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. Furthermore, 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.

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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
mode $L_1$ 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 $A$ modes of hexagons is clear from Figure 2.

For instance, the $LA$–sequence of the benzenoid chain in Figure 1 is $LLLALLALLAALL$ 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 $〈x_1,x_2,...,x_n〉$ the class of isoarithmic benzenoid chains with the $LA$–sequence

$$L^{x_1}AL^{x_2}A...AL^{x_n}$$

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

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

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

$$K_n〈x_1,x_2,...,x_n〉 = (x_n + 1)K_{n-1}〈x_1,x_2,...,x_{n-1}〉 + K_{n-2}〈x_1,x_2,...,x_{n-2}〉.$$

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.

![Hexagonal Chain and Caterpillar Tree](image)

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

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Lemma 1. From Figure 5, the $K$–number of the graph $G$ is calculated by the following tri–diagonal determinantal expression\cite{9}:

$$
K_n(G) = det A_n = \begin{vmatrix}
    b + 2 & 1 & 0 \\
    1 & b + 2 & 1 \\
    0 & 1 & b + 2 \\
    \ddots & \ddots & \ddots \\
    0 & 1 & b + 2 \\
    0 & 1 & b + 2
\end{vmatrix}.
$$

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 $L^{x_1}AL^{x_2}A\ldots L^{x_{n-1}}AL^{x_n}$, then the number $K(H)$ of its Kekulé structures is equal to the $Z$–index of the caterpillar tree $C_n(x_1, x_2, \ldots, x_n)$\cite{7}.

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

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

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5}
\caption{Simple binary regularly cata–condensed benzenoids.}
\end{figure}
From this it is shown that the \( Z \)-index of the caterpillar trees coincides with Euler’s continuant like the following lemma.

**Lemma 3.** \( Z(C_n(x_1, x_2, \ldots, x_n)) = L_n(x_1, x_2, \ldots, x_n)[7] \).

### 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

\[
C(B_n(x)) = \binom{n + i + 1}{n - i}
\]

such that \( 0 \leq i \leq n \) and we take the point number of the path graph \( N = 2n + 1 \). The number of \( k \)-matchings of a path graph for \( 0 \leq k \leq \lfloor N/2 \rfloor \) 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 \( 0 \leq i \leq n \)

\[
C(B_n(x)) = \binom{n + 1}{n} \cdot \binom{n + 2}{n - 1} \cdot \cdots \cdot \binom{2n}{1} \cdot \binom{2n + 1}{0}
\]

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

\[
m(G, k) = \binom{2n + 1}{0} \cdot \binom{2n}{1} \cdot \cdots \cdot \binom{n + 2}{n - 1} \cdot \binom{n + 1}{n}
\]

It is clear that \( C(B_n(x)) \) 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 \( B_0(x) \), \( C(B_0(x)) = 1 \) equals to \( m(G, k) \) for \( N = 2 \times 0 + 1 = 1 \). For \( B_1(x) \), \( C(B_1(x)) = 1, 2 \) equal to \( m(G, k) \) for \( N = 2 \times 1 + 1 = 3 \). For \( B_2(x) \), \( C(B_2(x)) = 1, 4, 3 \) equal to \( m(G, k) \) for \( N = 2 \times 2 + 1 = 5 \).

**Lemma 4.** If \( b_1 + 1 = b_2 + 1 = \ldots = b_k + 1 = b + 1 \) (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])

\[ K_n(G) = \text{det}A_n = B_n(x). \]

**Proof.**

\[
\begin{align*}
K_1(G) &= |x + 2| = x + 2 = B_1(x) \\
K_2(G) &= \begin{vmatrix} x + 2 & 1 \\ 1 & x + 2 \end{vmatrix} = (x + 2)(x + 2) - 1 = x^2 + 4x + 3 = B_2(x) \\
K_3(G) &= \begin{vmatrix} 1 & x + 2 & 1 \\ 0 & 1 & x + 2 \end{vmatrix} = x^3 + 6x^2 + 10x + 4 = B_3(x)
\end{align*}
\]

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 notation \(K_n\) is the number of the repetition of the diagonal hexagons. We also take the number of the hexagons \(b_1 + 1\) 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.** \(K_n(G) = Z\left(C_{2n}(G)\right)\).

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

\[ K_{k+1}(G) = Z\left(C_{2k+2}(b + 1, 1, b, 1, \ldots, b, 1)\right). \]

By assumption

\[ K_k(G) = Z\left(C_{2k}(b + 1, 1, b, 1, \ldots, b, 1)\right) \]

and

\[ K_{k-1}(G) = Z\left(C_{2k-2}(b + 1, 1, b, 1, \ldots, b, 1)\right). \]

By Lemma 1,

\[
K_{k+1}(G) = (b + 2)K_k(G) - K_{k-1}(G) = (b + 2)Z(C_{2k}(G)) - Z(C_{2k-2}(G))
\]

\[
= bZ(C_{2k}(G)) + 2[Z(C_{2k-1}(G)) + Z(C_{2k-2}(G))] - Z(C_{2k-2}(G))
\]

\[
= bZ(C_{2k}(G)) + Z(C_{2k-1}(G)) + Z(C_{2k-1}(G)) + Z(C_{2k-2}(G))
\]

\[
= Z(C_{2k+1}(G)) + Z(C_{2k}(G)) = Z(C_{2k+2}(G))
\]

Therefore, \(K_n(G) = Z\left(C_{2n}(G)\right)\) for all \(n\).
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 $K_3(G) = \text{det} A = 56$. Now we use the corresponding caterpillar tree of the hexagonal chain as the follows:

![Figure 6](image)

**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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