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Algebraic structure count of some cyclic hexagonal-square chains on the Möbius strip

Olga Bodroža-Pantić
Department of Mathematics and Informatics, Trg D. Obradovića 4, University of Novi Sad, 21000 Novi Sad, Serbia
E-mail: bodroza@im.ns.ac.yu

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The concept of ASC (Algebraic structure count) is introduced into theoretical organic chemistry by Wilcox as the difference between the number of so-called "even" and "odd" Kekulé structures of a conjugated molecule. Precisely, algebraic structure count (ASC-value) of the bipartite graph G corresponding to the skeleton of a conjugated hydrocarbon is defined by $\mathrm{ASC}\{G\} \stackrel{\mathrm{def}}{=} \sqrt{|\det A|}$ where A is the adjacency matrix of G. The determination of algebraic structure count of (bipartite) cyclic hexagonal-square chains in the the class of plane such graphs is known. In this paper we expand these considerations on the non-plane class. An explicit combinatorial formula for ASC is deduced in the special case when all hexagonal fragments are isomorphic.

KEY WORDS: algebraic structure count, Kekulé structure

AMS subject classification (2001): 05C70, 05C50, 05B50, 05A15

1. Introduction

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

$$\mathrm{ASC}\{G\} \stackrel{\mathrm{def}}{=} \sqrt{|\det A|},$$

where A is the adjacency matrix of G.

The thermodynamic stability of an alternant hydrocarbon is related to the ASC-value for the bipartite graph which represents its skeleton. The basic application of ASC is in the following. Among two isomeric conjugated hydrocarbons (whose related graphs have an equal number of vertices and an equal number of edges), the one having greater ASC will be more stable. In particular, if $\mathrm{ASC} = 0$, then the respective hydrocarbon is extremely reactive and usually does not exist [4, 5].

In the case of the bipartite plane graphs containing only circuits of the length of the form $4s + 2\,(s = 1, 2, \ldots)$ (benzenoid hydrocarbons) all perfect matchings are of the same parity [8]. Consequently, in this case ASC coincides with the number of perfect matchings, i.e. K-value.

The enumeration of perfect matchings (Kekulé structures) is a classical problem in the theoretical chemistry of polycyclic conjugated molecules with a plethora of known counting formulae and several hundreds of published papers [7]. This can be attributed to the fact that simple and powerful recursive method exists for the calculation of K-values which is based on the formula $K\{G\} = K\{G-e\} + K\{G-(e)\}$ ($G-e$ stands for the subgraph obtained from the graph G by deleting the edge e of G and $G-(e)$ stands for the subgraph obtained from G by deleting both the edge e and its terminal vertices).

On the other hand, there are very few works dealing with ASC. Ten years ago prof. Ivan Gutman with his colleagues started the systematic study of the algebraic structure count (ASC) [11] – [17]. Although there are three possible formulas:

$$\left.\begin{array}{l} \mathrm{ASC}\{G\} = \mathrm{ASC}\{G-e\} + \mathrm{ASC}\{G-(e)\}, \\ \mathrm{ASC}\{G\} = \mathrm{ASC}\{G-e\} - \mathrm{ASC}\{G-(e)\}, \\ \mathrm{ASC}\{G\} = \mathrm{ASC}\{G-(e)\} - \mathrm{ASC}\{G-e\}. \end{array}\right\} \tag{1}$$

– the *Gutman formulas* [10], [18] for the algebraic structure count, it turned out that for evaluating the ASC-values of some concrete bipartite graphs the following theorem [6] was much more useful.

Theorem 1. Two perfect matchings are of opposite parity if one is obtained from the other by cyclically rearranging of an even number edges within a single circuit. If the number of cyclically rearranged double bonds is odd, then the respective two perfect matchings are of equal parity.

By a *hexagonal (unbranched) chain* H we mean a finite, plane graph obtained by concatenating m $(m \geqslant 1)$ 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.

The *Cyclic hexagonal-square chain* $C_n = C_n(H_1, H_2, \ldots, H_n)$ is a connected, bipartite 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* (figure 1). Square α_i $(r_i p_{i+1} q_{i+1} s_i)$ connects two terminal cells (hexagons) of H_i and H_{i+1} for $i = 1, 2, \ldots, n-1, n$ $(H_{n+1} \stackrel{\mathrm{def}}{=} H_1)$ 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

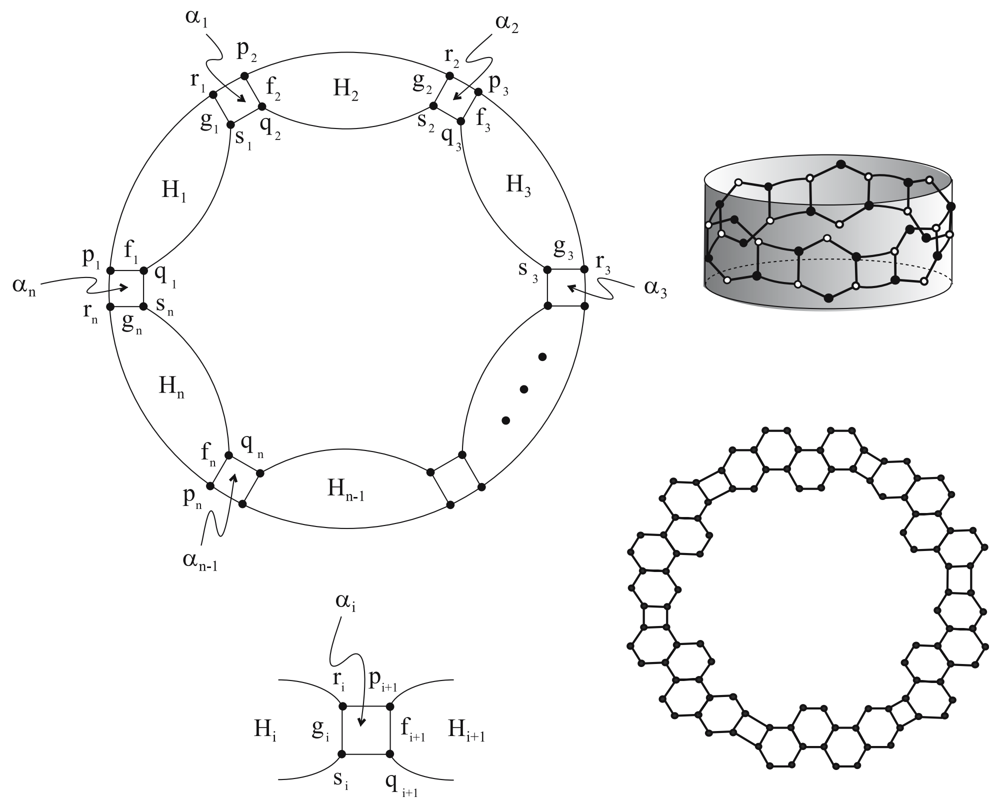

Figure 1. The plane cyclic hexagonal-square chains.

f_{i+1} ($f_{n+1} \stackrel{\text{def}}{=} f_1$), respectively. Their end vertices are r_i, s_i and p_{i+1}, q_{i+1} respectively, as it is shown in figure 1 and figure 2.

Note that if $p_{n+1} = p_1$ and $q_{n+1} = q_1$, then the graph is the plane one, i.e. it can be drawn on a plane without self-crossing of its edges (figure 1). Otherwise, if $p_1 = q_{n+1}$ and $q_1 = p_{n+1}$, then the graph is not the plane one, but it can be drawn on a Möbius strip without self-crossing of its edges (figure 2).

The graphs H_i ($i = 1, \ldots, n$) are said to be mutually *isomorphic* if for every $i \in \{1, \ldots, n-1\}$ 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_{i+1} such that the following conditions are fulfilled:

(i) two vertices x and x' are adjacent in H_i iff $\varphi(x)$ and $\varphi(x')$ are adjacent in H_{i+1}; and

(ii) in the case of the plane C_n:

$$\varphi(p_i) = p_{i+1}, \varphi(q_i) = q_{i+1}, \varphi(r_i) = r_{i+1} \quad \text{and} \quad \varphi(s_i) = s_{i+1};$$

or

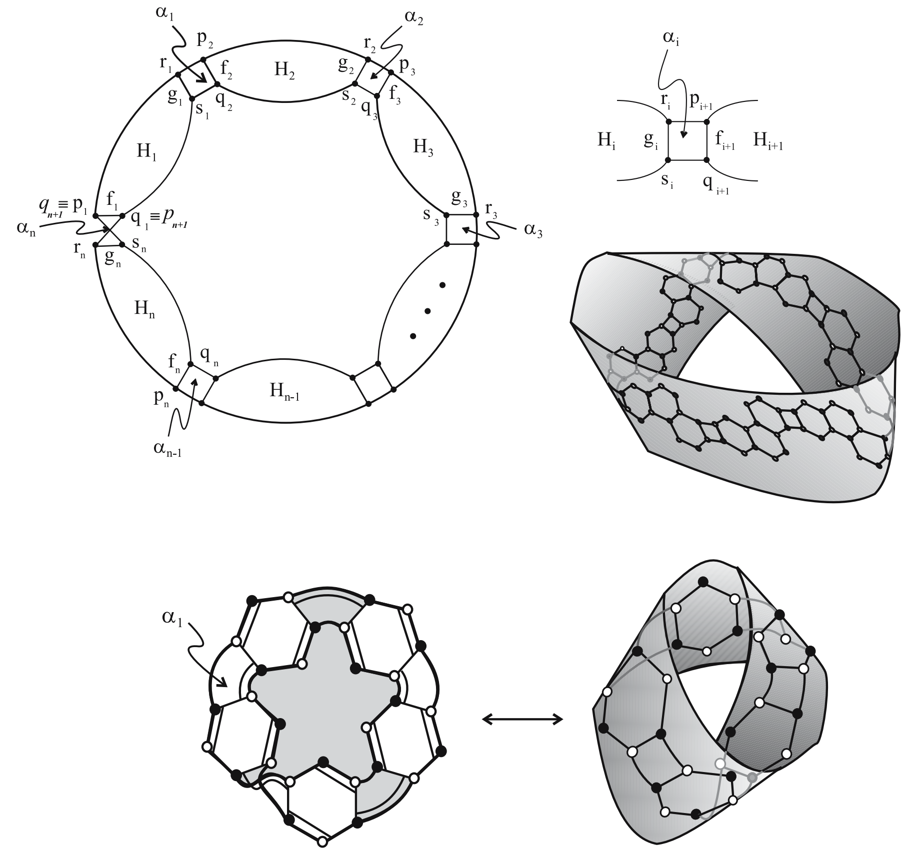

Figure 2. The non-plane cyclic hexagonal-square chains.

in the case of the non-plane C_n:

$$\varphi(p_i) = q_{i+1}, \varphi(q_i) = p_{i+1}, \varphi(r_i) = s_{i+1} \quad \text{and} \quad \varphi(s_i) = r_{i+1}.$$

Note that in the first case 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.* In the second case there is only one *external circuit* which is the boundary of the infinite region (on the Möbius strip). In [16] the following theorem is proved.

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

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

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

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

The aim of this paper is to prove the following result:

Theorem 3. If all hexagonal chains H_i $(i = 1, 2, \ldots, n)$ in the non-plane graph C_n are mutually isomorphic and l is the number of edges in the path from the vertex q_1 to the vertex s_1 which does not contain vertices p_1 and r_1, then

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

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

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

2. Preliminaries

For the plane graphs in which every cell is a circuit of length of the form $4s + 2$ $(s = 1, 2, \ldots)$ (for example molecular graphs of benzenoid hydrocarbons like hexagonal chains H_i), all perfect matchings are of equal parity and $\mathrm{ASC}\{G\} = K\{G\}$. The enumeration of K-values for these graphs is well-known problem [9]. There are several equivalent (different) explicit formulas for the K-number of the hexagonal chains [20], [21]. For example, it is known for a long time [8] that the number of perfect matchings of the zig-zag chain of n hexagons is equal to the $(n + 2)$-th Fibonacci number $(F_0 = 0, F_1 = 1; F_{k+2} = F_{k+1} + F_k, k \geqslant 0)$ and the number of perfect matchings of the linear chain of n hexagons is equal to $n + 1$.

Consider the non-plane graph C_n. Note that the number of vertices in H_i is $4m_i + 2$ where m_i is the number of hexagons in H_i. The requirement of the graph C_n to be bipartite and non-plane implies that n is odd.

In order to distinguish edges of α_i in C_n we can represent them graphically by two vertical and two horizontal lines as it is shown in figure 2. Consider now a perfect matching of C_n. Observe that 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 figure 3 (these edges are marked by double lines).

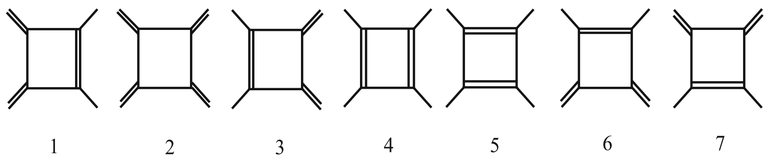

Figure 3. The seven modes in which double bonds can be arranged in and around a square.

Definition 1. The arrangement word of a perfect matching of the graph C_n is the word $u = u_1 u_2 \dots u_n$ from the set $\{1, 2, \dots, 6, 7\}^n$, 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 $i = 1, \dots, n$.

For example, the arrangement words of the perfect matchings represented in Figures 4a, 4b, and 4c are $u = 7766666$, $u = 2244443$, and 2231313, respectively.

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

3. Good perfect matchings

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

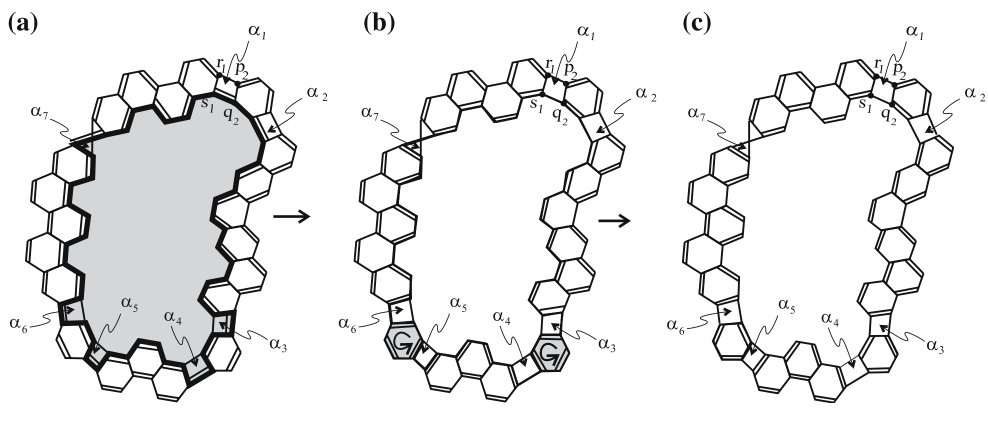

Figure 4. The arrangement words: (a) 7766666, (b) 2244443, (c) 2231313.

Note that the edge of a square which belongs to the external circuit (horizontal lines in figure 4) are 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* [8]. Denote the graphs $H_i - (f_i) - (g_i)$, $H_i - (f_i) - g_i$, $H_i - f_i - (g_i)$ and $H_i - f_i - g_i$ 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 the number $K_{i,1}$ represents the number of all perfect matchings of H_i which contain both edges f_i and g_i; the number $K_{i,2}$ represents the number of all perfect matchings of H_i which contain f_i and do not contain g_i; the number $K_{i,3}$ represents the number of all perfect matchings of H_i which contain g_i and do not contain f_i; the number $K_{i,4}$ represents 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 disjoined 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 $j_1 j_2 \ldots j_n$ of the alphabet $\{1, 2, 3, 4\}$ in the following way: If the considered perfect matching induces in H_i a perfect matching which is assigned to the graph $H_{i,j}$, then $j_i = j$. For example, the word $j_1 j_2 \ldots j_n$ for the perfect matching which is represented in figure 4c, is 4434141. Note that by choosing the edges of a perfect matching of C_n in H_i and H_{i+1} $(i = 1, \ldots, n;\ H_{n+1} \stackrel{\text{def}}{=} H_1)$ we must not generate one of modes 4 and 5 of arrangements of the perfect matching in the square between H_i and H_{i+1} i.e. the subwords $j_i j_{i+1}$ $(i = 1, \ldots, n-1)$ and word $j_n j_1$ 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

$$\kappa\{C_n\} = \sum_{\substack{j_1 j_2 \ldots j_n \in \{1,2,3,4\}^n \\ j_n j_1,\, j_i j_{i+1} \notin \{11, 12, 31, 32\};\ 1 \leqslant i \leqslant n-1}} K_{1,j_1} K_{2,j_2} \cdots K_{n,j_n}.$$

Let

$$M_i = \begin{bmatrix} 0 & 0 & K_{i,3} & K_{i,4} \\ K_{i,1} & K_{i,2} & K_{i,3} & K_{i,4} \\ 0 & 0 & K_{i,3} & K_{i,4} \\ K_{i,1} & K_{i,2} & K_{i,3} & K_{i,4} \end{bmatrix},$$

where

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

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.

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

4. Determination of the ASC-value for an arbitrary non-plane cyclic hexagonal-square chain

In order to determine the value ASC$\{C_n\}$ we shall consider the remaining perfect matchings of C_n i.e. the ones whose arrangement words contain at least one of numbers 6 and/or 7. Note that the number of vertices of H_i $(i = 1, \ldots, n)$ is even. Consequently, if an arrangement word u contains at least one of numbers 6 and/or 7 then this word belongs to the set $\{6, 7\}^n$ i.e. all its letters are 6 and/or 7. Moreover, the number of perfect matchings of C_n with such arrangement words is exactly two. If the colours of the vertices p_{i+1} and r_{i+1} are different then $u_{i+1} = u_i$ i.e. the subword $u_i u_{i+1} \in \{66, 77\}$; if the colours of the vertices p_{i+1} and r_{i+1} are identical then the subword $u_i u_{i+1} \in \{67, 76\}$.
Further, for each arrangement word $u \equiv u_1 u_2 \ldots u_n$ there is another one $\overline{u} \equiv \overline{u}_1 \overline{u}_2 \cdots \overline{u}_n$ which is "complementary" in the sense that

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

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. Note that their union makes the external circuit. Let's examine the parities of them. Since we can obtain one of them from the other by cyclically rearranging the edges (double bonds) within the external circuit, it depends on the number of vertices of C_n.

If the number n is even then these perfect matchings are of opposite parity (one of them is obtained from the other by cyclically rearranging an even number of double bonds). So, ASC$\{C_n\} = \kappa\{C_n\}$, for n-even.

Consider now the case when the number n is odd. The length of the external circuit is then $\equiv 2 \pmod 4$. Consequently, these perfect matchings are of equal parity (one of them is obtained from the other by cyclically rearranging an odd number of double bonds). Denote the path from the vertex q_i to the vertex s_i which does not contain vertices p_i and r_i by $\widehat{q_i s_i}$ and the number of vertices of this path by c_i. Observe the arrangement word in which $u_n = 6$ and the circuit $\widehat{q_1 s_1}\widehat{q_2 s_2}\ldots\widehat{q_{n-1}s_{n-1}}\widehat{q_n s_n} r_n$. Let $i_1, i_2 \ldots, i_k$ $(i_1 \leqslant i_2 \leqslant \cdots \leqslant i_k)$ $(0 \leqslant k \leqslant n-1)$ be indices of letters 6 in the subword $u_1 u_2 \ldots u_{n-1}$ of the arrangement word u. In the case $k \neq 0$, if we remove edges $s_{i_j} q_{i_j+1}$ for $j = 1, \ldots, k$ in the considered circuit and add edges $s_{i_j} r_{i_j}, r_{i_j} p_{i_j+1}$ and $p_{i_j+1} q_{i_j+1}$ $(j = 1, \ldots, k)$, then we obtain a new circuit whose length is $c + 1 + 2k$ (indicated by bold lines in figure 4a), where $c = \Sigma_{i=1}^{n} c_i$. Rearranging edges of the perfect matching in this circuit we obtain a perfect matching with the arrangement word in $\{1, 2, 3, 4\}^n$ (figure 4b). But, we can always rearrange the edges of the obtained perfect matching within some of fragments H_i to obtain a good perfect matching (figure 4c). So, if the number of rearranged edges (in the first step) $(c+1+2k)/2$ is even, then $\mathrm{ASC}\{C_n\} = \kappa\{C_n\} - 2$; otherwise $\mathrm{ASC}\{C_n\} = \kappa\{C_n\} + 2$.

According to the foregoing we can formulate the following theorem.

Theorem 4. If C_n is the non-plane graph, then

$$ASC\{C_n\} = \begin{cases} \kappa\{C_n\}, & \text{if } n \text{ is even ;} \\ \kappa\{C_n\} - 2, & \text{if } n \text{ is odd and } c + 1 + 2k \equiv 0 \pmod 4; \\ \kappa\{C_n\} + 2, & \text{if } n \text{ is odd and } c + 1 + 2k \equiv 2 \pmod 4), \end{cases}$$

where c is the sum of numbers of vertices in all paths $\widehat{q_i s_i}$ for $i = 1, \ldots, n$; k is the number of letters 6 in the subword $u_1 u_2 \ldots u_{n-1}$ of the arrangement word u (in wich $u_n = 6$) and $\kappa\{C_n\}$ is determined by lemma 2.

5. Proof of theorem 3

Let now all hexagonal chains H_i, $i = 1, 2, \ldots, n$ be mutually isomorphic. Note that the number n have to be odd. (The condition for the non-plane graph C_n to be bipartite in the case when all hexagonal chains are isomorphic requires that p_i and r_i are of the same colour.) Let us introduce the following notions:

$$M \stackrel{\text{def}}{=} M_1 = M_2 = \cdots = M_n$$
$$K_j \stackrel{\text{def}}{=} K_{1,j} = K_{2,j} = \cdots = K_{n,j}, \quad j = 1, \ldots, 4.$$

In this case we can obtain both a recurrence relation and an explicit formula for the number of good perfect matchings of C_n. □

Lemma 3. In the case of isomorphic hexagonal chains H_i $(i = 1, \ldots, n)$ the following relation holds

$$\kappa\{C_n\} = (K_2 + K_3 + K_4)\kappa\{C_{n-1}\} + (K_1 K_4 - K_2 K_3)\kappa\{C_{n-2}\}$$

with initial conditions

$$\kappa\{C_1\} = K_2 + K_3 + K_4 \text{ and } \kappa\{C_2\} = (K_2 + K_3 + K_4)^2 + 2(K_1 K_4 - K_2 K_3).$$

Proof. The characteristic equation of M is

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

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 $n \geqslant 2$. Consequently,

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

for $n \geqslant 2$. Using lemma 2 we obtain the desired recurrence relation for $\kappa\{C_n\}$. □

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

$$L = K_2 + K_3 + K_4 \qquad \text{and} \qquad D = \sqrt{L^2 + 4(K_1K_4 - K_2K_3)}. \tag{3}$$

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

Lemma 4. In the case of isomorphic hexagonal chains H_i $(i = 1, \dots, n)$

$$\kappa\{C_n\} = [(L - D)^n + (L + D)^n]/2^n,$$

where L and D are given by (3).

In order to complete the proof of theorem 3 consider the perfect matchings with arrangement words 6767…676 and 7676…767. Let l be the number of edges of $\widehat{q_1s_1}$. If $l \equiv 2 \pmod 4$ (note that the number of edges of $\widehat{p_1r_1}$ is $\equiv l \pmod 4$)), then the number $c + 1 + 2k = (2k + 1)(l + 1) + 1 + 2k \equiv l + 2 \equiv 0 \pmod 4$ (figure 5a). In that case $ASC\{C_n\} = \kappa\{C_n\} - 2$ (theorem 4). If $l \equiv 0 \pmod 4$, then we obtain $c + 1 + 2k = (2k + 1)(l + 1) + 1 + 2k \equiv l + 2 \equiv 2 \pmod 4$ (figure 5b). In that case ASC $\{C_n\} = \kappa\{C_n\} + 2$. Using lemma 4 we obtain the statement of theorem 3.

Example. For the both graphs in figure 5 the numbers $K_1 - K_4$ are equal, i.e. $K_1 = K_2 = K_4 = 1$ and $K_3 = 2$ and $\kappa(C_7) = \dfrac{(4 - 2\sqrt{3})^7 + (4 + 2\sqrt{3})^7}{2^7} = 10084$. However, for the graph in figure 5a, $l = 6 \equiv 2 \pmod 4$, which implies ASC $(C_7) = 10084 - 2 = 10082$. For the graph in figure 5b, $l = 8 \equiv 0 \pmod 4$, which implies ASC $(C_7) = 10084 + 2 = 10086$.

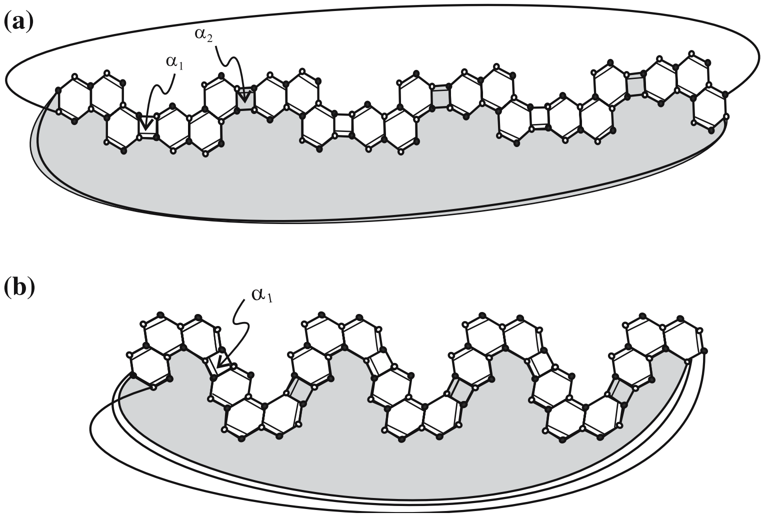

Figure 5. $\mathrm{ASC}(C_7) = 10084 - 2 = 10082$, (b) $\mathrm{ASC}(C_7) = 10084 + 2 = 10086$.

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