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Some Relations between Kekulé Structure and Morgan−Voyce Polynomials

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ABSTRACT

In this paper, Kekulé structures of benzenoid chains are considered. It has been shown that the coefficients of a $B_n(x)$ Morgan Voyce polynomial equal to the number of k–matchings ($m(G, k)$) of a path graph which has $N = 2n + 1$ points. Furtermore, two relations are obtained between regularly zig–zag non-branched catacondensed benzenoid chains and Morgan–Voyce polynomials and between regularly zig−zag non branched catacondensed benzenoid chains and their corresponding caterpillar trees.

1. INTRODUCTION

A benzenoid system is obtained by using the regular hexagons consecutively so that two hexagons are either disjoint or have a common edge [1]. An example of benzenoid chain is illustrated in Figure 1.

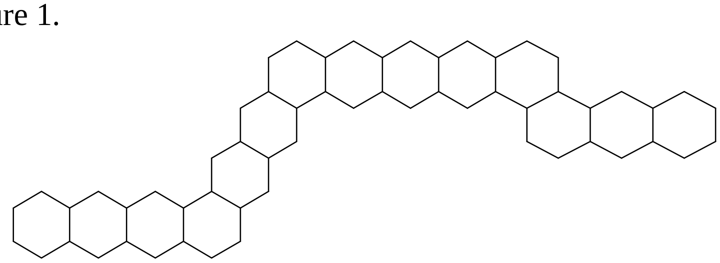

Figure 1. A Benzenoid Chain.

In connection with the benzenoid chains the LA–sequence is defined as an ordered h–tuple ($h > 1$) of the symbols L and A. The i–th symbol is L if the i–th hexagon is of

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modeL_1 or L_2. The i–th symbol is A if the i–th hexagon is of mode A. The definition of L_1, L_2 and Amodes of hexagons is clear from Figure 2.

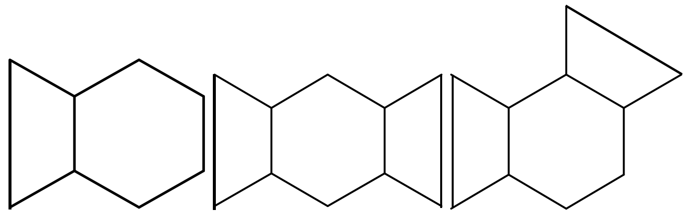

Figure 2. Illustration of L_1, L_2 and A modes of hexagons, respectively.

For instance, the LA–sequence of the benzenoid chain in Figure 1 is $LLLALLALLLAALL$ or, in the abbreviated form $L^3AL^2AL^3A^2L^2$. Each perfect matching of a benzenoid system (if any exists) represents a Kekulé structure. The number of Kekulé structures of benzenoid chains is called its“K number”. The K–number of a benzenoid chain is calculated by its LA–sequence.

Balaban and Tomescu coined the term isoarithmicity for the benzenoid chains which their K numbers are same [2]. It is denoted by $\langle x_1, x_2, \ldots, x_n\rangle$ the class of isoarithmic benzenoid chains with the LA–sequence

$$L^{x_1}AL^{x_2}A \ \ldots AL^{x_n}$$

where $n \geq 1$, and $x_1 \geq 1,\ x_n \geq 1,\ x_i \geq 0$ for $i = 2,3, \ldots, n-1$. For example isoarithmic class of the benzenoid chain which is depicted in Figure 1 is $\langle 3,2,3,0,2\rangle$.

Every benzenoid chain can be represented in this form. It is denoted by $K_n\langle x_1, x_2, \ldots, x_n\rangle$ the number of Kekulé structures of the chain $\langle x_1, x_2, \ldots, x_n\rangle$.It is defined for the initial terms of the K numbers such that ([1]) $K_0 = 1$,$K_1\langle x_1\rangle = 1 + x_1$.

Theorem 1. If $n \geq 2$ then for arbitrary $x_1 \geq 1,\ x_n \geq 1,\ x_i \geq 0,\ (i = 2,3, \ldots, n-1)$, the following recurrence relation holds [1]

$$K_n\langle x_1, x_2, \ldots, x_n\rangle = (x_n + 1)K_{n-1}\langle x_1, x_2, \ldots, x_{n-1}\rangle + K_{n-2}\langle x_1, x_2, \ldots, x_{n-2}\rangle.$$

2. THE HOSOYA INDEX AND MORGAN–VOYCE POLYNOMIALS

The Hosoya or Z–index was defined by Hosoya in 1971 [3] and the Hosoya index of a graph G is denoted by $Z(G)$. The $Z(G)$, is the total number of k–matchings which are the number of k choosing from a graph G such that the k lines are non–adjacent where N is the number of points.

Definition 1. The number of k–matchings is denoted by $m(G,k)$ and the $Z(G)$ is defined as $Z(G) = \sum_{k=0}^{\lfloor N/2\rfloor} m(G,k)$ such that $m(G,0) = 1$ for any graph G.

Theorem 2. The number of k–matchings of the path graph is calculated by the following equation [4]

$$m(G, k) = \binom{N-k}{k}, \text{ for } 0 \leq k \leq \lfloor N/2 \rfloor.$$

Relations between topological indices and some orthogonal polynomials for example Hermite, Laguerre and Chebyshev polynomials were found by Hosoya ([5]). Another relation between the sextet polynomial of a hexagonal chain and the matching polynomial of a caterpillar tree was discovered by Gutman [6]. As a result of this paper, it has been shown that the K–number of a hexagonal chain is equal to the Hosoya index of the corresponding caterpillar [7]. For instance, corresponding caterpillar tree of the hexagonal chain which is depicted in Figure 1 is on the below.

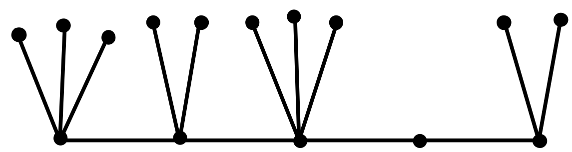

Figure 3. The hexagonal chain in Figure 1 has 14 hexagons and the corresponding caterpillar tree has 14 edges.

The caterpillar tree of the hexagonal chain in Figure 3 is $C_5(4, 3, 4, 1, 3)$.

Definition 2. The Morgan–Voyce polynomials $B_n(x)$ is defined by [8] as

$$B_n(x) = \sum_{i=0}^{n} \binom{n+i+1}{n-i} x^i$$

and the first five Morgan–Voyce polynomials are found from this equation like that

$$B_0(x) = 1$$
$$B_1(x) = x + 2$$
$$B_2(x) = x^2 + 4x + 3$$
$$B_3(x) = x^3 + 6x^2 + 10x + 4$$
$$B_4(x) = x^4 + 8x^3 + 21x^2 + 20x + 5 .$$

3. Regularly Zig–Zag Non–branched Catacondensed Benzenoids

The Kekulé number of regularly zig–zag non-branched cata condensed benzenoids was found by He, He and Xie [9] by Peak–Valley matrix.

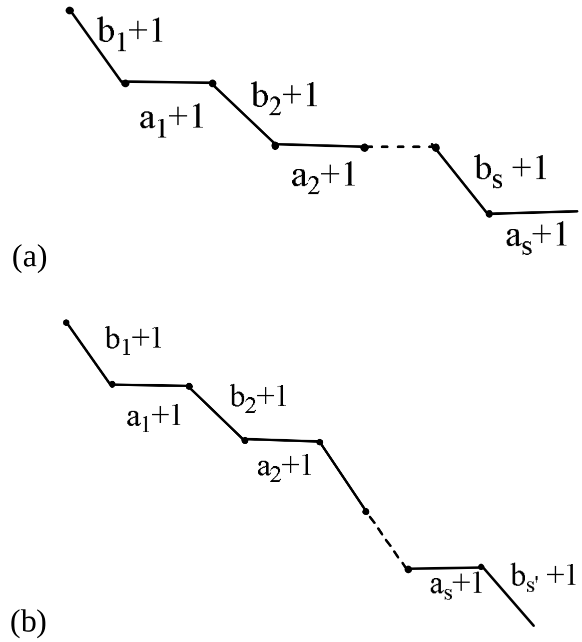

Figure 4. Dualist graph of a general non-branched cata–condensed benzenoids.

In Figure 4, $a_i \in$ $(i = 1,2,\dots s)$ and $b_i \in$ $(i = 1,2,\dots s')$ where $s' = s$ for Figure 4(a) and $s' = s + 1$ for Figure 4(b). $a_i + 1$ and $b_i + 1$ represent the numbers of linearly condensed six–membered rings horizontally and diagonally, respectively. For the benzenoid shown in Figure 4(a) and 4(b), the Peak–Valley matrix is as follows.

$$A_n = \begin{bmatrix} t_1 & 1 & 0 & & & \\ 1 & t_2 & 1 & & 0 & \\ 0 & 1 & t_3 & & & \\ & & & \ddots & 1 & 0 \\ & 0 & & 1 & t_{-1} & 1 \\ & & & 0 & 1 & t \end{bmatrix}$$

where $t_i = \begin{cases} b_{k+1} + 2, & if\ i = \sum_{j=0}^{k} a_j + 1 \\ 2, & if\ i \neq \sum_{j=0}^{k} a_j + 1 \end{cases}$, $k = 1,2,\dots,s;\ i = 1,2,\dots,$. Here is the number of peaks (or valleys) in a graph G. The Kekulé number of a graph G is shown by $K_n(G)(\ n = 1,\dots,\ )$.

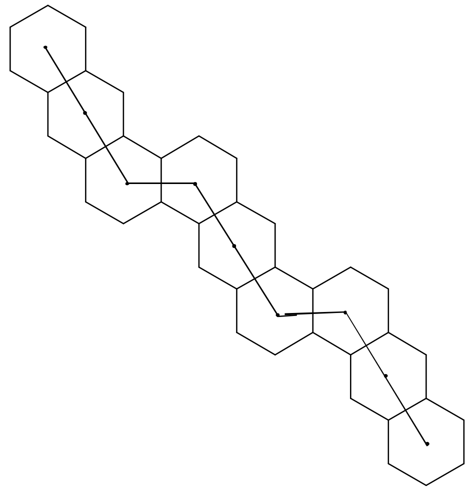

Figure 5. Simple binary regularly cata–condensed benzenoids.

Lemma 1. From Figure 5, the K–number of the graph G is calculated by the following tri–diagonal determinantal expression[9]:

$$K_{\mathrm{n}}(G) = detA_n = \begin{vmatrix} b+2 & 1 & 0 & & & \\ 1 & b+2 & 1 & & 0 & \\ 0 & 1 & b+2 & & & \\ & & & \ddots & 1 & 0 \\ & 0 & & 1 & b+2 & 1 \\ & & & 0 & 1 & b+2 \end{vmatrix}.$$

The order of the above determinant is $s+1$, where s is the repeat times of horizontal linear segments on the graph$G$.

4. CONTINUANTS AND CATERPILLAR TREES

Lemma 2. If H is a hexagonal chain whose LA–sequence is $L^{x_1}AL^{x_2}A \dots L^{x_{n-1}}AL^{x_n}$, then the number $K(H)$ of its Kekulé structures is equal to the Z–index of the caterpillar tree $C_n(x_1, x_2, \dots, x_n)$[7].

If it is written $C(H)$ for caterpillar tree of a H hexagonal chain, Lemma 2 is equivalent to the equality $K(H) = \mathrm{Z}(C(H))$.

Definition 3. The continuants (or continuant polynomials) are introduced by Euler [10] as $L_n(x_1, x_2, \dots, x_n) = x_n L_{n-1}(x_1, x_2, \dots, x_{n-1}) + L_{n-2}(x_1, x_2, \dots, x_{n-2})$ with initial conditions $L_0() = 1$, $L_1(x_1) = x_1$ and $L_2(x_1, x_2) = x_1 x_2 + 1$.

From this it is shown that the Z–index of the caterpillar trees coincides with Euler 's continuant like the following lemma.

Lemma 3. $Z\big(C_n(x_1, x_2, \dots, x_n)\big) = L_n(x_1, x_2, \dots, x_n)$[7].

5. MAIN RESULTS

Theorem 3. The coefficients of a $B_n(x)$ Morgan–Voyce polynomial are equal to the number of k–matchings ($m(G,k)$) of a path graph which has $N = 2n + 1$ points.

Proof. We denote the coefficients of Morgan–Voyce polynomials with

$$C\big(B_n(x)\big) = \binom{n+i+1}{n-i}$$

such that $0 \le i \le n$ and we take the point number of the path graph $N = 2n + 1$. The number of k–matchings of a path graph for $0 \le k \le \lfloor N/2 \rfloor$ is

$$m(G,k) = \binom{N-k}{k}$$

and $\lfloor N/2 \rfloor = \lfloor (2n+1)/2 \rfloor = n$ by the definition of the Hosoya index. Now we demonstrate the coefficients of the Morgan–Voyce polynomials in combinatorial form with respectively for $0 \le i \le n$

$$C\big(B_n(x)\big) = \binom{n+1}{n}, \binom{n+2}{n-1}, \dots, \binom{2n}{1}, \binom{2n+1}{0}$$

and $m(G,k) = \binom{N-k}{k}$ for $0 \le k \le \lfloor N/2 \rfloor = n$ with respectively

$$m(G,k) = \binom{2n+1}{0}, \binom{2n}{1}, \dots, \binom{n+2}{n-1}, \binom{n+1}{n}.$$

It is clear that $C\big(B_n(x)\big)$ and $m(G,k)$ are same in reverse order. From this we say for every n^{th} degree Morgan–Voyce polynomial there is a path graph (P_N) which has $N = 2n + 1$ points such that the coefficients of the Morgan–Voyce polynomials equal to the number of k–matchings of P_N.

Example 1. We show an application of the previous theorem for the first three Morgan–Voyce polynomials. For $B_0(x)$, $C\big(B_0(x)\big) = 1$ equals to $m(G,k)$ for $N = 2 \times 0 + 1 = 1$. For $B_1(x)$, $C\big(B_1(x)\big) = 1, 2$ equal to $m(G,k)$ for $N = 2 \times 1 + 1 = 3$. For $B_2(x)$,$C\big(B_2(x)\big) = 1, 4, 3$ equal to $m(G,k)$ for $N = 2 \times 2 + 1 = 5$.

Lemma 4. If $b_1 + 1 = b_2 + 1 = \cdots = b_s + 1 = b + 1$ (numbers of the regular hexagons on diagonal wise are same) like in Figure 5 and we take x instead of b_i, then (the right equation is used to express many properties of the Morgan–Voyce polynomials like in [8])

$$K_n(G) = detA_n = B_n(x).$$

Proof.

$$K_1(G) = \begin{vmatrix} x+2 \end{vmatrix} = x+2 = B_1(x)$$

$$K_2(G) = \begin{vmatrix} x+2 & 1 \\ 1 & x+2 \end{vmatrix} = (x+2)(x+2)-1 = x^2+4x+3 = B_2(x)$$

$$K_3(G) = \begin{vmatrix} x+2 & 1 & 0 \\ 1 & x+2 & 1 \\ 0 & 1 & x+2 \end{vmatrix} = x^3+6x^2+10x+4 = B_3(x)$$

and by the determinant of the tri–diagonal matrix in Lemma 1,

$$K_n(G) = B_n(x) = (x+2)B_{n-1}(x) - B_{n-2}(x).$$

In Lemma 1, the (n) indice on the notatin K_n is the number of the repetition of the diagonal hexagons. We also take the number of the hexagons $b_i + 1$ on diagonal wise like the previous lemma. For Figure 5, $b_1 + 1 = b_2 + 1 = \cdots = b_s + 1 = b + 1$ and its corresponding caterpillar tree is $C_{2n}(b+1, 1, b, 1, \ldots, b, 1)$.

There is a relation between the K–number of the hexagonal chain in Figure 5 and Z–index of its corresponding caterpillar tree as noted in the next theorem.

Theorem 4. $K_n(G) = Z\big(C_{2n}(G)\big)$.

Proof. Induct on n. For $n = 1$, $K_1(G) = Z\big(C_2(b+1, 1)\big) = b + 2$, as desired. We assume that the equality is true for $n \le k$ and we will show that it is true for $n = k + 1$. This means

$$K_{k+1}(G) = Z\big(C_{2k+2}(b+1, 1, b, 1, \ldots, b, 1)\big).$$

By assumption

$$K_k(G) = Z\big(C_{2k}(b+1, 1, b, 1, \ldots, b, 1)\big)$$

and

$$K_{k-1}(G) = Z\big(C_{2k-2}(b+1, 1, b, 1, \ldots, b, 1)\big).$$

By Lemma 1,

$$\begin{aligned} K_{k+1}(G) &= (b+2)K_k(G) - K_{k-1}(G) \\ &= (b+2)Z(C_{2k}(G)) - Z(C_{2k-2}(G)) \\ &= bZ(C_{2k}(G)) + 2[Z(C_{2k-1}(G)) + Z(C_{2k-2}(G))] - Z(C_{2k-2}(G)) \\ &= bZ(C_{2k}(G)) + Z(C_{2k-1}(G)) + Z(C_{2k-1}(G)) + Z(C_{2k-2}(G)) \\ &= Z(C_{2k+1}(G)) + Z(C_{2k}(G)) = Z(C_{2k+2}(G)) \end{aligned}$$

This complete the proof.

Example 2. We calculate the Kekulé number of simple binary regularly catacondensed benzenoid in Figure 5 by two ways mentioned in the Theorem 4. The matrix form of K–number of the chain shown in Figure 5 is

$$K_3(G) = \begin{bmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 4 \end{bmatrix}$$

and $K_3(G) = detA = 56$. Now we use the corresponding caterpillar tree of the hexagonal chain as the follows:

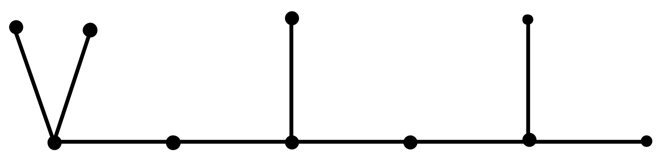

Figure 6. The hexagonal chain in Figure 5 has 9 hexagons and the corresponding caterpillar tree has 9 edges.

This caterpillar tree is denoted by $C_6(3,1,2,1,2,1)$ and $Z(C_6(3,1,2,1,2,1) = 56$. So that $K_3(G) = Z(C_6(3,1,2,1,2,1)$.

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