PUBLICATIONS DE L'INSTITUT MATHÉMATIQUE
Nouvelle série, tome 62 (76), 1997, 1–12

ALGEBRAIC STRUCTURE COUNT OF SOME CYCLIC HEXAGONAL-SQUARE CHAINS

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Communicated by Slobodan Simić

Abstract. Algebraic structure count (ASC-value) of a bipartite graph G is defined by $ASC\{G\} = \sqrt{|\det A|}$, where A is the adjacency matrix of G. In the case of bipartite, plane graphs in which every face-boundary (cell) is a circuit of length $4s+2$ $(s = 1, 2, \dots)$, this number is equal to the number of the perfect matchings (K-value) of G. However, if some of the circuits are of length $4s$ $(s = 1, 2, \dots)$, then the problem of evaluation of ASC-value becomes more complicated. In this paper the algebraic structure count of the class of cyclic hexagonal-square chains is determined. An explicit combinatorial formula for ASC is deduced in the special case when all hexagonal fragments are isomorphic.

Introduction. The *algebraic structure count* (ASC-value) of a bipartite graph G is defined by

$$ASC\{G\} := \sqrt{|\det A|},$$

where A is the adjacency matrix of G. In chemistry, the thermodynamic stability of a hydrocarbon is related to the ASC-value of the graph which represents its skeleton. In recent papers [**3**]–[**7**] formulas for ASC for some classes of bipartite, plane graphs containing some circuits of length $4s$ $(s = 1, 2, \dots)$ are deduced.

A *perfect matching* (*1-factor*) of G is a selection of edges of G such that each vertex of G belongs to exactly one selected edge. In chemistry, perfect matchings are called the Kekulé structures of the molecule whose skeleton is represented by the graph G.

By a *hexagonal (unbranched) chain* H we mean a finite, plane graph obtained by concatenating m $(m \geq 1)$ circuits of length 6 which we call *hexagons* in such a way that any two adjacent hexagons (cells) have exactly one edge in common, each cell is adjacent to exactly two other cells, except terminal cells which are adjacent to exactly one other cell each and no one vertex belongs to more than two hexagons. Figure 1 shows one of the possible hexagonal chains consisting of 15 hexagons.

AMS Subject Classification (1991): Primary 05C70, 05B50, 05A15

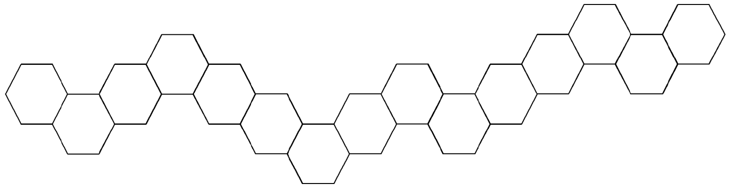

Fig. 1

There are several equivalent (different) explicit formulas for the number K of the hexagonal chains [**8**]–[**10**]. For example, it is known for a long time [**2**] that the number of perfect matchings of the zig-zag chain of n hexagons (Fig. 2a) is equal to the $(n+2)$-th Fibonacci number ($F_0 = 0$, $F_1 = 1$; $F_{k+2} = F_{k+1} + F_k$, $k \geq 0$) and the number of perfect matchings of the linear chain of n hexagons (Fig. 2b) is $n+1$.

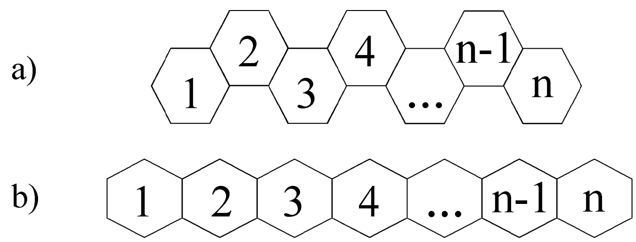

Fig. 2

The *cyclic hexagonal-square chain* $C_n = C_n(H_1, H_2, \ldots, H_n)$ considered in this paper is a connected, bipartite, plane graph which consists of n hexagonal unbranched chains $H_1, H_2, \ldots, H_n$, cyclically concatenated by circuits of length 4 which we call *squares* (Fig. 3). Square α_i connects two terminal cells (hexagons) of H_i and H_{i+1} for $i = 1, 2, \ldots, n-1, n$ ($H_{n+1} := H_1$) in such a way that every vertex of α_i belongs to exactly one hexagon. Denote the edges of α_i belonging to H_i and H_{i+1} by g_i and f_{i+1} ($f_1 := f_{n+1}$) respectively and their end-vertices by r_i, s_i and p_{i+1}, q_{i+1} ($p_1 := p_{n+1}$, $q_1 := q_{n+1}$) respectively, as it is shown in Fig. 3. Note that the graph C_n contains two face-boundaries which are different from squares and hexagons (the one of their regions is infinite). We call them *external circuits.* The vertices of α_i are denoted in such a way that vertices p_i and r_i ($i = 1, \ldots, n$) belong to the boundary of the infinite region and the vertices $s_1, q_2, s_2, q_3, \ldots, q_n, s_n, q_1$ belonging to the other external circuit are cyclically arranged in a clockwise direction.

The graphs H_i and H_j are said to be *isomorphic* if there is a $(1,1)$-mapping $y = \varphi(x)$ of the vertex set of the graph H_i onto the vertex set of the graph H_j such that: (i) two vertices x and x' are adjacent in H_i iff $\varphi(x)$ and $\varphi(x')$ are adjacent in H_j; (ii) $\varphi(p_i) = p_j$, $\varphi(q_i) = q_j$, $\varphi(r_i) = r_j$ and $\varphi(s_i) = s_j$.

In what follows we denote the subgraph obtained from G by deleting the edge e by $G - e$ and the subgraph obtained from G by deleting both the edge e and its terminal vertices by $G - (e)$.

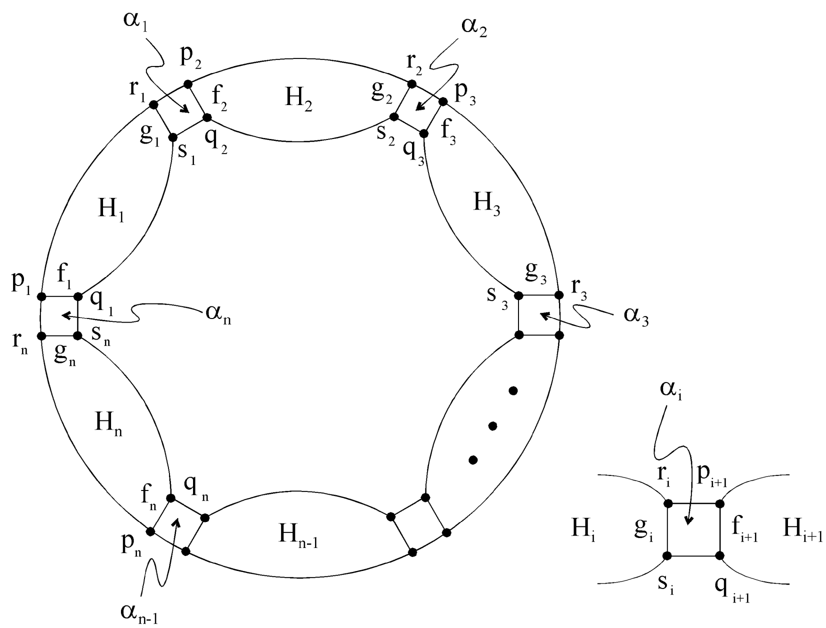

Fig. 3

Our aim is to prove the following result:

THEOREM 1. *If all the hexagonal chains H_i $(i = 1, 2, \dots, n)$ in the graph C_n are mutually isomorphic, then*

$$ASC\{C_n\} = \begin{cases} ((L-D)^n + (L+D)^n)/2^n, & \text{if } n \text{ is odd;} \\ ((L-D)^n + (L+D)^n)/2^n - 2, & \text{if } n \text{ is even} \end{cases}$$

where $L = K_2 + K_3 + K_4$, $D = \sqrt{L^2 + 4(K_1K_4 - K_2K_3)}$ and:

$$\begin{aligned} K_1 &= K\{H_i - (f_i) - (g_i)\} \\ K_2 &= K\{H_i - (f_i) - g_i\} \\ K_3 &= K\{H_i - f_i - (g_i)\} \\ K_4 &= K\{H_i - f_i - g_i\}. \end{aligned}$$

Preliminaries. All the graphs considered are assumed to be connected, planar, bipartite graphs whose all circuits are of even length. Define a binary relation ρ in the set of all perfect matchings of G in the following way.

Definiion 1. Two perfect matchings P_1 and P_2 are ρ-related iff the union of the sets of edges of P_1 and P_2 forms an even number of circuits of length $4s$ $(s = 1, 2, \dots)$.

It can be proved that ρ is an equivalence relation and subdivides the set of perfect matchings into two equivalence classes [**2**]. In [**2**] this relation is called "being of the same parity" and the numbers of elements of these classes are denoted by K_+ and K_-. We have the following theorem (Dewar and Longuet-Higgins [**2**]).

Theorem 2. *For the determinant of the adjacency matrix A of the graph G we have* $\det A = (-1)^n (K_+ - K_-)^2$.

This theorem yields the following corollary

Corollary 1. *For the algebraic structure count of the graph G there holds*

$$ASC\{G\} = |K_+ - K_-|.$$

In the case of graphs in which every cell is a circuit of length of the form $4s + 2$ $(s = 1, 2, \dots)$ (for example molecular graphs of benzenoid hydrocarbons), all perfect matchings are in the same class [**2**]. This implies

$$ASC\{G\} = K\{G\}, \tag{2}$$

where $K\{G\}$ is the number of perfect matchings of G. The enumeration of K-values for these graphs is well-known problem [**1**].

If some cells are allowed to be of length $4s$ $(s = 1, 2, \dots)$ (non-benzenoid hydrocarbons) then (1) need not be true. In such a case the following theorem, which follows directly from Definition 1, can be useful for evaluating the ASC-value.

Theorem 3. *Two perfect matchings are in distinct classes (of opposite parity) if one is obtained from the other by cyclically rearranging of an even number edges within a single circuit.*

Consider the graph C_n. Let m_i be the number of hexagons in H_i. Note that the number of vertices in H_i and C_n are equal to $4m_i + 2$ and $\sum_{i=1}^{n}(4m_i + 2) = 2n + 4\sum_{i=1}^{n} m_i$ respectively. Denote lengths of external circuits by c_1 and c_2 (the order is not important). The requirement for the graph C_n to be bipartite implies that the numbers c_1 and c_2 must be even. Note that the union of the external circuits represents the spanning subgraph of C_n, so:

$$c_1 + c_2 = 2n + 4\sum_{i=1}^{n} m_i \tag{2}$$

In order to distinguish edges of α_i we can represent them graphically by two vertical and two horizontal lines as in Fig. 3. Consider now a perfect matching of C_n. Observe that the edges belonging to the perfect matching can be arranged in and around a square in seven different ways (*modes* 1–7), as it is shown in Fig. 4 (these edges are marked by double lines).

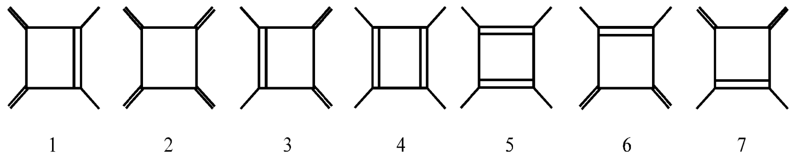

Fig. 4

Definition 2. The arrangement word of a perfect matching of the graph C_n is the word $u = u_1u_2\ldots u_n$ from $\{1,2,\ldots,6,7\}^n$, where u_i is the mode (1–7) of the arrangement of edges of the perfect matching in and around the square α_i for $i = 1,\ldots,n$.

For example, the arrangement words of the perfect matchings represented in Figures 5a and 5b are $u = 21322$ and $u = 77777$ respectively. (We can imagine that our position of observation of squares is inside the finite region whose boundary is the external circuit containing edges represented by lower horizontal lines and our motion (rotation) is in a clockwise direction.)

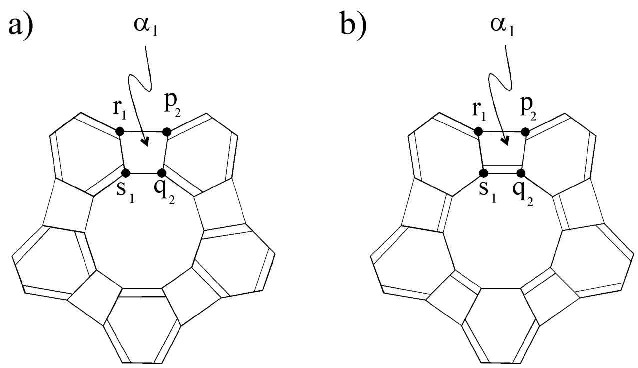

Fig. 5

The modes 4 and 5 (Fig. 4) are interconverted by rearranging two (an even number) edges of the considered perfect matching. Therefore, using Theorem 3, it follows that the perfect matchings of C_n, with arrangement of edges in and around a square α_i ($1 \le i \le n$) of modes 4 and 5, can be divided into pairs of opposite sign. It implies, by Corollary 1, that the perfect matchings in which the mode 4 or 5 appears for any α_i ($1 \le i \le n$) can be excluded from the consideration, when the algebraic structure count is evaluated.

Good perfect matchings. *Definition* 3. The perfect matchings are called good if their arrangement words belong to $\{1,2,3\}^n$.

Note that the edge of a square which belongs to one of the external circuits (horizontal lines in Fig. 4) is never in a good perfect matching. This means that every good perfect matching of the graph C_n induces in every hexagonal chain H_i $(i=1,\ldots,n)$ a perfect matching of H_i i.e., the edges of a good perfect matching of C_n can be rearranged only within each fragment H_i $(i=1,2,\ldots,n)$. Hence all good perfect matchings are of equal parity.

In order to determine the value $ASC\{C_n\}$, determine at first the number of all good perfect matchings of C_n using the so-called *transfer matrix method* [**2**]. Denote the graphs $H_i-(f_i)-(g_i)$, $H_i-(f_i)-g_i$, $H_i-f_i-(g_i)$ and $H_i-f_i-g_i$ (Fig. 3) by $H_{i,1}$, $H_{i,2}$, $H_{i,3}$, $H_{i,4}$ and their K-values by $K_{i,1}$, $K_{i,2}$, $K_{i,3}$ and $K_{i,4}$, respectively. Observe that $K_{i,1}$ is the number of all perfect matchings of H_i which contain both edges f_i and g_i; $K_{i,2}$ is the number of all perfect matchings of H_i which contain f_i and do not contain g_i; $K_{i,3}$ is the number of all perfect matchings of H_i which contain g_i and do not contain f_i; $K_{i,4}$ is the number of all perfect matchings of H_i which do not contain any of edges f_i and g_i. In this way, the set of all perfect matchings of H_i is divided into four disjointed classes. These classes (i.e., their elements) are said to be assigned to the corresponding graphs $H_{i,j}$ $(j=1,\ldots,4)$.

Associate with each good perfect matching of C_n a word $j_1j_2\ldots j_n$ of the alphabet $\{1,2,3,4\}$ in the following way: If the considered perfect matching induces in H_i a perfect matching assigned to the graph $H_{i,j}$, then $j_i=j$. For example, the word $j_1j_2\ldots j_n$ for the perfect matching represented in Fig. 5a, is 44144. Note that by choosing the edges of a perfect matching of C_n in H_i and H_{i+1} $(i=1,\ldots,n;$ $H_{n+1}:=H_1)$ we must not generate one of the modes 4 and 5 of arrangements of the perfect matching in the square between H_i and H_{i+1} i.e., the subwords j_ij_{i+1} $(i=1,\ldots,n-1)$ and subword j_nj_1 must not belong to the set $\{11,12,31,32\}$. According to the foregoing we obtain the following statement.

Lemma 1. *If we denote the number of all good perfect matchings of C_n by $\kappa\{C_n\}$, then*

$$\kappa\{C_n\}=\sum_{\substack{j_1j_2\ldots j_n\in\{1,2,3,4\}^n\\ j_nj_1,\,j_ij_{i+1}\notin\{11,12,31,32\}\\ 1\le i\le n-1}} K_{1,j_1}K_{2,j_2}\cdots K_{n,j_n}\quad\square$$

Let

$$M_i=\begin{bmatrix}0 & 0 & K_{i,3} & K_{i,4}\\ K_{i,1} & K_{i,2} & K_{i,3} & K_{i,4}\\ 0 & 0 & K_{i,3} & K_{i,4}\\ K_{i,1} & K_{i,2} & K_{i,3} & K_{i,4}\end{bmatrix}\quad\text{where}\quad \begin{aligned}K_{i,1}&=K\{H_i-(f_i)-(g_i)\}\\ K_{i,2}&=K\{H_i-(f_i)-g_i\}\\ K_{i,3}&=K\{H_i-f_i-(g_i)\}\\ K_{i,4}&=K\{H_i-f_i-g_i\}.\end{aligned}$$

Then the previous lemma can be written in the following form.

LEMMA 2. *The number of good perfect matchings of the graph C_n is equal to the sum of entries of the main diagonal of the matrix $M_1 \cdot M_2 \cdots M_n$ i.e.,*

$$\kappa\{C_n\} = \mathrm{tr}(M_1 \cdot M_2 \cdots M_n)$$

Determination of the ASC-value for an arbitrary cyclic hexagonal-square chain. In order to determine $ASC\{C_n\}$ we shall consider the remaining perfect matchings of C_n i.e., the ones whose arrangement words contain 6 and/or 7.

Definition 4. The edges of the graph C_n are called internal if they do not belong to the external circuits.

LEMMA 3. *Let the word $u \equiv u_1 u_2 \ldots u_n$ be the arrangement word of a perfect matching M and $u_i \in \{6, 7\}$ $(1 \leq i \leq n)$. Then no internal edge of C_n is in M.*

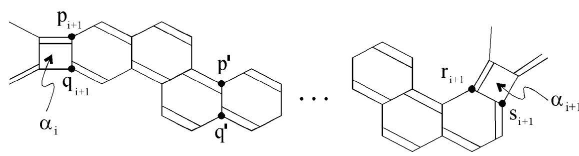

Fig. 6

Proof. Consider an internal edge $p'q'$ of C_n and denote the part of C_n between the edges $p_{i+1}q_{i+1}$ and $p'q'$ (one of two possible hexagonal-square chains which contain both edges $p_{i+1}q_{i+1}$ and $p'q'$) by L' (Fig. 6). Note that exactly one of the vertices p_{i+1} and q_{i+1} is connected in M to a vertex which does not belong to the subgraph L'. Since the number of vertices in L' is even, exactly one of the vertices p' and q' is connected in M to a vertex which does not belong to L'. Consequently, the edge $p'q'$ cannot be in M. $\square$

LEMMA 4. *If an arrangement word u contains 6 and/or 7, then this word belongs to $\{6, 7\}^n$ i.e., all its letters are 6 and/or 7. There are exactly two perfect matchings of C_n with such arrangement words.*

Proof. The proof of Lemma 3 implies the first part of the lemma. Moreover, if the colours of the vertices p_{i+1} and r_{i+1} (Fig. 6) are different, then $u_{i+1} = u_i$ i.e., $u_i u_{i+1} \in \{66, 77\}$; if the colours of the vertices p_{i+1} and r_{i+1} are identical, then $u_i u_{i+1} \in \{67, 76\}$. Further, for each arrangement of the word $u \equiv u_1 u_2 \ldots u_n$ there is another one $\overline{u} \equiv \overline{u}_1 \overline{u}_2 \ldots \overline{u}_n$ which is "complementary" in the sense that

$$\overline{u}_i = \begin{cases} 6, & \text{if } u_i = 7 \\ 7, & \text{if } u_i = 6 \end{cases} \qquad \text{for } i = 1, \ldots, n.$$

For each of these two only possible arrangement words (u and $\overline{u}$) from the set $\{6, 7\}^n$ there exists exactly one perfect matching because no internal edge of C_n

can be in it (Lemma 3). Consequently, there are exactly two perfect matchings (we shall denote them by $\mathcal{U}$ and $\overline{\mathcal{U}}$) with arrangement words from the set $\{6,7\}^n$. $\square$

In order to examine the parities of $\mathcal{U}$ and $\overline{\mathcal{U}}$ (refer to Definition 1) note that we can obtain one of them from the other by cyclically rearranging the edges at first within one of external circuits and then within the other external circuit.

Further, if the number n is odd, then the length of one of external circuits is $\equiv 0 \pmod 4$ and the length of the other one is $\equiv 2 \pmod 4$. According to the foregoing and Theorem 3 we obtain that the perfect matchings $\mathcal{U}$ and $\overline{\mathcal{U}}$ are of opposite parity. Consequently, $ASC\{C_n\} = \kappa\{C_n\}$. A graph C_n presented in Fig. 5 is an example of such a case.

Consider now the case when the number n is even. The length of both of the external circuits is $c_1 \equiv c_2 \equiv 0 \pmod 4$ or $c_1 \equiv c_2 \equiv 2 \pmod 4$. For both of these two subcases we obtain that $\mathcal{U}$ and $\overline{\mathcal{U}}$ are of equal parity. We distinguish two possibilities.

Possibility I: words u and $\overline{u}$ consist of the same letters i.e., $u = 66\dots6$ and $\overline{u} = 77\dots7$. If we cyclically rearrange the edges of $\mathcal{U}$ within one of the external circuits which contains vertices $p_1, r_1, p_2, r_2, \dots, p_n, r_n$ (Figure 9), we obtain a good perfect matching. The number of rearranged edges is even for the case $c_1 \equiv c_2 \equiv 0 \pmod 4$ and odd for the case $c_1 \equiv c_2 \equiv 2 \pmod 4$. This implies (Theorem 3) that the perfect matchings $\mathcal{U}$ and $\overline{\mathcal{U}}$ are of opposite parity with good perfect matchings of C_n in the first case and of the equal parity with good perfect matchings of C_n in the second case. So we obtain

$$ASC\{C_n\} = \begin{cases} \kappa\{C_n\} - 2, & \text{if } c_1 \equiv c_2 \equiv 0 \pmod 4; \\ \kappa\{C_n\} + 2, & \text{if } c_1 \equiv c_2 \equiv 2 \pmod 4 \end{cases} \tag{3}$$

Possibility II: Both the letters 6 and 7 appear in the word u. Let $i_1, i_2 \dots, i_k$ $(i_1 \le i_2 \le \dots \le i_k)$ be indices of letters 7 in arrangement word u. Observe the external circuit which contains vertices $p_1, r_1, p_2, r_2, \dots, p_n, r_n$. If we remove edges $r_{i_j}p_{i_j+1}$ for $j = 1, \dots, k$ $(p_{n+1} := p_1)$ and add edges $r_{i_j}s_{i_j}$, $s_{i_j}q_{i_j+1}$ and $q_{i_j+1}p_{i_j+1}$ $(j = 1, \dots, k)$, then we obtain a new circuit of length $c + 2k$ (indicated by bold lines in Fig. 7 and Fig. 8). Rearranging edges of the perfect matching $\mathcal{U}$ in this circuit we obtain a good perfect matching. The number $(c+2k)/2$ of rearranged edges can be even, as in example in Fig. 7 or odd, as in example in Fig. 8. This implies

$$ASC\{C_n\} = \begin{cases} \kappa\{C_n\} - 2, & \text{if } c + 2k \equiv 0 \pmod 4; \\ \kappa\{C_n\} + 2, & \text{if } c + 2k \equiv 2 \pmod 4. \end{cases} \tag{4}$$

Note that the relation (3) is just a special case of (4) for $k = 0$. According to the foregoing we can state the following theorem.

THEOREM 4. *We have*

$$ASC\{C_n\} = \begin{cases} \kappa\{C_n\}, & \textit{if } n \textit{ is odd;} \\ \kappa\{C_n\} - 2, & \textit{if } n \textit{ is even and } c + 2k \equiv 0 \pmod 4; \\ \kappa\{C_n\} + 2, & \textit{if } n \textit{ is even and } c + 2k \equiv 2 \pmod 4 \end{cases}$$

where c is the length of an external circuit; k is the number of letters 6 (or 7) in the arrangement word u (or $\overline{u}$) and $\kappa\{C_n\}$ is determined by Lemma 2. $\square$

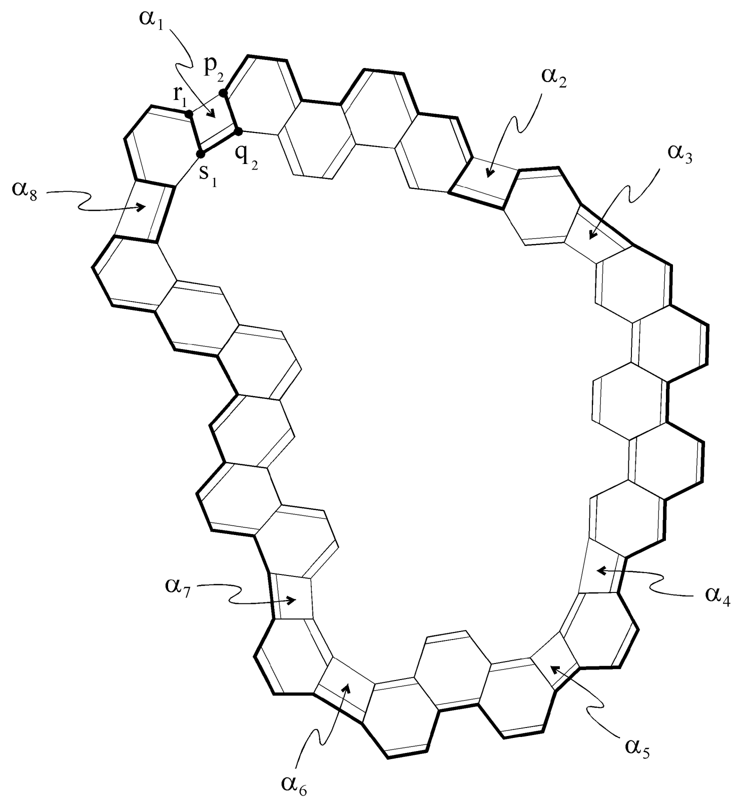

Fig. 7

Proof of Theorem 1. Let now all hexagonal chains H_i be mutually isomorphic in such a way that all edges f_i, $i = 1, \ldots, n$ are mutually corresponded and all edges g_i, $i = 1, \ldots, n$ are mutually corresponded too. We introduce the following notions:

$$m := m_1 = m_2 = \ldots = m_n$$
$$M := M_1 = M_2 = \ldots = M_n$$
$$K_j := K_{1,j} = K_{2,j} = \ldots = K_{n,j}, \quad j = 1, \ldots, 4.$$

We can obtain both a recurrence relation and an explicit formula for the number of good perfect matchings of C_n.

LEMMA 5. *In the case of isomorphic hexagonal chains H_i ($i = 1, \ldots, n$) we have*

$$\kappa\{C_n\} = (K_2 + K_3 + K_4)\kappa\{C_{n-1}\} + (K_1K_4 - K_2K_3)\kappa\{C_{n-2}\}$$

with initial conditions

$$\kappa\{C_1\} = K_2 + K_3 + K_4$$
$$\kappa\{C_2\} = (K_2 + K_3 + K_4)^2 + 2(K_1K_4 - K_2K_3)$$

Proof. The characteristic equation of M is

$$\lambda^4 - (K_2 + K_3 + K_4)\lambda^3 + (K_2K_3 - K_1K_4)\lambda^2 = 0. \tag{5}$$

Using the Cayley-Hamilton theorem we obtain

$$M^n - (K_2 + K_3 + K_4)M^{n-1} + (K_2K_3 - K_1K_4)M^{n-2} = 0$$

for $n \geq 2$. Consequently,

$$\operatorname{tr}(M^n) - (K_2 + K_3 + K_4)\operatorname{tr}(M^{n-1}) + (K_2K_3 - K_1K_4)\operatorname{tr}(M^{n-2}) = 0$$

for $n \geq 2$. Using Lemma 2 we obtain the desired recurrence relation for $\kappa\{C_n\}$. $\square$

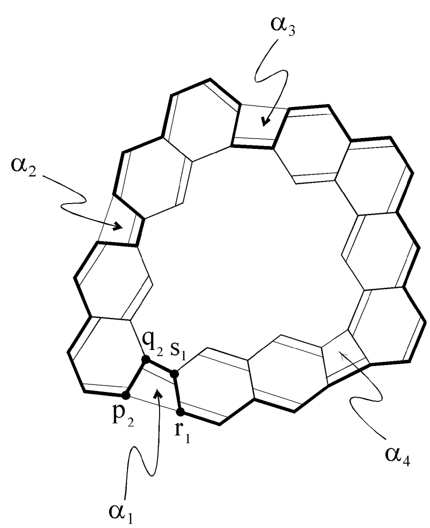

Fig. 8

The eigenvalues of the matrix M are $\lambda_1 = \lambda_2 = 0$, $\lambda_3 = (L - D)/2$ and $\lambda_4 = (L + D)/2$, where

$$L = K_2 + K_3 + K_4 \text{ and } D = \sqrt{L^2 + 4(K_1K_4 - K_2K_3)} \tag{6}$$

Since $\operatorname{tr}(M^n) = \sum_{i=1}^{4} \lambda_i^n$ we obtain the following statement.

LEMMA 6. *For $\kappa\{C_n\}$ we have $\kappa\{C_n\} = [(L-D)^n + (L+D)^n]/2^n$, where L and D are given by* (6). $\square$

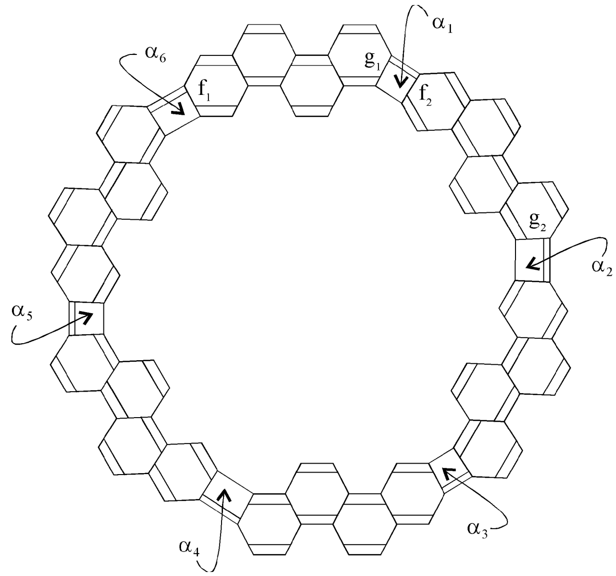

Fig. 9

Example 1. For the graph C_5 from Fig. 5 we obtain $K_1 = 1$, $K_2 = K_3 = 0$, $K_4 = 1$. Using Lemma 6 we get $\kappa\{C_5\} = 11$.

Example 2. The graph C_6 from Fig. 9 consists of six isomorphic hexagonal zig-zag chains for which $K_1 = F_3 = 2$, $K_2 = F_2 = 1$, $K_3 = F_4 = 3$, $K_4 = F_3 = 2$. Using Lemma 6 we get $\kappa\{C_6\} = ((6-2\sqrt{10})^6 + (6+2\sqrt{10})^6)/2^6 = 54758$.

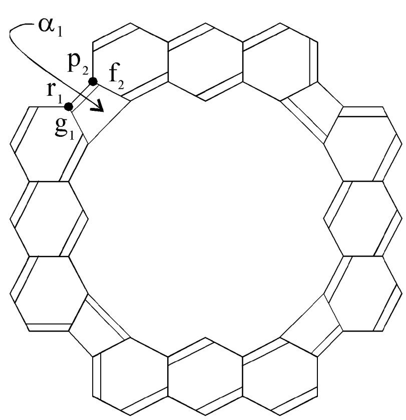

Fig. 10

Example 3. The graph C_4 from Fig. 10 consists of four isomorphic linear chains for which $K_1 = 2$, $K_2 = K_3 = 1$, $K_4 = 0$. Using Lemma 6 again, we get $\kappa\{C_4\} = 2$.

In order to complete the proof of Theorem 1 consider the perfect matchings $\mathcal{U}$ and $\overline{\mathcal{U}}$ again. The graph C_n is bipartite in the case when all hexagonal chains are isomorphic is equivalent to the following one: *If p_i and r_i are of the same colour, then n must be even.* In the case when p_i and r_i are of the same colour (Fig. 10) we have $u = 6767\ldots 67$ and $n = 2k$. The number of edges of the external circuit from p_i to r_i is even; so we obtain $c + 2k \equiv 0 \pmod 4$. In another case, when p_i and r_i are of different colours (Fig. 9) we get $u = 66\ldots 6$ and $k = 0$. The number of edges in the external circuit from p_i to r_i is odd. So, if n is even, then we obtain again that $c + 2k \equiv 0 \pmod 4$. Using Theorem 4 and Lemma 6 we obtain the assertion of Theorem 1. $\square$

Example 4. The graph in Fig. 5 (Example 1) is an example for the case n-odd and the graphs in Fig. 9 and Fig. 10 (Examples 2 and 3) are examples for the case n-even. In the first case we get $ASC\{C_5\} = \kappa\{C_5\} = 11$ and in the second two cases $ASC\{C_6\} = \kappa\{C_6\} - 2 = 54756$ and $ASC\{C_4\} = \kappa\{C_4\} - 2 = 2 - 2 = 0$.

Acknowledgement. The author is grateful to Prof. Ivan Gutman for useful discussions and many valuable comments.

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(Received 05 07 1996)
(Revised 30 04 1997)