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Extremal hexagonal chains concerning k-matchings and k-independent sets *

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Denote by $\mathcal{B}_n$ the set of the hexagonal chains with n hexagons. For any $B_n \in \mathcal{B}_n$, let $m_k(B_n)$ and $i_k(B_n)$ be the numbers of k-matchings and k-independent sets of B_n, respectively. In the paper, we show that for any hexagonal chain $B_n \in \mathcal{B}_n$ and for any $k \geqslant 0$, $m_k(L_n) \leqslant m_k(B_n) \leqslant m_k(Z_n)$ and $i_k(L_n) \geqslant i_k(B_n) \geqslant i_k(Z_n)$, with left equalities holding for all k only if $B_n = L_n$, and the right equalities holding for all k only if $B_n = Z_n$, where L_n and Z_n are the linear chain and the zig-zag chain, respectively. These generalize some related results known before.

KEY WORDS: hexagonal chain, graph, invariants, benzenoid hydrocarbons, k-matching, k-independent set

1. Introduction

Let $G = (V, E)$ be a graph with the vertex set $V(G)$ and the edge set $E(G)$. Let e and x be an edge and a vertex in G, respectively. We will denote by $G - e$ the graph obtained from G by removing edge e, and by $G - x$ the graph obtained from G by removing vertex x (and all its incident edges). Let S be a subset of $V(G)$. We denote by $G - S$ the graph obtained from G by removing all the vertices of S. Our standard reference for graph theoretical terminology is [1].

Two edges of a graph G are said to be independent if they are not incident. A subset M of $E(G)$ is called a matching of G if any two edges of M are independent in G. We denote by $m(G)$ the number of matchings of G. A matching M is called a k-matching if $|M| = k$. We denote by $m_k(G)$ the number of k-matchings of G. Obviously, $m(G) = \sum_k m_k(G)$.

Two vertices of a graph G are said to be independent if they are not adjacent. A subset I of $V(G)$ is called an independent set of G if any two vertices of I are independent in G. We denote by $i(G)$ the number of independent sets of G. An independent set I is

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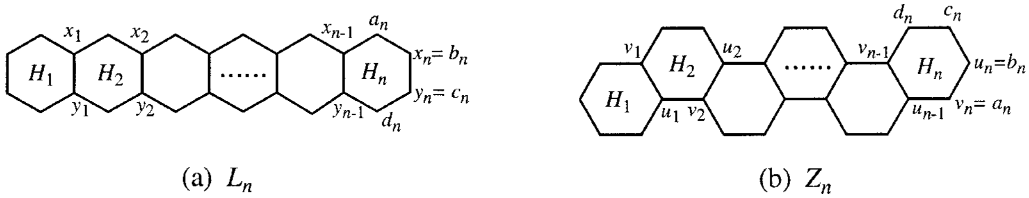

Figure 1.

said to be k-independent if $|I| = k$. We denote by $i_k(G)$ the number of k-independent sets of G. Obviously, $i(G) = \sum_k i_k(G)$.

It is well known that the two graph invariants $m(G)$ and $i(G)$ are important ones in structural chemistry. They are nowadays commonly called "the Hosoya index" and "the Merrifield–Simmons index", respectively.

A hexagonal system is regarded as a 2-connected plane graph in which every finite region is a regular hexagon of unit side length. Hexagonal systems are of great importance for theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons.

A hexagonal chain is a hexagonal system with the properties that (a) it has no vertex belonging to three hexagons, and (b) it has no hexagon adjacent to more than two hexagons. Hexagonal chains are the graph representations of an important subclass of benzenoid molecules, namely, of the so-called unbranched catacondensed benzenoids. The structure of those graphs is apparently the simplest among all hexagonal systems. A great deal of mathematical and mathematico-chemical results on hexagonal chains were obtained (see, for example, [2–4]).

We denote by $\mathcal{B}_n$ the set of the hexagonal chains with n hexagons. Let $B_n \in \mathcal{B}_n$. If the subgraph of B_n induced by the vertices with degree 3 is a matching with $n-1$ edges, then B_n is called a linear chain and denoted by L_n. If the subgraph of B_n induced by the vertices with degree 3 is a path, then B_n is called a zig-zag chain and denoted by Z_n. Figures 1(a) and (b) illustrate L_n and Z_n, respectively.

It is easy to see that $\mathcal{B}_1 = \{L_1\} = \{Z_1\}$, $\mathcal{B}_2 = \{L_2\} = \{Z_2\}$ and $\mathcal{B}_3 = \{L_3, Z_3\}$.

In 1993, Gutman discussed the extremal hexagonal chains with respect to some topological invariants. About the Hosoya index and the Merrifield–Simmons index, he obtained the following

Theorem 1 (Gutman [5]). For any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n$,

(a) $m(L_n) \leqslant m(B_n)$ with equality holding only if $B_n = L_n$,

(b) $i(L_n) \geqslant i(B_n)$ with equality holding only if $B_n = L_n$.

In [6], the first author of this paper obtained the following result, which is conjectured by Gutman in [5].

Theorem 2 (Zhang [6]). For any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n$,

(a) $m(B_n) \leqslant m(Z_n)$ with equality holding only if $B_n = Z_n$,

(b) $i(B_n) \geqslant i(Z_n)$ with equality holding only if $B_n = Z_n$.

In this paper, we refine this result as follows:

Theorem 3. For any $B_n \in \mathcal{B}_n$ and for each $k \geqslant 0$,

$$m_k(L_n) \leqslant m_k(B_n) \leqslant m_k(Z_n).$$

Moreover, the equality of the left-hand side (right-hand side, respectively) holds for each k only if $B_n = L_n$ ($B_n = Z_n$, respectively).

Theorem 4. For any $B_n \in \mathcal{B}_n$ and for each $k \geqslant 0$,

$$i_k(Z_n) \leqslant i_k(B_n) \leqslant i_k(L_n).$$

Moreover, the equality of the left-hand side (right-hand side, respectively) holds for each k only if $B_n = Z_n$ ($B_n = L_n$, respectively).

One can see that theorems 1 and 2 are immediate consequences of theorems 3 and 4, respectively.

In order to prove theorems 3 and 4, we consider the following two polynomials: Z-polynomial and Y-polynomial.

The Z-polynomial (called Z-counting polynomial) was defined by Hosoya [7] as

$$Z(G) = \sum_k m_k(G)x^k,$$

which is a special case of the matching polynomial defined by Farrell [8], and has essentially the same combinatorial contents as the matching polynomial.

According to independent sets, Y-polynomial is defined as

$$Y(G) = \sum_k i_k(G)x^k.$$

Let $f(x) = \sum_{k=0}^{n} a_k x^k$ and $g(x) = \sum_{k=0}^{n} b_k x^k$ be two polynomials of x. We say $f(x) \preceq g(x)$, if for each k, $0 \leqslant k \leqslant n$, $a_k \leqslant b_k$. We say $f(x) \prec g(x)$, if for each k, $0 \leqslant k \leqslant n$, $a_k \leqslant b_k$, and there exists some k such that $a_k < b_k$.

We will prove the following two theorems, which are equivalent to theorems 3 and 4, respectively.

Theorem 5. For any $n \geqslant 1$ and for any $B_n \in \mathcal{B}_n$,

(a) if $B_n \neq L_n$ then $Z(B_n) \succ Z(L_n)$, and

(b) if $B_n \neq Z_n$ then $Z(B_n) \prec Z(Z_n)$.

Theorem 6. For any $n \geqslant 1$ and for any $B_n \in \mathcal{B}_n$,

(a) if $B_n \neq L_n$ then $Y(B_n) \prec Y(L_n)$, and

(b) if $B_n \neq Z_n$ then $Y(B_n) \succ Y(Z_n)$.

Obviously, theorems 5 and 6 hold for $n = 1, 2$. Thus, we suppose that $n \geqslant 3$ below.

2. Some preliminaries

Among the many properties of $Z(G)$ and $Y(G)$ ([7–10] etc.) we mention the following results which will be useful to the material which follows.

Claim 1. Let G be a graph consisting of two components G_1 and G_2. Then

(a) $Z(G) = Z(G_1)Z(G_2)$,

(b) $Y(G) = Y(G_1)Y(G_2)$.

Claim 2.

(a) Let uv be an edge of G. Then $Z(G) = Z(G - uv) + xZ(G - u - v)$.

(b) Let u be a vertex of G and N_u be the subset of $V(G)$ containing the vertex u and its neighbors. Then $Y(G) = Y(G - u) + xY(G - N_u)$.

Claim 3. For each $uv \in E(G)$:

(a) $Z(G) - Z(G - u) - xZ(G - u - v) \succeq 0$,

(b) $Y(G) - Y(G - u) - xY(G - u - v) \preceq 0$.

Moreover, the equalities of (a) and (b) hold only if v is the unique neighbor of u.

Any element B_n of $\mathcal{B}_n$ can be obtained from an appropriately chosen graph $B_{n-1} \in \mathcal{B}_{n-1}$ by attaching to it a new hexagon H (figure 2).

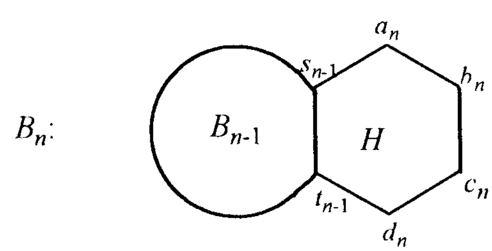

Figure 2.

3. The proof of theorem 5

In this section, we will use the notation G for $Z(G)$, when it would lead to no confusion.

Referring to figure 2, by claims 1(a) and 2(a) we have

$$\begin{aligned} B_n = {} & \big(1+3x+x^2\big)B_{n-1} + \big(x+2x^2\big)\big\{(B_{n-1}-s_{n-1}) + (B_{n-1}-t_{n-1})\big\} \\ & + \big(x^2+x^3\big)(B_{n-1}-s_{n-1}-t_{n-1}), \end{aligned} \tag{1}$$

$$B_n - s = \begin{cases} (1+2x)B_{n-1} + \big(x+x^2\big)(B_{n-1}-t_{n-1}), & \text{if } s = a_n, \\ (1+x)B_{n-1} + x(B_{n-1}-t_{n-1}) & \\ \quad + \big(x+x^2\big)(B_{n-1}-s_{n-1}) + x^2(B_{n-1}-s_{n-1}-t_{n-1}), & \text{if } s = b_n, \\ (1+x)B_{n-1} + \big(x+x^2\big)(B_{n-1}-t_{n-1}) & \\ \quad + x(B_{n-1}-s_{n-1}) + x^2(B_{n-1}-s_{n-1}-t_{n-1}), & \text{if } s = c_n, \\ (1+2x)B_{n-1} + \big(x+x^2\big)(B_{n-1}-s_{n-1}), & \text{if } s = d_n \end{cases} \tag{2}$$

and

$$B_n - s - t = \begin{cases} (1+x)B_{n-1} + x(B_{n-1}-t_{n-1}), & \text{if } s = a_n, t = b_n, \\ B_{n-1} + x(B_{n-1}-t_{n-1}) + x(B_{n-1}-s_{n-1}) & \\ \quad + x^2(B_{n-1}-s_{n-1}-t_{n-1}), & \text{if } s = b_n, t = c_n, \\ (1+x)B_{n-1} + x(B_{n-1}-s_{n-1}), & \text{if } s = c_n, t = d_n. \end{cases} \tag{3}$$

According to formulas (2), (3) and claim 3(a), it follows that:

Lemma 1. For any $B_n \in \mathcal{B}_n$ $(n \geqslant 2)$ (see figure 2), we have

(a) $B_n - b_n \prec B_n - d_n$ and $B_n - c_n \prec B_n - a_n$,

(b) $B_n - b_n - c_n \prec B_n - a_n - b_n$ and $B_n - b_n - c_n \prec B_n - c_n - d_n$,

(c) $(B_n - b_n) + (B_n - c_n) \prec (B_n - a_n) + (B_n - b_n)$ and $(B_n - b_n) + (B_n - c_n) \prec (B_n - c_n) + (B_n - d_n)$.

By lemma 1, we get

Lemma 2. Let L_n $(n \geqslant 2)$ be a linear chain (see figure 1(a)). Then

(a) $L_n - x_n = L_n - y_n \prec L_n - a_n = L_n - d_n$,

(b) $L_n - x_n - y_n \prec L_n - a_n - x_n = L_n - y_n - d_n$,

(c) $(L_n - x_n) + (L_n - y_n) \prec (L_n - a_n) + (L_n - x_n) = (L_n - y_n) + (L_n - d_n)$.

Lemma 3. Let Z_n $(n \geqslant 3)$ be a zig-zag chain (see figure 1(b)). Then

(a) $Z_n - u_n \prec Z_n - c_n \prec Z_n - v_n$ and $Z_n - u_n \prec Z_n - d_n \prec Z_n - v_n$,

(b) $Z_n - u_n - c_n \prec Z_n - c_n - d_n \prec Z_n - u_n - v_n$,

(c) $(Z_n - u_n) + (Z_n - c_n) \prec (Z_n - c_n) + (Z_n - d_n) \prec (Z_n - u_n) + (Z_n - v_n)$.

Proof. We show the following two facts.

Fact 1. For any $B_n \in \mathcal{B}_n$ $(n \geqslant 3)$, if $B_{n-1} - s_{n-1} \prec B_{n-1} - t_{n-1}$ then

(a) $B_n - b_n \prec B_n - c_n \prec B_n - a_n$ and $B_n - b_n \prec B_n - d_n \prec B_n - a_n$,

(b) $B_n - b_n - c_n \prec B_n - c_n - d_n \prec B_n - a_n - b_n$,

(c) $(B_n - b_n) + (B_n - c_n) \prec (B_n - c_n) + (B_n - d_n) \prec (B_n - a_n) + (B_n - b_n)$.

Proof of fact 1. By (2) and (3), it is easy to see the following:

$$(B_n - a_n) - (B_n - d_n) = \left(x + x^2\right)\left\{(B_{n-1} - t_{n-1}) - (B_{n-1} - s_{n-1})\right\},$$
$$(B_n - c_n) - (B_n - b_n) = x^2\left\{(B_{n-1} - t_{n-1}) - (B_{n-1} - s_{n-1})\right\},$$
$$(B_n - a_n - b_n) - (B_n - c_n - d_n) = x\left\{(B_{n-1} - t_{n-1}) - (B_{n-1} - s_{n-1})\right\}$$

and

$$\left\{(B_n - a_n) + (B_n - b_n)\right\} - \left\{(B_n - c_n) + (B_n - d_n)\right\} = x\left\{(B_{n-1} - t_{n-1}) - (B_{n-1} - s_{n-1})\right\}.$$

By the hypothesis $B_{n-1} - s_{n-1} \prec B_{n-1} - t_{n-1}$ we get $(B_n - d_n) \prec (B_n - a_n)$, $(B_n - b_n) \prec (B_n - c_n)$, $(B_n - c_n - d_n) \prec (B_n - a_n - b_n)$ and $(B_n - c_n) + (B_n - d_n) \prec (B_n - a_n) + (B_n - b_n)$. Thus, fact 1 follows by lemma 1. This completes the proof of fact 1. □

Fact 2. Let Z_n be a zig-zag chain (see figure 1(b)). Then

$$Z_1 - u_1 = Z_1 - v_1 \quad \text{and} \quad Z_i - u_i \prec Z_i - v_i, \quad 2 \leqslant i \leqslant n.$$

Proof of fact 2. Obviously, $Z_1 - u_1 = Z_1 - v_1$. For $2 \leqslant i \leqslant n$, we have by (2)

$$(Z_i - v_i) - (Z_i - u_i) = x\left\{Z_{i-1} - (Z_{i-1} - u_{i-1}) - x(Z_{i-1} - u_{i-1} - v_{i-1})\right\} + x^2\left\{(Z_{i-1} - v_{i-1}) - (Z_{i-1} - u_{i-1})\right\}.$$

Thus, by claim 3(a), if $Z_{i-1} - u_{i-1} \preceq Z_{i-1} - v_{i-1}$ then $Z_i - u_i \prec Z_i - v_i$. Hence, by induction we can show for each $2 \leqslant i \leqslant n$, $Z_i - u_i \prec Z_i - v_i$. This completes the proof of fact 2. □

From facts 1 and 2 we get lemma 3 immediately. □

In order to use induction to prove theorem 5, we will prove the following result which contains more contents than that of theorem 5.

Theorem 7. For any hexagonal chain $B_n \in \mathcal{B}_n$ $(n \geqslant 3)$,

(a) $L_n - x_n \preceq B_n - s \preceq Z_n - v_n$, where $s \in \{a_n, b_n, c_n, d_n\}$,

(b) $L_n - x_n - y_n \preceq B_n - s - t \preceq Z_n - u_n - v_n$, where $st \in \{a_n b_n, b_n c_n, c_n d_n\}$,

(c) $(L_n - x_n) + (L_n - y_n) \preceq (B_n - s) + (B_n - t) \preceq (Z_n - u_n) + (Z_n - v_n)$, where $st \in \{a_n b_n, b_n c_n, c_n d_n\}$,

(d) $L_n \preceq B_n \preceq Z_n$.

Moreover, the equalities of the left-hand side of (a)–(d) hold only if $B_n = L_n$ and $\{s, t\} = \{x_n, y_n\}$; and the equalities of the right-hand side of (a)–(d) hold only if $B_n = Z_n$ and $\{s, t\} = \{u_n, v_n\}$.

Proof of theorem 7. First we note that if $B_n = L_n$ then the left-hand side parts of (a)–(d) hold by lemma 2; and if $B_n = Z_n$ then the right-hand side parts of (a)–(d) hold by lemma 3. Consequently, when we prove the left-hand side parts we may assume that $B_n \neq L_n$. Similarly, when we prove the right-hand side parts we may assume that $B_n \neq Z_n$.

We prove theorem 7 by induction.

(i) First we consider the case $n = 3$. In this case, $\mathcal{B}_3 = \{L_3, Z_3\}$.

(a) We show that $L_3 - x_3 \prec Z_3 - s$, where $s \in \{v_3, u_3, c_3, d_3\}$. By lemma 3(a), it suffices to show that $L_3 - x_3 \prec Z_3 - u_3$. By (2) we have

$$\begin{aligned} L_3 - x_3 &= (1+x)L_2 + x(L_2 - y_2) + \left(x + x^2\right)(L_2 - x_2) + x^2(L_2 - x_2 - y_2), \\ Z_3 - u_3 &= (1+x)Z_2 + x(Z_2 - v_2) + \left(x + x^2\right)(Z_2 - u_2) + x^2(Z_2 - u_2 - v_2) \\ &= (1+x)L_2 + x(L_2 - a_2) + \left(x + x^2\right)(L_2 - x_2) + x^2(L_2 - x_2 - a_2). \end{aligned}$$

By lemma 2(a) we get $L_2 - y_2 \prec L_2 - a_2$ and $L_2 - x_2 - y_2 \prec L_2 - x_2 - a_2$. Thus, $L_3 - x_3 \prec Z_3 - u_3$.

Similarly, we can show that $L_3 - s \prec Z_3 - v_3$, where $s \in \{a_3, x_3, y_3, d_3\}$.

(b) We show that $L_3 - x_3 - y_3 \prec Z_3 - s - t$, where $st \in \{v_3 u_3, u_3 c_3, c_3 d_3\}$. By lemma 3(b) it suffices to show that $L_3 - x_3 - y_3 \prec Z_3 - u_3 - c_3$.

By (3) we have

$$\begin{aligned} L_3 - x_3 - y_3 &= L_2 + x(L_2 - x_2) + x(L_2 - y_2) + x^2(L_2 - x_2 - y_2), \\ Z_3 - u_3 - c_3 &= Z_2 + x(Z_2 - v_2) + x(Z_2 - u_2) + x^2(Z_2 - u_2 - v_2) \\ &= L_2 + x(L_2 - a_2) + x(L_2 - x_2) + x^2(L_2 - a_2 - x_2). \end{aligned}$$

Thus, by lemma 2(a) we have $L_3 - x_3 - y_3 \prec Z_3 - u_3 - c_3$.

Similarly, we can show that $L_3 - s - t \prec Z_3 - u_3 - v_3$, where $st \in \{a_3 x_3, x_3 y_3, y_3 d_3\}$.

(c) By (a) we have that $(L_3 - x_3) \prec (Z_3 - u_3)$ and $(L_3 - y_3) \prec (Z_3 - c_3)$. Thus, we get that $(L_3 - x_3) + (L_3 - y_3) \prec (Z_3 - u_3) + (Z_3 - c_3)$. By lemma 3(c) we get that $(L_3 - x_3) + (L_3 - y_3) \prec (Z_3 - s) + (Z_3 - t)$, where $st \in \{v_3 u_3, u_3 c_3, c_3 d_3\}$.

Similarly, we can prove that $(L_3 - s) + (L_3 - t) \prec (Z_3 - u_3) + (Z_3 - v_3)$, where $st \in \{a_3 x_3, x_3 y_3, y_3 d_3\}$.

(d) Now we show that $L_3 \prec Z_3$. By (1), we get

$$\begin{aligned} L_3 &= \left(1+3x+x^2\right)L_2 + \left(x+2x^2\right)\left\{(L_2-x_2)+(L_2-y_2)\right\} \\ &\quad + \left(x^2+x^3\right)(L_2-x_2-y_2), \\ Z_3 &= \left(1+3x+x^2\right)Z_2 + \left(x+2x^2\right)\left\{(Z_2-v_2)+(Z_2-u_2)\right\} \\ &\quad + \left(x^2+x^3\right)(Z_2-y_2-v_2), \\ &= \left(1+3x+x^2\right)L_2 + \left(x+2x^2\right)\left\{(L_2-a_2)+(L_2-x_2)\right\} \\ &\quad + \left(x^2+x^3\right)(L_2-x_2-a_2). \end{aligned}$$

By lemma 2 we get that $L_3 \prec Z_3$.

Therefore, theorem 7 holds for $n = 3$.

(ii) Suppose the theorem true for all hexagonal chains with fewer than n hexagons. Let B_n be a hexagonal chain with $n \geqslant 4$ hexagons, which is obtained from $B_{n-1} \in \mathcal{B}_{n-1}$ by attaching to it a new hexagon H (figure 2).

(a) We show that if $B_n \neq L_n$ then $L_n - x_n \prec B_n - s$, where $s \in \{a_n, b_n, c_n, d_n\}$. By lemma 1(a), it suffices to show that $L_n - x_n \prec B_n - b_n$ and $L_n - x_n \prec B_n - c_n$. By (2), we have

$$\begin{aligned} L_n - x_n &= (1+x)L_{n-1} + x(L_{n-1}-y_{n-1}) + \left(x+x^2\right)(L_{n-1}-x_{n-1}) \\ &\quad + x^2(L_{n-1}-x_{n-1}-y_{n-1}), \\ B_n - b_n &= (1+x)B_{n-1} + x(B_{n-1}-t_{n-1}) + \left(x+x^2\right)(B_{n-1}-s_{n-1}) \\ &\quad + x^2(B_{n-1}-s_{n-1}-t_{n-1}). \end{aligned}$$

By the inductive hypotheses we have $L_{n-1} \preceq B_{n-1}$, $L_{n-1} - y_{n-1} \preceq B_{n-1} - t_{n-1}$, $L_{n-1} - x_{n-1} \preceq B_{n-1} - s_{n-1}$ and $L_{n-1} - x_{n-1} - y_{n-1} \preceq B_{n-1} - s_{n-1} - t_{n-1}$. Since $B_n \neq L_n$, either $B_{n-1} \neq L_{n-1}$ or $\{s_{n-1}, t_{n-1}\} \neq \{x_{n-1}, y_{n-1}\}$, and hence, at least one of the four inequalities is strict. Therefore, we get that $L_n - x_n \prec B_n - b_n$. Similarly, we can show that $L_n - x_n \prec B_n - c_n$.

Similarly, we can show that if $B_n \neq Z_n$ then $B_n - s \prec Z_n - v_n$, where $s \in \{a_n, b_n, c_n, d_n\}$.

(b) We show that if $B_n \neq L_n$, then $L_n - x_n - y_n \prec B_n - s - t$, where $st \in \{a_n b_n, b_n c_n, c_n d_n\}$. By lemma 1(b), it suffices to show that $L_n - x_n - y_n \prec B_n - b_n - c_n$. By (3), we have

$$\begin{aligned} L_n - x_n - y_n &= L_{n-1} + x(L_{n-1}-y_{n-1}) + x(L_{n-1}-x_{n-1}) \\ &\quad + x^2(L_{n-1}-x_{n-1}-y_{n-1}), \\ B_n - b_n - c_n &= B_{n-1} + x(B_{n-1}-t_{n-1}) + x(B_{n-1}-s_{n-1}) \\ &\quad + x^2(B_{n-1}-s_{n-1}-t_{n-1}). \end{aligned}$$

By the inductive hypotheses $L_{n-1} \preceq B_{n-1}$, $L_{n-1} - y_{n-1} \preceq B_{n-1} - t_{n-1}$, $L_{n-1} - x_{n-1} \preceq B_{n-1} - s_{n-1}$ and $L_{n-1} - x_{n-1} - y_{n-1} \preceq B_{n-1} - s_{n-1} - t_{n-1}$. Since $B_n \neq L_n$, either $B_{n-1} \neq L_{n-1}$ or $\{s_{n-1}, t_{n-1}\} \neq \{x_{n-1}, y_{n-1}\}$, and hence, at least one of the four inequalities is strict. Therefore, we get that $L_n - x_n - y_n \prec B_n - b_n - c_n$.

Similarly, we can show that if $B_n \neq Z_n$, then $B_n - s - t \prec Z_n - v_n - u_n$, where $st \in \{a_n b_n, b_n c_n, c_n d_n\}$.

(c) By (a) we have that $(L_n - x_n) \prec (B_n - b_n)$ and $(L_n - y_n) \prec (B_n - c_n)$. Thus, we get that $(L_n - x_n) + (L_n - y_n) \prec (B_n - b_n) + (B_n - c_n)$. By lemma 1(c), we get that if $B_n \neq L_n$ then $(L_n - x_n) + (L_n - y_n) \prec (B_n - s) + (B_n - t)$, where $st \in \{a_n b_n, b_n c_n, c_n d_n\}$.

We show that if $B_n \neq Z_n$ then $(B_n - s) + (B_n - t) \prec (Z_n - u_n) + (Z_n - v_n)$, where $st \in \{a_n b_n, b_n c_n, c_n d_n\}$. By lemma 1(c), it suffices to show that $(B_n - a_n) + (B_n - b_n) \prec (Z_n - u_n) + (Z_n - v_n)$ and $(B_n - c_n) + (B_n - d_n) \prec (Z_n - u_n) + (Z_n - v_n)$.

By (2), we have

$$\begin{aligned}(B_n - a_n) + (B_n - b_n) &= (2 + 3x)B_{n-1} + \left(x + x^2\right)\left\{(B_{n-1} - s_{n-1}) + (B_{n-1} - t_{n-1})\right\}\\ &\quad + x(B_{n-1} - t_{n-1}) + x^2(B_{n-1} - s_{n-1} - t_{n-1}),\\ (Z_n - u_n) + (Z_n - v_n) &= (2 + 3x)Z_{n-1} + \left(x + x^2\right)\left\{(Z_{n-1} - u_{n-1}) + (Z_{n-1} - v_{n-1})\right\}\\ &\quad + x(Z_{n-1} - v_{n-1}) + x^2(Z_{n-1} - u_{n-1} - v_{n-1}).\end{aligned}$$

By the inductive hypotheses we have $B_{n-1} \preceq Z_{n-1}$, $(B_{n-1} - t_{n-1}) \preceq (Z_{n-1} - v_{n-1})$, $(B_{n-1} - s_{n-1}) + (B_{n-1} - t_{n-1}) \preceq (Z_{n-1} - u_{n-1}) + (Z_{n-1} - v_{n-1})$ and $B_{n-1} - s_{n-1} - t_{n-1} \preceq Z_{n-1} - u_{n-1} - v_{n-1}$. Since $B_n \neq Z_n$, either $B_{n-1} \neq Z_{n-1}$ or $\{s_{n-1}, t_{n-1}\} \neq \{u_{n-1}, v_{n-1}\}$, and hence, at least one of the four inequalities is strict. Therefore, we get that $(B_n - a_n) + (B_n - b_n) \prec (Z_n - u_n) + (Z_n - v_n)$. Similarly, we can prove that $(B_n - c_n) + (B_n - d_n) \prec (Z_n - u_n) + (Z_n - v_n)$.

(d) We show that if $B_n \neq L_n$, then $L_n \prec B_n$. By (1), we get

$$\begin{aligned}L_n &= \left(1 + 3x + x^2\right)L_{n-1} + \left(x + 2x^2\right)\left\{(L_{n-1} - x_{n-1}) + (L_{n-1} - y_{n-1})\right\}\\ &\quad + \left(x^2 + x^3\right)(L_{n-1} - x_{n-1} - y_{n-1}),\\ B_n &= \left(1 + 3x + x^2\right)B_{n-1} + \left(x + 2x^2\right)\left\{(B_{n-1} - s_t) + (B_{n-1} - t_{n-1})\right\}\\ &\quad + \left(x^2 + x^3\right)(B_{n-1} - s_{n-1} - t_{n-1}).\end{aligned}$$

By the inductive hypotheses we have $L_{n-1} \preceq B_{n-1}$, $(L_{n-1} - x_{n-1}) + (L_{n-1} - y_{n-1}) \preceq (B_{n-1} - s_{n-1}) + (B_{n-1} - t_{n-1})$ and $L_{n-1} - x_{n-1} - y_{n-1} \preceq B_{n-1} - s_{n-1} - t_{n-1}$. Since $B_n \neq L_n$, either $B_{n-1} \neq L_{n-1}$ or $\{s_{n-1}, t_{n-1}\} \neq \{x_{n-1}, y_{n-1}\}$, and hence, at least one of the three inequalities is strict. Therefore, we get that $L_n \prec B_n$.

Similarly we can show that if $B_n \neq Z_n$, then $B_n \prec Z_n$.

The proof of theorem 7 is complete. □

4. The proof of theorem 6

In this section, we will use the notation G for $Y(G)$, when it would lead to no confusion.

The Y-polynomial and Z-polynomial conform to similar, but not identical recurrence relations. Our proof of theorem 6 follows a similar pattern of reasoning as the proof of theorem 5, and will be outlined in an abbreviated form.

Referring to figure 2, by claims 1(b) and 2(b) we have

$$\begin{aligned} B_n = {} & (1+2x)B_{n-1} + \big(x+x^2\big)\big\{(B_{n-1}-s_{n-1})+(B_{n-1}-t_{n-1})\big\} \\ & + x^2(B_{n-1}-s_{n-1}-t_{n-1}), \end{aligned} \tag{1'}$$

$$B_n - s = \begin{cases} (1+2x)B_{n-1} + \big(x+x^2\big)(B_{n-1}-t_{n-1}), & \text{if } s = a_n, \\ (1+x)B_{n-1} + x(B_{n-1}-t_{n-1}) & \\ \quad + \big(x+x^2\big)(B_{n-1}-s_{n-1}) + x^2(B_{n-1}-s_{n-1}-t_{n-1}), & \text{if } s = b_n, \\ (1+x)B_{n-1} + \big(x+x^2\big)(B_{n-1}-t_{n-1}) & \\ \quad + x(B_{n-1}-s_{n-1}) + x^2(B_{n-1}-s_{n-1}-t_{n-1}), & \text{if } s = c_n, \\ (1+2x)B_{n-1} + \big(x+x^2\big)(B_{n-1}-s_{n-1}), & \text{if } s = d_n \end{cases} \tag{2'}$$

and

$$B_n - s - t = \begin{cases} (1+x)B_{n-1} + x(B_{n-1}-t_{n-1}), & \text{if } s = a_n, t = b_n, \\ B_{n-1} + x(B_{n-1}-t_{n-1}) + x(B_{n-1}-s_{n-1}) & \\ \quad + x^2(B_{n-1}-s_{n-1}-t_{n-1}), & \text{if } s = b_n, t = c_n, \\ (1+x)B_{n-1} + x(B_{n-1}-s_{n-1}), & \text{if } s = c_n, t = d_n. \end{cases} \tag{3'}$$

According to formulas (2′), (3′) and claim 3(b), it follows that

Lemma 1′. For any $B_n \in \mathcal{B}_n$ $(n \geqslant 2)$ (see figure 2), we have

(a) $B_n - b_n \succ B_n - d_n$ and $B_n - c_n \succ B_n - a_n$,

(b) $B_n - b_n - c_n \succ B_n - a_n - b_n$ and $B_n - b_n - c_n \succ B_n - c_n - d_n$,

(c) $(B_n - b_n) + (B_n - c_n) \succ (B_n - a_n) + (B_n - b_n)$ and $(B_n - b_n) + (B_n - c_n) \succ (B_n - c_n) + (B_n - d_n)$.

By lemma 1′, we get

Lemma 2′. Let L_n $(n \geqslant 2)$ be a linear chain (see figure 1(a)). Then

(a) $L_n - x_n = L_n - y_n \succ L_n - a_n = L_n - d_n$,

(b) $L_n - x_n - y_n \succ L_n - a_n - x_n = L_n - y_n - d_n$,

(c) $(L_n - x_n) + (L_n - y_n) \succ (L_n - a_n) + (L_n - x_n)$ and $(L_n - x_n) + (L_n - y_n) \succ (L_n - y_n) + (L_n - d_n)$.

Similarly to the proof of lemma 3, we can get

Lemma 3′. Let Z_n $(n \geqslant 3)$ be a zig-zag chain (see figure 1(b)). Then

(a) $Z_n - u_n \succ Z_n - c_n \succ Z_n - v_n$ and $Z_n - u_n \succ Z_n - d_n \succ Z_n - v_n$,

(b) $Z_n - u_n - c_n \succ Z_n - c_n - d_n \succ Z_n - u_n - v_n$,

(c) $(Z_n - u_n) + (Z_n - c_n) \succ (Z_n - c_n) + (Z_n - d_n) \succ (Z_n - u_n) + (Z_n - v_n)$.

In order to use induction to prove theorem 6, we will prove the following result which contains more contents than that of theorem 6.

Theorem 8. For any hexagonal chain $B_n \in \mathcal{B}_n$ $(n \geqslant 3)$,

(a) $L_n - x_n \succeq B_n - s \succeq Z_n - v_n$, where $s \in \{a_n, b_n, c_n, d_n\}$,

(b) $L_n - x_n - y_n \succeq B_n - s - t \succeq Z_n - u_n - v_n$, where $st \in \{a_nb_n, b_nc_n, c_nd_n\}$,

(c) $(L_n - x_n) + (L_n - y_n) \succeq (B_n - s) + (B_n - t) \succeq (Z_n - u_n) + (Z_n - v_n)$, where $st \in \{a_nb_n, b_nc_n, c_nd_n\}$,

(d) $L_n \succeq B_n \succeq Z_n$.

Moreover, the equalities of the left-hand side of (a)–(d) hold only if $B_n = L_n$ and $\{s, t\} = \{x_n, y_n\}$; and the equalities of the right-hand side of (a)–(d) hold only if $B_n = Z_n$ and $\{s, t\} = \{u_n, v_n\}$.

Proof of theorem 8. Using lemmas 1′, 2′ and 3′, theorem 8 can be proved in a fully similar manner to the proof of theorem 7. □

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