + 34w_1^2 w_2^2 w_6 + 18w_1^2 w_2 w_4^2 + 10w_1^2 w_2 w_8$ $+ 6w_1^2 w_4 w_6 + 2w_1^2 w_{10} + 13w_2^6 + 20w_2^4 w_4 + 10w_2^3 w_6 + 9w_2^2 w_4^2 + 5w_2^2 w_8 + 6w_2 w_4 w_6 + 2w_2 w_{10} + w_4^3$ $+ 2w_4 w_8 + w_6^2 + w_{12}$.

The following corollary is immediate from Theorem 3 using Lemma 2.

Corollary 3.1

$$\begin{aligned} \phi(S_n; \underline{x}) &= (x^2 - 1) \phi(S_{n-1}; \underline{x}) - (2x^2 + 1) \phi(S_{n-2}; \underline{x}) \\ &\quad - 2 \sum_{r=2}^n \left[(-1)^{r-1} x^2 + 1 \right] \phi(S_{n-r-1}; \underline{x}) \quad (n > 0), \end{aligned}$$

with

$$\phi(S_0; \underline{x}) = x^2 - 1, \quad \phi(S_{-1}; \underline{x}) = 1 \quad \text{and} \quad \phi(S_{-k}; \underline{x}) = 0, \quad \text{for } k > 1.$$

The following table gives the values of $\phi(S_n; \underline{x})$ for $n = 1, 2, 3, 4$ and 5 .

Table 4

Characteristic Polynomials of Rectangular Chains

n	$\phi(S_n; x)$
1	$x^4 - 4x^2$
2	$x^6 - 7x^4 + 7x^2 - 1$
3	$x^8 - 10x^6 + 23x^4 - 10x^2 + 1$
4	$x^{10} - 13x^8 + 48x^6 - 52x^4 + 16x^2$
5	$x^{12} - 16x^{10} + 82x^8 - 154x^6 + 101x^4 - 22x^2 + 1$

5 CIRCUIT POLYNOMIALS AND CHARACTERISTIC POLYNOMIALS OF PENTAGONAL CHAINS

The case of the pentagonal chain is a more difficult one. Again, Theorem 1 can be applied. In this case H will be the linear pentagonal chain with n cells. We will denote this graph by F_n . G will be F_{n-1} and $k=5$. As before, we will take xy to be a terminal edge (see Figure 2(i)). The graphs $G-x$, $G-y$ and $G-x-y$ are shown below in Figures 2(ii), (iii) and (iv) respectively. For convenience in analysis and also for brevity of notation, we will denote these three graphs by A_n , B_n and D_n respectively.

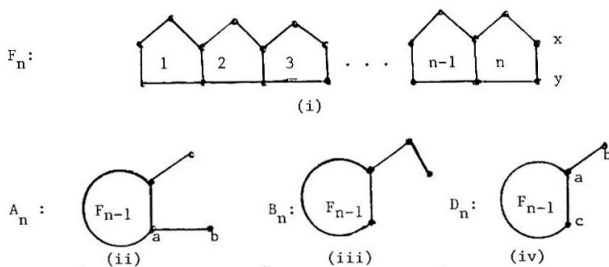


Figure 2

It is clear from the diagrams that A_1 , B_1 and D_1 are the chains P_4 , P_4 and P_3 respectively.

It can be easily confirmed that F_n has $3n+2$ and therefore G has $3n-1$ nodes. In considering the summation term of the theorem (see Equation (1)) P_2 will be x itself and P_{3n-1} , the path containing all the nodes of G . The paths in G with x and y as endnodes will contain $j=2+3m$ nodes, for $0 \leq m \leq n-1$. The removal of P_2 leaves D_{n-1} . The removal of P_5 leaves D_{n-2} . Generally, the removal of P_{2+3m} from G leaves the graph D_{n-m-1} (we take D_0 to be the empty graph). Therefore we get from Equation (1),

$$G^* = \sum_{m=0}^{n-1} w_{3m+5} D_{n-m-1}.$$

By applying the reduction process to A_n , by deleting edge ab (see Figure 2(ii)) and then the edge incident to the node of valency 1 in A_n - $a-b$, we get

$$A_n = w_1 D_n + w_2^2 D_{n-1} + w_1 w_2 B_{n-1}. \quad (3)$$

Also, by similar applications of the reduction process to B_n and D_n , we get

$$B_n = w_2 F_{n-1} + w_1 D_n \quad (4)$$

and

$$D_n = w_1 F_{n-1} + w_2 A_{n-1}. \quad (5)$$

By substituting for B_{n-1} in Equation (3), using Equation (4), we get

$$A_n = w_1 D_n + (w_2^2 + w_1^2 w_2) D_{n-1} + w_1 w_2^2 F_{n-2}. \quad (6)$$

Hence by substituting the above formulae for the circuit polynomials of $G-x (=A_n)$, $G-y (=B_n)$, $G-x-y (=D_n)$ and G^* , into Theorem 1, we get after simplifications,

$$F_n = w_1 w_2 F_{n-1} + w_2^2 (w_1^2 + w_2) F_{n-2} + (w_1^2 + w_2) D_n + w_1 w_2 (w_1^2 + 2w_2) D_{n-1} + \sum_{m=0}^{n-1} w_{3m+5} D_{n-m-1}. \quad (7)$$

We now require an explicit recurrence for the circuit polynomial of the

graph D_n . To this end, we apply the reduction to D_n by deleting the edge a (see Figure 2(iii)). The graph $D_n - ab$ will be F_{n-2} with P_4 and P_2 attached to the ends of a terminal edge uv . Call this graph $G_{n-2,4,2}$. $D_n - ab$ will consist of D_{n-1} together with an isolated node. An analysis similar to the one above for G^* will show that

$$D_n^* = w_1 \sum_{m=0}^{n-2} w_{3m+5} D_{n-m-2} .$$

Apply the reduction process to $G_{n-2,4,2}$ by deleting uv . This yields

$$G_{n-2,4,2} = G_{n-3,6,3} + w_2 P_1 P_3 D_{n-2} + P_1 P_3 \sum_{m=0}^{n-4} w_{3m+5} D_{(n-2)-m-1} .$$

Similarly,

$$G_{n-3,6,3} = G_{n-4,8,4} + w_2 P_2 P_5 D_{n-3} + P_2 P_5 \sum_{m=0}^{n-5} w_{3m+5} D_{(n-3)-m-1} .$$

Hence by similar repeated applications of the reduction process to the edge-deleted graphs until we obtain the chain P_{3n} , we add the resulting contributions to get

$$\begin{aligned} G_{n-2,4,2} = D_n - ab = P_{3n} + w_2 \sum_{r=1}^{n-2} P_{2n-2r-1} P_{n-r-1} D_r \\ + \sum_{r=1}^{n-2} P_{2n-2r-1} P_{n-r-1} \sum_{m=0}^{r-1} w_{3m+5} D_{r-m-1} . \end{aligned}$$

From Lemma 1 we get the following result which gives an explicit recurrence

for D_n .

Lemma 3

$$\begin{aligned} C(D_n; \underline{w}) = C(P_{3n}; \underline{w}) + w_2 \sum_{r=1}^{n-1} C(P_{2n-2r-1}; \underline{w}) C(P_{n-r-1}; \underline{w}) C(D_r; \underline{w}) \\ + \sum_{r=1}^{n-1} C(P_{2n-2r-1}; \underline{w}) C(P_{n-r-1}; \underline{w}) \sum_{m=0}^{r-1} w_{3m+5} C(D_{r-m-1}; \underline{w}) \quad (n > 1) , \end{aligned}$$

where

$$C(D_1; \underline{w}) = C(P_3; \underline{w}) = w_1^3 + 2w_1 w_2 \quad \text{and} \quad C(D_0; \underline{w}) = 1 .$$

Hence we have the following theorem using Equation (7).

Theorem 4

$$\begin{aligned}
 C(F_n; \underline{w}) &= w_1 w_2 C(F_{n-1}; \underline{w}) + w_2^2 (w_1^2 + w_2) C(F_{n-2}; \underline{w}) \\
 &\quad + (w_1^2 + w_2) C(D_n; \underline{w}) + w_1 w_2 (w_1^2 + 2w_2) C(D_{n-1}; \underline{w}) \\
 &\quad + \sum_{m=0}^{n-1} w_{3m+5} C(D_{n-m-1}; \underline{w}) \quad (n > 0),
 \end{aligned}$$

where

$$C(F_0; \underline{w}) = w_1^2 + w_2 \text{ and } C(D_n; \underline{w}) \text{ is given above in Lemma 3.}$$

The following tables give the polynomials $C(D_n; \underline{w})$ and $C(F_n; \underline{w})$, for $n=1, 2, 3$ and 4 .

Table 5

Circuit Polynomials of the Graphs \mathcal{D}_n

n	$C(D_n; \underline{w})$
1	$w_1^3 + 2w_1 w_2$
2	$w_1^6 + 6w_1^4 w_2 + 8w_1^2 w_2^2 + w_2^3 + w_1 w_5$
3	$w_1^9 + 10w_1^7 w_2 + 31w_1^5 w_2^2 + 32w_1^3 w_2^3 + 6w_1 w_2^4 + 5w_1^2 w_2 w_5 + 2w_1^4 w_5 + w_1 w_8$
4	$w_1^{12} + 14w_1^{10} w_2 + 70w_1^8 w_2^2 + 152w_1^6 w_2^3 + 136w_1^4 w_2^4 + 35w_1^2 w_2^5 + w_2^6 + 3w_1^7 w_5 + 18w_1^5 w_2 w_5$ $+ 26w_1^3 w_2^2 w_5 + 4w_1 w_2^3 w_5 + w_1^2 w_5^2 + 2w_1^4 w_8 + 5w_1^2 w_2 w_8 + w_1 w_{11}$

Table 6

Circuit Polynomials of Pentagonal Chains

n	$C(F_n; w)$
1	$w_1^5 + 5w_1^3w_2 + 5w_1w_2^2 + w_5$
2	$w_1^8 + 9w_1^6w_2 + 24w_1^4w_2^2 + 20w_1^2w_2^3 + 4w_1w_2w_5 + 2w_1^3 + w_5 + 2w_2^4 + w_8$
3	$w_1^{11} + 13w_1^9w_2 + 59w_1^7w_2^2 + 113w_1^5w_2^3 + 85w_1^3w_2^4 + 15w_1w_2^5 + 16w_1^4w_2w_5 + 20w_1^2w_2^2w_5 + 4w_1w_2w_8$ $+ 3w_1^6w_5 + 2w_1^3w_8 + w_1w_5^2 + 2w_2^3w_5 + w_{11}$
4	$w_1^{14} + 17w_1^{12}w_2 + 110w_1^{10}w_2^2 + 342w_1^8w_2^3 + 528w_1^6w_2^4 + 370w_1^4w_2^5 + 85w_1^2w_2^6 + 3w_2^7 + 4w_1^9w_5$ $+ 36w_1^7w_2w_5 + 102w_1^5w_2^2w_5 + 98w_1^3w_2^3w_5 + 16w_1w_2^4w_5 + 3w_1^4w_5^2 + 7w_1^2w_2w_5^2 + 3w_1^6w_8 + 16w_1^4w_2w_8$ $+ 20w_1^2w_2^2w_8 + 2w_2^3w_8 + 2w_1w_5w_8 + 2w_1^3w_{11} + 4w_1w_2w_{11} + w_{14}$.

The following results are immediate from Lemma 3 and Theorem 4.

Lemma 4

$$\begin{aligned} \phi(D_n; x) &= \phi(P_{3n}; x) - \sum_{r=1}^{n-1} \phi(P_{2n-2r-1}; x) \phi(P_{n-r-1}; x) \phi(D_r; x) \\ &\quad - 2 \sum_{r=1}^{n-1} \phi(P_{2n-2r-1}; x) \phi(P_{n-r-1}; x) \sum_{m=0}^{r-1} \phi(D_{r-m-1}; x) \quad (n > 1), \end{aligned}$$

with

$$\phi(D_0; x) = 1, \quad \phi(D_1; x) = \phi(P_3; x) = x^3 - 2x.$$

Theorem 5

$$\begin{aligned} \phi(F_n; x) &= -x \phi(F_{n-1}; x) + (x^2 - 1) \phi(F_{n-2}; x) \\ &\quad + (x^2 - 1) \phi(D_n; x) - x(x^2 - 2) \phi(D_{n-1}; x) \\ &\quad - 2 \sum_{m=0}^{n-1} \phi(D_{n-m-1}; x) \quad (n > 0), \end{aligned}$$

where

$$\phi(F_0; x) = x^2 - 1 \text{ and } \phi(D_n; x) \text{ is given above in Lemma 4.}$$

The following tables are analogons to Tables 5 and 6 respectively.

Table 7

Characteristic Polynomials of the Graphs D_n

n	$\phi(D_n; x)$
1	$x^3 - 2x$
2	$x^6 - 6x^4 + 8x^2 - 2x - 1$
3	$x^9 - 10x^7 + 31x^5 - 4x^4 - 3x^3 + 10x^2 + 4x$
4	$x^{12} - 14x^{10} + 70x^8 - 6x^7 - 152x^6 + 36x^5 + 132x^4 - 52x^3 - 21x^2 + 6x + 1$

Table 8

Characteristic Polynomials of Pentagonal Chains

n	$\phi(F_n; x)$
1	$x^5 - 5x^3$
2	$x^8 - 9x^6 + 24x^4 - 4x^3 - 20x^2 + 8x$
3	$x^{11} - 13x^9 + 59x^7 - 6x^6 - 113x^5 + 32x^4 + 81x^3 - 40x^2 - 3x + 2$
4	$x^{14} - 17x^{12} + 110x^{10} - 8x^9 - 342x^8 + 72x^7 + 522x^6 - 204x^5 - 326x^4 + 192x^3 + 17x^2 - 16x - 1$

6 μ -POLYNOMIALS OF POLYGONAL CHAINS

Suppose that the graph G contains r distinct cycles Z_1, Z_2, \dots, Z_r and that the cycle Z_i is given the weight w_i . Suppose also that each node of G is given a weight u and each edge, a weight v . Then the weight vector \underline{w} will be $(u, v, w_1, w_2, \dots, w_r)$. Let us denote this new weight vector by \underline{w}' . Throughout this section we will assume that the weight vector is \underline{w}' .

The following lemma gives the connection between the μ -polynomial $\mu(G; \underline{t}, x)$ of G and $C(G; \underline{w}')$. It is taken from [5]. \underline{t} is the vector (t_1, t_2, \dots, t_r) .

Lemma 5

$$\mu(G; \underline{t}, x) = C(G; (x, -1, 2t_1, 2t_2, \dots, 2t_r)).$$

i.e. $\mu(G; \underline{t}, x)$ is obtained from $C(G; \underline{w}')$, by replacing u by x , v by -1 and w_i by $2t_i$.

The following result is immediate from Lemmas 1 and 5.

Lemma 6

$$\mu(G; \underline{t}, x) = \mu(G'; \underline{t}, x) - \mu(G''; \underline{t}, x) + \mu(G^*; \underline{t}, x).$$

The μ -polynomial version of Theorem 1 can be easily obtained from Lemma 6. We will therefore omit its proof. The result is given in the following theorem in which, for brevity, $\mu(G)$ is written $\mu(G; \underline{t}, x)$.

Theorem 6

$$\begin{aligned} \mu(H; \underline{t}, x) = & \mu(P_{k-2}) \mu(G) - \mu(P_{k-3}) [\mu(G-x) + \mu(G-y)] \\ & + \sum_{P_j} t_{r(j)} \mu(G-P_j), \end{aligned}$$

where $t_{r(j)}$ is the weight assigned to the cycle $Z_{r(j)}$ consisting of the chain P_k and a path P_j in G with x and y as end nodes and the summation is taken over all such paths P_j in G .

Theorem 6 can be used as a basis for finding explicit recurrences for the μ -polynomials of polygonal chains. The analyses will be similar to those given in Sections 3, 4 and 5.

REFERENCES

- [1] E.J. Farrell, J. Comb. Theory B, 26, 111 (1979).
- [2] E.J. Farrell, Discrete Math. 25, 121 (1979).
- [3] E.J. Farrell, J. Comb. Theory B, 27 75 (1979).
- [4] E.J. Farrell, Discrete Math. 39, 31 (1982).
- [5] E.J. Farrell and I. Gutman, A Note on the Circuit polynomial and its Relation to the μ -Polynomial, submitted.
- [6] I. Gutman, Acta Chimica (Budapest) 99, 145 (1979).
- [7] I. Gutman, Chem. Phys. Letters 66, 595 (1979).
- [8] I. Gutman, Z. Naturforsch. 35a, 458 (1980).
- [9] I. Gutman and O.E. Polansky, Theoret. Chem. Acta 60, 203 (1981).
- [10] F. Harary, "Graph Theory and Theoretical Physics", F. Harary editor, Academic Press, London and New York, 1967.
- [11] F. Harary and E. Palmer, "Graphical Enumeration" Academic Press, New York and London, 1973.
- [12] O.E. Polansky and M. Zander, J. Mol. Struct. 84, 361 (1981).
- [13] O.E. Polansky and A. Graovac, Match 13, 151 (1982).
- [14] A. Graovac, O.E. Polansky and N.N. Tyutyulkov, Croat. Chem. Acta 56, 325 (1983).
- [15] A. Graovac, I. Gutman and O.E. Polansky, Monatsh. Chem. 115, 1 (1984).

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