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Extremal polygonal chains on k-matchings *

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ABSTRACT: "k-matching" of a graph G is a set of k independent edges of G. The sum of k-matching of G is nowadays commonly called the Hosoya index. Denote by An the set of h-polygonal chains with n congruent regular h-polygons (h greater than 4). In this paper, we determine the the extremal polygon chains on k-matchings in the set of molecular graphs An. Thus we extend the main results (for h = 6) of [9], [10], and [11] to a more general case.

1 Introduction

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

A matching of G is a subset $M \subseteq E(G)$ in which any two edges are not incident. A matching M is called a k-matching if $|M| = k$. We denote by $m(G)$ the number of matchings of G, and denote by $m_k(G)$ the number of k-matchings of G. It is obvious that $m(G) = \sum_{k\geq 0} m_k(G)$. The graph invariant $m(G)$ introduced by Hosoya [2] is nowadays

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commonly called the Hosoya index. It is important in structural chemistry and it has been extensively studied (the details see [3] chapter 11 and references cited therein and the recent publications [4-7]).

A polygonal chain is a 2-connected simple graph G obtained by identifying a finite number of congruent regular polygons (called basic polygons) one by one such that each vertex of G has degree 2 or 3 and each basic polygon, except the first one and the last one, is adjacent to exactly two basic polygons. In other words, a polygonal chain is obtained by adding some chords to a closed polygonal curve C in the 3-dimensional Euclidean space so that C is divided into congruent regular polygons. We note that a polygonal chain may be geomitrically non-planar. A polygonal chain is called an h-polygonal chain if its basic polygons are h-polygons.

For $h \geq 6$, we denote by $\mathcal{A}_n$ the set of h-polygonal chains with n basic polygons (for example, when $h = 7$, $\mathcal{A}_2$ denote heptalene and $\mathcal{A}_3$ denote heptaphen respectively; when $h = 8$, $\mathcal{A}_2$ denote octalene and $\mathcal{A}_3$ denote octaphen respectively). For $A_n \in \mathcal{A}_n$, let H be the subgraph of A_n induced by the vertices of degree 3. A polygonal chain A_n is called a chain of type one and denoted as Z_n^1 if H is a path. A_n is called a chain of type two and denoted as Z_n^2 if it satisfies the following two conditions: (1) H is an $n-1$-matching; and (2) each basic polygon C_i of A_n, except the first and the last, has exactly two distinct edges in H, in which the first one is shared with C_{i-1} and the last one is shared with C_{i+1}. And from the first one to the last one have clockwise distance 2 (i.e., they are connected through a clockwise path with two edges not in H.)

Illustrative examples for Z_n^1 and Z_n^2 are shown in Figures 1 (a) and 1 (b), where $h = 8$. It is easy to see that for hexagonal chains, Z_n^1 are exactly the zig-zag chains (see Figure 2 (b)) and Z_n^2 are exactly the linear chains (see Figure 2 (a)). Note that $\mathcal{A}_1 = \{Z_1^1\} = \{Z_1^2\}$ and $\mathcal{A}_2 = \{Z_2^1\} = \{Z_2^2\}$ (when $h = 8$, the molecule have been considered by chemist [8]).

In 1993, Gutman discussed the extremal hexagonal chains with respect to three topological invariants : Hosoya index, largest eigenvalue and Merrified-Simmons index. His work greatly stimulated the study of extremal polygonal chains with respective to different types of topological invariants. On the Hosoya index, he obtained the following

Theorem 1.1 (Gutman [9]) For any $n \geq 1$ and any hexagonal chain $A_n \in \mathcal{A}_n, m(L_n) \leq m(A_n)$ with equality holding only if $A_n = L_n$, where $m(L_n)$ is the number of matchings of L_n and L_n denote the linear chain (see Figure 2 (a)).

In [10], L. Zhang proved the following result, which is conjectured by Gutman in [9].

Theorem 1.2 (Zhang [10]) For any $n \geq 1$ and any hexagonal chain $A_n \in \mathcal{A}_n, m(A_n) \leq m(Z_n)$ with equality holding only if $A_n = Z_n$, where Z_n denotes the zig-zag chain (see Figure

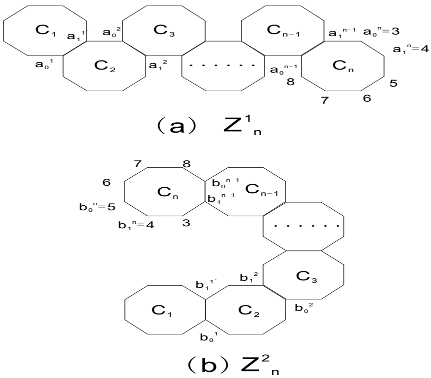


Fig 1: Chains of type one and type two

2 (b)).

In [11], L. Zhang and one of the present authors determined the extremal hexagonal chains with respect to k-matchings

Theorem 1.3 For any $n \geq 1$ and any hexagonal chain $A_n \in \mathcal{A}_n$,

$$m_k(L_n) \leq m_k(A_n) \leq m_k(Z_n).$$

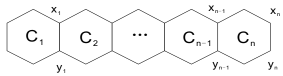
Moreover, the equalities on the left side holds for all k only if $A_n = L_n$; and the equalities on the right side hold for all k only if $A_n = Z_n$, where L_n and Z_n denote the linear chain and the zig-zag chain, respectively. (See Figures 2 (a) and 2 (b))

Clearly, Theorem 1.3 implies Theorem 1.1 and Theorem 1.2.

In [12, 13], Zhang , Wang and Li determined the extremal hexagonal chains concerning the total π-electron energy, which are similar to the extremal chains in [9-11] (see Figure 2).

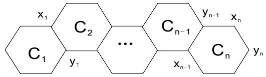
In [14], J. Rada and A. Tineo considered the polygonal chains and showed that among all polygonal chains with polygons of $4n-2$ vertices ($n \geq 2$), the linear polygonal chain has minimal energy. In their paper, they gave an example to show that the above result does not hold for octagonal chains. Such an example was also found for polyomino chains in [15]. These results show that we can not unify the solution of extreme h-polygonal chain problem concerning the total π-electron energy even when restricting h to be even integers .

To our surprise, we found that we can get a unified result of extremal h-polygonal chains on k-matchings for all integers $h \geq 6$. Our main results are as follows



(a) the minimal hexagonal chains concerning their k-matching

L_n



(b) the maximal hexagonal chains concerning their k-matching

Z_n

Fig 2: Extremal hexagonal chains

Theorem 1.4 Let $\mathcal{A}_n$ be the set of h-polygonal chains ($h \geq 6$). For any $A_n \in \mathcal{A}_n$, the following inequalities hold for all $k \geq 0$,

$$m_k(Z_n^2) \leq m_k(A_n) \leq m_k(Z_n^1).$$

Moreover, the equalities on the left side hold for all k only if $A_n = Z_n^2$; and the equalities on the right side hold for all k only if $A_n = Z_n^1$.

The cases of $h = 4, h = 3$ need different approach. The result for $h = 4$ is already given in [15], and the extremal polyomino chains concerning the k-matchings can be found in Figure 3. The case $h = 3$ is to be considered in another paper. For the case of $h = 5$ (pentagonal chains), a shorter proof can be provided. We will discuss it elsewhere. Some other results on pentagonal chains can be found in [16, 17].

In order to prove Theorem 1.4, we need to consider the Z-polynomial (Z-counting polynomial) introduced by Hosoya [2]:

$$Z(G) = \sum_k m_k(G)x^k (m_0(G) = 1).$$

Note that this is a kind of matching polynomial defined later by mathematicians in [18] and [19].

We will prove a result (Theorem 1.5) equivalent to Theorem 1.4, which involves a quasi-ordering defined as follows. 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 $a_k \leq b_k$ for all k. If $f(x) \preceq g(x)$ and there exists some k such that $a_k < b_k$, then we say $f(x) \prec g(x)$.

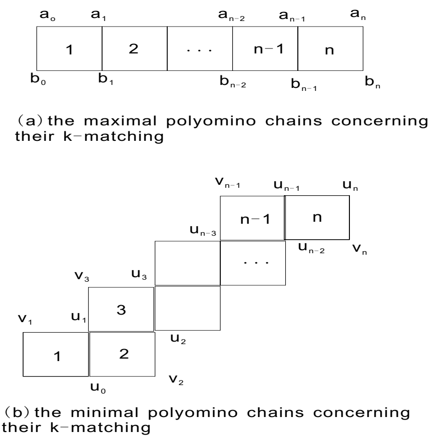


Fig 3: Extremal polyomino chains

Theorem 1.5 Let $\mathcal{A}_n$ be the set of h-polygonal chains ($h \geq 6$), for any $n \geq 3$ and for any $A_n \in \mathcal{A}_n$,

(a) If $A_n \neq Z_n^2$, then $Z(A_n) \succ Z(Z_n^2)$.

(b) If $A_n \neq Z_n^1$, then $Z(A_n) \prec Z(Z_n^1)$.

2 Some preliminaries

We mention some auxiliary results from [2, 18-20] as follows.

Claim 2.1 Let G be a graph consisting of two components G_1 and G_2, then $Z(G) = Z(G_1) \cdot Z(G_2)$.

Claim 2.2 Let uv be an edge of G, then $Z(G) = Z(G - uv) + xZ(G - u - v)$.

Claim 2.3 For each $uv \in E(G), Z(G) - Z(G - u) - xZ(G - u - v) \succeq 0$, Moreover, the equalities hold only if v is the unique neighbor of u .

In the following, we will use the notation G for $Z(G)$, when it would lead to no confusion. Some lemmas we need are as follows.

Lemma 2.4 Let A, B denote two disjoint graphs and a, b denote vertices in A, B respectively. Let X be the graph obtained from the union of A, B by adjoining the edge ab (see figure 4), then $X = AB + x(A - a)(B - b)$. (1).

Proof: From Claim 2.2, we can obtain the result immediately.

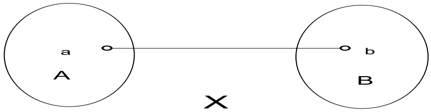


Fig 4:

As usual, we denote by P_n the path with n vertices. We also define $Z(P_n) = P_n$, If we apply Lemma 2.4 with $A = a$ and $B = P_n$, we obtain

$$P_{n+1} = P_n + xP_{n-1}(n \geq 0)(P_0 = P_1 = 1, P_{-1} = 0, P_{-2} = \frac{1}{x}) \tag{2}$$

From Claim 2.2 and Lemma 2.4 we have

$$P_{p+q} = P_pP_q + xP_{p-1}P_{q-1}(p, q \geq 0) \tag{3}$$

Lemma 2.5 Let G, A, B be three pairwise disjoint graphs. Two distinct vertices u, v belong to G and two vertices a, b belong to A and B respectively. Let Y be the graph obtained from the union $A \bigcup G \bigcup B$ by adjoining the edges au, bv (see figure 5), then

$$Y = ABG + x[A(B-b)(G-v) + (A-a)B(G-u)]$$
$$+x^2(A-a)(B-b)(G-u-v). \tag{4}$$

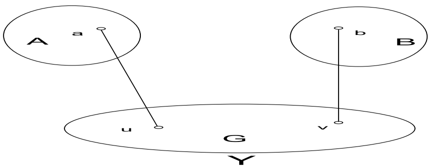


Fig 5:

Proof: It follows from repeated applications of Lemma 2.4. □

Remark 2.6 Let $A = P_p, B = P_q$, and a, b be endpoints of A, B respectively. Using Lemma 2.5, we have

$$Y = P_pP_qG + x[P_pP_{q-1}(G-v) + P_{p-1}P_q(G-u)] + x^2P_{p-1}P_{q-1}(G-u-v). \tag{5}$$

Any element A_n of $\mathcal{A}_n$ can be obtained from an appropriately chosen graph $A_{n-1} \in \mathcal{A}_{n-1}$ by attaching to it a new polygon C (figure 6).

Referring to figure 6, by Claims 2.1, Claim2.2 and Remark 2.6 we have

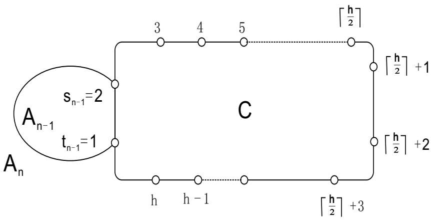


Fig 6:

$$A_n = P_{h-2}A_{n-1} + xP_{h-3}\{(A_{n-1} - s_{n-1}) + (A_{n-1} - t_{n-1})\}$$
$$+x^2P_{h-4}(A_{n-1} - s_{n-1} - t_{n-1}) \quad (6)$$
$$A_n - l = P_{l-3}P_{h-l}A_{n-1} + x[P_{l-4}P_{h-l}(A_{n-1} - s_{n-1}) + P_{l-3}P_{h-l-1}(A_{n-1} - t_{n-1})]$$
$$+x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1})(l \in \{3, 4, \cdots, h\}) \quad (7)$$

(In this paper, l denote both a vertex of h-polygon and the nature number labeling the vertex.)

and

$$A_n - l - (l + 1)$$
$$= P_{l-3}P_{h-l-1}A_{n-1} + x[P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1}) + P_{l-3}P_{h-l-2}(A_{n-1} - t_{n-1})]$$
$$+x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1}) \quad (8)$$

3 The proof of theorem 1.5

Now we are in the position to prove our main results. First we give the following two lemmas.

Lemma 3.1 Let Z_n^1 $(n \geq 2)$ be the chain of type one (see figure 1(a)). Then

(a) $Z_n^1 - a_1^n \prec Z_n^1 - l \prec Z_n^1 - a_0^n$,

(b) $Z_n^1 - a_1^n - 5 \prec Z_n^1 - l - (l + 1) \prec Z_n^1 - a_0^n - a_1^n$,

(c) $(Z_n^1 - a_1^n) + (Z_n^1 - 5) \prec (Z_n^1 - l) + (Z_n^1 - (l + 1)) \prec (Z_n^1 - a_0^n) + (Z_n^1 - a_1^n)$,

where $l \in \{5, 6, \cdots, h\}$.

Lemma 3.2 Let Z_n^2 $(n \geq 2)$ be the chain of type two (see figure 1(b)). Then

(a) $Z_n^2 - b_1^n \prec Z_n^2 - l \prec Z_n^2 - 3$,

(b) $Z_n^2 - b_1^n - b_0^n \prec Z_n^2 - l - (l + 1) \prec Z_n^2 - 3 - b_1^n$,

(c) $(Z_n^2 - b_1^n) + (Z_n^2 - b_0^n) \prec (Z_n^2 - l) + (Z_n^2 - (l+1)) \prec (Z_n^2 - 3) + (Z_n^2 - b_1^n)$,

where $l \in \{5, 6, \cdots, h\}$.

In order to prove the two lemmas, we need the following two claims.

Claim 3.3 For any $A_n \in \mathcal{A}_n$ $(n \geq 2)$, if $A_{n-1} - s_{n-1} \preceq A_{n-1} - t_{n-1}$ (see figure 6), then

(a) $A_n - 4 \prec A_n - l \prec A_n - 3$,

(b) $A_n - 4 - 5 \prec A_n - l - (l+1) \prec A_n - 3 - 4$,

(c) $(A_n - 4) + (A_n - 5) \prec (A_n - l) + (A_n - (l+1)) \prec (A_n - 3) + (A_n - 4)$.

where $l \in \{(5), (6), \cdots, (h)\}$

Proof of Claim 3.3: (a) By (7), $A_n - 3 = P_{h-3}A_{n-1} + xP_{h-4}(A_{n-1} - t_{n-1})$

$$A_n - 4 = P_1P_{h-4}A_{n-1} + x[P_0P_{h-4}(A_{n-1} - s_{n-1}) + P_1P_{h-5}(A_{n-1} - t_{n-1})] \\ +x^2P_0P_{h-5}(A_{n-1} - s_{n-1} - t_{n-1}) \\ = P_{h-4}A_{n-1} + xP_{h-4}(A_{n-1} - s_{n-1}) + xP_{h-5}(A_{n-1} - t_{n-1}) \\ +x^2P_{h-5}(A_{n-1} - s_{n-1} - t_{n-1})$$

$$A_n - l = P_{l-3}P_{h-l}A_{n-1} + x[P_{l-4}P_{h-l}(A_{n-1} - s_{n-1}) + P_{l-3}P_{h-l-1}(A_{n-1} - t_{n-1})] \\ +x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1})(3 \leq l \leq h)$$

So $(A_n - 3) - (A_n - l)$

$$= (P_{h-3} - P_{l-3}P_{h-l})A_{n-1} + (xP_{h-4} - xP_{l-3}P_{h-l-1})(A_{n-1} - t_{n-1}) - xP_{l-4}P_{h-l}(A_{n-1} - s_{n-1}) \\ -x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1})$$

(Apply eqs(2) (3)) $= xP_{l-4}P_{h-l-1}A_{n-1} + x^2P_{l-4}P_{h-l-2}(A_{n-1} - t_{n-1})$

$$-xP_{l-4}(P_{h-l-1} + xP_{h-l-2})(A_{n-1} - s_{n-1}) - x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1}) \\ = xP_{l-4}P_{h-l-1}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})] \\ +x^2P_{l-4}P_{h-l-2}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})] \succ 0$$

Let $l = 4$, we obtain

$$(A_n - 3) - (A_n - 4) = xP_{h-5}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})] \\ +x^2P_{h-6}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})]$$

Consequently,

$$(A_n - 4) - (A_n - l) = [(A_n - 4) - (A_n - 3)] + [(A_n - 3) - (A_n - l)]$$

$= -xP_{h-5}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})] - x^2P_{h-6}[(A_{n-1} - t_{n-1}) - (A_{n-1} -$

$s_{n-1})] + xP_{l-4}P_{h-l-1}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$+x^2P_{l-4}P_{h-l-2}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})]$

$= -x^2P_{l-5}P_{h-l-2}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$-x^3P_{l-5}P_{h-l-3}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})] \prec 0$

(Where $P_{h-5} - P_{l-4}P_{h-l-1} = P_{(l-4)+(h-l-1)} - P_{l-4}P_{h-l-1} = xP_{l-5}P_{h-l-2}$

and $P_{h-6} - P_{l-4}P_{h-l-2} = xP_{l-5}P_{h-l-3}$)

(b) By (8), $A_n - l - (l+1) = P_{l-3}P_{h-l-1}A_{n-1}$

$+x[P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1}) + P_{l-3}P_{h-l-2}(A_{n-1} - t_{n-1})]$

$+x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1})$

Let $l = 3$, we obtain

$A_n - 3 - 4 = P_{h-4}A_{n-1} + xP_{h-5}(A_{n-1} - t_{n-1})$

Consequently,

$[A_n - 3 - 4] - [A_n - l - (l+1)] = (P_{h-4} - P_{l-3}P_{h-l-1})A_{n-1} - xP_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1})$

$+(xP_{h-5} - xP_{l-3}P_{h-l-2})(A_{n-1} - t_{n-1}) - x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1})$

$= xP_{l-4}P_{h-l-2}A_{n-1} - xP_{l-4}(P_{h-l-2} + xP_{h-l-3})(A_{n-1} - s_{n-1})$

$+x^2P_{l-4}P_{h-l-3}(A_{n-1} - t_{n-1}) - x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1})$

$= xP_{l-4}P_{h-l-2}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$+x^2P_{l-4}P_{h-l-3}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})] \succ 0$

Let $l = 4$, we obtain

$(A_n - 3 - 4) - (A_n - 4 - 5) = xP_{h-6}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$+x^2P_{h-7}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})]$

Consequently,

$(A_n-4-5)-[A_n-l-(l+1)] = [(A_n-4-5)-(A_n-3-4)]+[(A_n-3-4)-(A_n-l-(l+1))]$

$= -xP_{h-6}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$-x^2P_{h-7}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})]$

$+xP_{l-4}P_{h-l-2}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$+x^2P_{l-4}P_{h-l-3}[(A_{n-1} - t_{n-1}) - (A_{n-1} - s_{n-1})]$

$= -x^2P_{l-5}P_{h-l-3}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$-x^3P_{l-5}P_{h-l-4}[(A_{n-1}-t_{n-1})-(A_{n-1}-s_{n-1})]\prec 0$

(c) $(A_n-3)+(A_n-4)-(A_n-l)-[A_n-(l+1)] = P_{h-3}A_{n-1}+xP_{h-4}(A_{n-1}-t_{n-1})+P_{h-4}A_{n-1}$
$+xP_{h-4}(A_{n-1}-s_{n-1})+xP_{h-5}(A_{n-1}-t_{n-1})+x^2P_{h-5}(A_{n-1}-s_{n-1}-t_{n-1})$
$-P_{l-3}P_{h-l}A_{n-1}-xP_{l-4}P_{h-l}(A_{n-1}-s_{n-1})-xP_{l-3}P_{h-l-1}(A_{n-1}-t_{n-1})$
$-x^2P_{l-4}P_{h-l-1}(A_{n-1}-s_{n-1}-t_{n-1})-P_{l-2}P_{h-l-1}A_{n-1}-xP_{l-3}P_{h-l-1}(A_{n-1}-s_{n-1})$
$-xP_{l-2}P_{h-l-2}(A_{n-1}-t_{n-1})-x^2P_{l-3}P_{h-l-2}(A_{n-1}-s_{n-1}-t_{n-1})$
$=(P_{h-3}+P_{h-4}-P_{l-3}P_{h-l}-P_{l-2}P_{h-l-1})A_{n-1}$
$+(xP_{h-4}+xP_{h-5}-xP_{l-3}P_{h-l-1}-xP_{l-2}P_{h-l-2})(A_{n-1}-t_{n-1})$
$+(xP_{h-4}-xP_{l-4}P_{h-l}-xP_{l-3}P_{h-l-1})(A_{n-1}-s_{n-1})$
$+(x^2P_{h-5}-x^2P_{l-4}P_{h-l-1}-x^2P_{l-3}P_{h-l-2})(A_{n-1}-s_{n-1}-t_{n-1})$
$=xP_{l-4}P_{h-l-2}A_{n-1}+x^2P_{l-4}P_{h-l-3}(A_{n-1}-t_{n-1})-xP_{l-4}(P_{h-l-2}+xP_{h-l-3})(A_{n-1}-s_{n-1})$
$-x^2P_{l-4}P_{h-l-2}(A_{n-1}-s_{n-1}-t_{n-1})$

(Where by (2) and (3) the coefficient of $A_{n-1}=P_{h-3}+P_{h-4}-P_{l-3}P_{h-l}-P_{l-2}P_{h-l-1}$
$=P_{(l-3)+(h-l)}+P_{h-4}-P_{l-3}P_{h-l}-P_{l-2}P_{h-l-1}=xP_{l-4}P_{h-l-1}-P_{l-2}P_{h-l-1}+P_{h-4}$
$=-P_{l-3}P_{h-l-1}+P_{h-4}=xP_{l-4}P_{h-l-2}$,
the coefficient of $A_{n-1}-t_{n-1}=xP_{h-4}+xP_{h-5}-xP_{l-3}P_{h-l-1}-xP_{l-2}P_{h-l-2}$
$=(xP_{h-4}-xP_{l-3}P_{h-l-1})-xP_{l-2}P_{h-l-2}+xP_{h-5}=x^2P_{l-4}P_{h-l-2}-xP_{l-2}P_{h-l-2}+xP_{h-5}$
$=-xP_{l-3}P_{h-l-2}+xP_{h-5}=x^2P_{l-4}P_{h-l-3}$,
the coefficient of $A_{n-1}-s_{n-1}=xP_{h-4}-xP_{l-4}P_{h-l}-xP_{l-3}P_{h-l-1}$
$=x^2P_{l-5}P_{h-l-1}-xP_{l-3}P_{h-l-1}=-xP_{l-4}P_{h-l-1}=-xP_{l-4}(P_{h-l-2}+xP_{h-l-3})$,
the coefficient of $A_{n-1}-s_{n-1}-t_{n-1}=x^2P_{h-5}-x^2P_{l-4}P_{h-l-1}-x^2P_{l-3}P_{h-l-2}$
$=x^3P_{l-5}P_{h-l-2}-x^2P_{l-3}P_{h-l-2}=-x^2P_{l-4}P_{h-l-2})$
$=xP_{l-4}P_{h-l-2}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]$
$+x^2P_{l-4}P_{h-l-3}[(A_{n-1}-t_{n-1})-(A_{n-1}-s_{n-1})]\succ 0$

Let $l=4$, we obtain

$[(A_n-3)+(A_n-4)]-[(A_n-4)+(A_n-5)]=xP_{h-6}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-$
$s_{n-1}-t_{n-1})]+x^2P_{h-7}[(A_{n-1}-t_{n-1})-(A_{n-1}-s_{n-1})]$

Consequently,

$$[(A_n-4)+(A_n-5)]-[(A_n-l)+(A_n-(l+1))]=\{[(A_n-4)+(A_n-5)]-[(A_n-3)+(A_n-4)]\}+\{[(A_n-3)+(A_n-4)]-[(A_n-l)+(A_n-(l+1))]\}$$
$$=-xP_{h-6}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]-x^2P_{h-7}[(A_{n-1}-t_{n-1})-(A_{n-1}-s_{n-1})]+xP_{l-4}P_{h-l-2}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]$$
$$+x^2P_{l-4}P_{h-l-3}[(A_{n-1}-t_{n-1})-(A_{n-1}-s_{n-1})]$$
$$=-x^2P_{l-5}P_{h-l-3}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]$$
$$-x^3P_{l-5}P_{h-l-4}[(A_{n-1}-t_{n-1})-(A_{n-1}-s_{n-1})]\prec 0$$

Claim 3.4 Let Z_n^1 be the chain of type one (see figure 1(a)) and Z_n^2 be the chain of type two (see figure 1(b)) respectively. Then $Z_1^2-b_0^1=Z_1^2-b_1^1,\ Z_1^1-a_0^1=Z_1^1-a_1^1$ and $Z_i^2-b_1^i\prec Z_i^2-b_0^i,\ Z_i^1-a_1^i\prec Z_i^1-a_0^i,\ 2\le i\le n$.

Proof of Claim 3.4 : Obviously, $Z_1^2-b_0^1=Z_1^2-b_1^1,\ Z_1^1-a_0^1=Z_1^1-a_1^1$. For $2\le i\le n$, by Claim 3.3 (a),

$$(Z_i^1-a_0^i)-(Z_i^1-a_1^i)=xP_{h-5}\{Z_{i-1}^1-(Z_{i-1}^1-a_1^{i-1})-x(Z_{i-1}^1-a_0^{i-1}-a_1^{i-1})\}$$
$$+x^2P_{h-6}\{(Z_{i-1}^1-a_0^{i-1})-(Z_{i-1}^1-a_1^{i-1})\}.$$

Thus, by Claim 2.3, if $(Z_{i-1}^1-a_1^{i-1})\preceq(Z_{i-1}^1-a_0^{i-1})$ then $(Z_i^1-a_1^i)\prec(Z_i^1-a_0^i)$. Hence, by induction we can show for each $2\le i\le n$, $(Z_i^1-a_1^i)\prec(Z_i^1-a_0^i)$.

Similarly, by Claim 3.3 (a) and Claim 2.3, we can show that $Z_i^2-b_1^i\prec Z_i^2-b_0^i,\ 2\le i\le n$. The proof of Claim 3.4 is complete.

From Claim 3.3 and Claim 3.4, we get Lemma 3.1 and Lemma 3.2 immediately.

In order to use induction to prove Theorem 1.5, we will prove the following result by induction.

Theorem 3.5 For any h-polygonal chain $A_n\in\mathcal{A}_n$ $(n\ge 3)$,

(a) $Z_n^2-b_1^n\preceq A_n-l\preceq Z_n^1-a_0^n$,

(b) $Z_n^2-b_1^n-b_0^n\preceq A_n-l-(l+1)\preceq Z_n^1-a_0^n-a_1^n$,

(c) $(Z_n^2-b_1^n)+(Z_n^2-b_0^n)\preceq(A_n-l)+(A_n-(l+1))\preceq(Z_n^1-a_0^n)+(Z_n^1-a_1^n)$,

where $l\in\{(3),(4),\cdots,(h)\}$.

(d) $Z_n^2\preceq A_n\preceq Z_n^1$.

Moreover, the equalities of the right-hand side of (a)-(d) hold only if $A_n=Z_n^1$ and $l,l+1$ denote a_0^n,a_1^n respectively; and the equalities of the left-hand side of (a)-(d) hold only if $A_n=Z_n^2$ and $l,l+1$ denote b_1^n,b_0^n respectively.

Proof of Theorem 3.5: First we note that if $A_n=Z_n^2$ then the left-hand side parts of (a)-(d) hold by Lemma 3.2; and if $A_n = Z_n^1$ then the right-hand side parts of (a)-(d) hold by Lemma 3.1. Consequently, when we prove the left-hand side parts we may assume that $A_n \neq Z_n^2$. Similarly, when we prove the right-hand side parts we may assume that $A_n \neq Z_n^1$.

We prove Theorem 3.5 by induction.

(i) First we consider the case $n = 3$.

(a) We show that if $A_3 \neq Z_3^1$ then $A_3 - l \prec Z_3^1 - a_0^3$.

By (7), let $n = 3$, then

$$A_3 - l = P_{l-3}P_{h-l}A_2 + x[P_{l-4}P_{h-l}(A_2 - s_2) + P_{l-3}P_{h-l-1}(A_2 - t_2)]$$
$$+x^2 P_{l-4}P_{h-l-1}(A_2 - s_2 - t_2)(3 \leq l \leq h)$$
$$= P_{l-3}P_{h-l}Z_2^1 + x[P_{l-4}P_{h-l}(Z_2^1 - s_2) + P_{l-3}P_{h-l-1}(Z_2^1 - t_2)]$$
$$+x^2 P_{l-4}P_{h-l-1}(Z_2^1 - s_2 - t_2)$$
$$Z_3^1 - a_0^3 = Z_3^1 - 3 = P_{h-3}Z_2^1 + xP_{h-4}(Z_2^1 - a_0^2)$$
$$(Z_3^1 - a_0^3) - (A_3 - l) = (P_{h-3} - P_{l-3}P_{h-l})Z_2^1 + xP_{h-4}(Z_2^1 - a_0^2) - xP_{l-4}P_{h-l}(Z_2^1 - s_2)$$
$$-xP_{l-3}P_{h-l-1}(Z_2^1 - t_2) - x^2 P_{l-4}P_{h-l-1}(Z_2^1 - s_2 - t_2)$$

(By Lemma 3.1 (a), we have $Z_2^1 - t_2 \preceq Z_2^1 - a_0^2$)

$$\succeq xP_{l-4}P_{h-l-1}Z_2^1 + x(P_{h-4} - P_{l-3}P_{h-l-1})(Z_2^1 - a_0^2) - xP_{l-4}(P_{h-l-1} + xP_{h-l-2})(Z_2^1 - s_2)$$
$$-x^2 P_{l-4}P_{h-l-1}(Z_2^1 - s_2 - t_2)$$
$$= xP_{l-4}P_{h-l-1}[Z_2^1 - (Z_2^1 - s_2) - x(Z_2^1 - s_2 - t_2)] + x^2 P_{l-4}P_{h-l-2}[(Z_2^1 - a_0^2) - (Z_2^1 - s_2)] \succ 0$$

Similarly, we can show that if $A_3 \neq Z_3^2$, then $Z_3^2 - b_1^3 \prec A_3 - l$.

(b) We show that if $A_3 \neq Z_3^1$, then $A_3 - l - (l+1) \prec Z_3^1 - a_0^3 - a_1^3$.

By (8), let $n = 3$, then

$$A_3 - l - (l+1) = P_{l-3}P_{h-l-1}Z_2^1$$
$$+x[P_{l-4}P_{h-l-1}(Z_2^1 - s_2) + P_{l-3}P_{h-l-2}(Z_2^1 - t_2)] + x^2 P_{l-4}P_{h-l-2}(Z_2^1 - s_2 - t_2)(3 \leq l \leq h)$$
$$Z_3^1 - a_0^3 - a_1^3 = Z_3 - 3 - 4 = P_{h-4}Z_2^1 + xP_{h-5}(Z_2^1 - a_0^2)$$
$$(Z_3^1 - a_0^3 - a_1^3) - (A_3 - l - (l+1)) = (P_{h-4} - P_{l-3}P_{h-l-1})Z_2^1 + xP_{h-5}(Z_2^1 - a_0^2)$$
$$-xP_{l-4}P_{h-l-1}(Z_2^1 - s_2) - xP_{l-3}P_{h-l-2}(Z_2^1 - t_2) - x^2 P_{l-4}P_{h-l-2}(Z_2^1 - s_2 - t_2)$$

(By Lemma 3.1 (a), we have $Z_2^1 - t_2 \preceq Z_2^1 - a_0^2$)

$$\succeq xP_{l-4}P_{h-l-2}Z_2^1 + x(P_{h-5} - P_{l-3}P_{h-l-2})(Z_2^1 - a_0^2)$$
$$-xP_{l-4}(P_{h-l-2} + xP_{h-l-3})(Z_2^1 - s_2) - x^2 P_{l-4}P_{h-l-2}(Z_2^1 - s_2 - t_2)$$

$= xP_{l-4}P_{h-l-2}[Z_2^1-(Z_2^1-s_2)-x(Z_2^1-s_2-t_2)]+x^2P_{l-4}P_{h-l-3}[(Z_2^1-a_0^2)-(Z_2^1-s_2)] \succ 0$

Similarly, we can show that if $A_3 \neq Z_3^2$, then $Z_3^2 - b_1^3 - b_0^3 \prec A_3 - l - (l+1)$.

(c) We show that if $A_3 \neq Z_3^1$, then $(A_3 - l) + (A_3 - (l+1)) \prec (Z_3^1 - a_0^3) + (Z_3^1 - a_1^3)$.

$(Z_3^1 - a_0^3) + (Z_3^1 - a_1^3) - (A_3 - l) - [A_3 - (l+1)]$

$= P_{h-3}Z_2^1 + xP_{h-4}(Z_2^1 - a_0^2) + P_{h-4}Z_2^1 + xP_{h-4}(Z_2^1 - a_1^2) + xP_{h-5}(Z_2^1 - a_0^2)$

$\quad +x^2P_{h-5}(Z_2^1 - a_0^2 - a_1^2) - P_{l-3}P_{h-l}Z_2^1 - xP_{l-4}P_{h-l}(Z_2^1 - s_2) - xP_{l-3}P_{h-l-1}(Z_2^1 - t_2)$

$\quad -x^2P_{l-4}P_{h-l-1}(Z_2^1 - s_2 - t_2) - P_{l-2}P_{h-l-1}Z_2^1 - xP_{l-3}P_{h-l-1}(Z_2^1 - s_2)$

$\quad -xP_{l-2}P_{h-l-2}(Z_2^1 - t_2) - x^2P_{l-3}P_{h-l-2}(Z_2^1 - s_2 - t_2)$

(By Lemma 3.1 (b), $Z_2^1 - a_0^2 - a_1^2 \succeq Z_2^1 - l - (l+1)$)

$\succeq (P_{h-3} + P_{h-4} - P_{l-3}P_{h-l} - P_{l-2}P_{h-l-1})Z_2^1 + xP_{h-4}[(Z_2^1 - a_0^2) + (Z_2^1 - a_1^2)]$

$\quad -xP_{l-3}P_{h-l-1}(Z_2^1 - s_2) - xP_{l-2}P_{h-l-2}(Z_2^1 - t_2) + xP_{h-5}(Z_2^1 - a_0^2)$

$\quad -xP_{l-4}P_{h-l}(Z_2^1 - s_2) - xP_{l-3}P_{h-l-1}(Z_2^1 - t_2)$

$\quad +(x^2P_{h-5} - x^2P_{l-4}P_{h-l-1} - x^2P_{l-3}P_{h-l-2})(Z_2^1 - a_0^2 - a_1^2) \qquad (*)$

Where by (2) and (3),

the coefficient of $Z_2^1 = P_{h-3} + P_{h-4} - P_{l-3}P_{h-l} - P_{l-2}P_{h-l-1}$

$= (P_{h-3} - P_{l-3}P_{h-l}) + P_{h-4} - P_{l-2}P_{h-l-1} = xP_{l-4}P_{h-l-1} + P_{h-4} - (P_{l-3} + xP_{l-4})P_{h-l-1}$

$= P_{h-4} - P_{l-3}P_{h-l-1} = xP_{l-4}P_{h-l-2}$,

the coefficient of $Z_2^1 - a_0^2 - a_1^2 = x^2P_{h-5} - x^2P_{l-4}P_{h-l-1} - x^2P_{l-3}P_{h-l-2}$

$= x^3P_{l-5}P_{h-l-2} - x^2P_{l-3}P_{h-l-2} = -x^2P_{l-4}P_{h-l-2}$,

because $P_{h-4} = P_{(l-3)+(h-l-1)} = P_{l-3}P_{h-l-1} + xP_{l-4}P_{h-l-2}$,

so, the coefficient of $Z_2^1 - s_2 = -xP_{l-3}P_{h-l-1} = x^2P_{l-4}P_{h-l-2} - xP_{h-4}$,

similarly, the coefficient of $Z_2^1 - t_2 = -xP_{l-2}P_{h-l-2} = x^2P_{l-3}P_{h-l-3} - xP_{h-4}$.

So,

$(*) = xP_{l-4}P_{h-l-2}Z_2^1 + xP_{h-4}[(Z_2^1 - a_0^2) + (Z_2^1 - a_1^2) - (Z_2^1 - s_2) - (Z_2^1 - t_2)]$

$\qquad +x^2P_{l-4}P_{h-l-2}(Z_2^1 - s_2) + x^2P_{l-3}P_{h-l-3}(Z_2^1 - t_2) + xP_{h-5}(Z_2^1 - a_0^2)$

$\qquad -xP_{l-4}(P_{h-l-1} + xP_{h-l-2})(Z_2^1 - s_2) - xP_{l-3}(P_{h-l-2} + xP_{h-l-3})(Z_2^1 - t_2)$

$\qquad -x^2P_{l-4}P_{h-l-2}(Z_2^1 - a_0^2 - a_1^2)$

$= xP_{l-4}P_{h-l-2}Z_2^1 + xP_{h-4}[(Z_2^1 - a_0^2) + (Z_2^1 - a_1^2) - (Z_2^1 - s_2) - (Z_2^1 - t_2)]$

$-xP_{l-4}P_{h-l-1}(Z_2^1 - s_2) - xP_{l-3}P_{h-l-2}(Z_2^1 - t_2) + xP_{h-5}(Z_2^1 - a_0^2)$

$-x^2P_{l-4}P_{h-l-2}(Z_2^1 - a_0^2 - a_1^2)$

(By Lemma 3.1 (a), $Z_2^1 - a_0^2 \succeq Z_2^1 - l$)

$\succeq xP_{l-4}P_{h-l-2}Z_2^1 + xP_{h-4}[(Z_2^1 - a_0^2) + (Z_2^1 - a_1^2) - (Z_2^1 - s_2) - (Z_2^1 - t_2)]$

$-xP_{l-4}P_{h-l-1}(Z_2^1 - a_0^2) - xP_{l-3}P_{h-l-2}(Z_2^1 - a_0^2) + xP_{h-5}(Z_2^1 - a_0^2)$

$-x^2P_{l-4}P_{h-l-2}(Z_2^1 - a_0^2 - a_1^2)$

$= xP_{l-4}P_{h-l-2}[Z_2^1 - (Z_2^1 - a_0^2) - x(Z_2^1 - a_0^2 - a_1^2)]$

$+xP_{h-4}[(Z_2^1 - a_0^2) + (Z_2^1 - a_1^2) - (Z_2^1 - s_2) - (Z_2^1 - t_2)] \succ 0$

Where the coefficient of $Z_2^1 - a_0^1 = xP_{h-5} - xP_{l-4}P_{h-l-1} - xP_{l-3}P_{h-l-2}$

$= x^2P_{l-5}P_{h-l-2} - x(P_{l-4} + xP_{l-5})P_{h-l-2}$

$= -xP_{l-4}P_{h-l-2}$

(d) By (6), let $n = 3$, then

$A_3 = P_{h-2}A_2 + xP_{h-3}\{(A_2 - s_2) + (A_2 - t_2)\} + x^2P_{h-4}(A_2 - s_2 - t_2)$

$= P_{h-2}Z_2^1 + xP_{h-3}\{(Z_2^1 - s_2) + (Z_2^1 - t_2)\} + x^2P_{h-4}(Z_2^1 - s_2 - t_2)$

$Z_3 = P_{h-2}Z_2^1 + xP_{h-3}\{(Z_2^1 - a_0^2) + (Z_2^1 - a_1^2)\} + x^2P_{h-4}(Z_2^1 - a_0^2 - a_1^2)$

Thus, by Lemma 3.1 (b) and (c), we get that $A_3 \prec Z_3^1$.

Similarly, we can prove that $Z_3^2 \prec A_3$.

Therefore, Theorem 3.5 holds for $n = 3$.

(ii) Suppose the Theorem true for all h-polygonal chains with fewer than n h-polygons. Let A_n be a h-polygonal chain with $n \geq 4$ h-polygons, which is obtained from $A_{n-1} \in \mathcal{A}_{n-1}$ by attaching to it a new h-polygon C (figure 6).

(a) We show that if $A_n \neq Z_n^1$, then $A_n - l \prec Z_n^1 - a_0^n$, where $l \in \{3, 4, \cdots, h\}$.

By (7), we have

$A_n - l = P_{l-3}P_{h-l}A_{n-1} + x[P_{l-4}P_{h-l}(A_{n-1} - s_{n-1}) + P_{l-3}P_{h-l-1}(A_{n-1} - t_{n-1})]$

$+x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1})(3 \leq l \leq h)$

$Z_n^1 - a_0^n = Z_n^1 - 3 = P_{h-3}Z_{n-1}^1 + xP_{h-4}(Z_{n-1}^1 - a_0^{n-1})$

$(Z_n^1 - a_0^n) - (A_n - l)$

$= P_{h-3}Z_{n-1}^1 - P_{l-3}P_{h-l}A_{n-1} + xP_{h-4}(Z_{n-1}^1 - a_0^{n-1}) - xP_{l-4}P_{h-l}(A_{n-1} - s_{n-1})$

$-xP_{l-3}P_{h-l-1}(A_{n-1} - t_{n-1}) - x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1})$

By the inductive hypotheses we have $A_{n-1} \preceq Z^1_{n-1}$ and $A_{n-1} - t_{n-1} \preceq Z^1_{n-1} - a_0^{n-1}$.

So $(Z^1_n - a^n_0) - (A_n - l) \succeq (P_{h-3} - P_{l-3}P_{h-l})A_{n-1} + x(P_{h-4} - P_{l-3}P_{h-l-1})(Z^1_{n-1} - a_0^{n-1})$

$-xP_{l-4}(P_{h-l-1} + xP_{h-l-2})(A_{n-1} - s_{n-1}) - x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1})$

$= xP_{l-4}P_{h-l-1}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$+x^2P_{h-4}P_{h-l-2}[(Z^1_{n-1} - a_0^{n-1}) - (A_{n-1} - s_{n-1})] \succ 0$

Similarly, we can show that if $A_n \neq Z^2_n$, then $Z^2_n - b^n_1 \prec A_n - l$, where $l \in \{3, 4, \cdots, h\}$.

(b) We show that if $A_n \neq Z^1_n$, then $A_n - l - (l+1) \prec Z^1_n - a^n_0 - a^n_1$, where $l \in \{3, 4, \cdots, h\}$.

By (8), we have

$A_n - l - (l + 1) = P_{l-3}P_{h-l-1}A_{n-1} + x[P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1})$

$+P_{l-3}P_{h-l-2}(A_{n-1} - t_{n-1})] + x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1})(3 \leq l \leq h)$

$Z^1_n - a^n_0 - a^n_1 = Z^1_n - 3 - 4 = P_{h-4}Z^1_{n-1} + xP_{h-5}(Z^1_{n-1} - a_0^{n-1})$

Consequently,

$(Z^1_n - a^n_0 - a^n_1) - (A_n - l - (l + 1))$

$= P_{h-4}Z^1_{n-1} - P_{l-3}P_{h-l-1}A_{n-1} + xP_{h-5}(Z^1_{n-1} - a_0^{n-1}) - xP_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1})$

$-xP_{l-3}P_{h-l-2}(A_{n-1} - t_{n-1}) - x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1})$

By the inductive hypotheses we have $A_{n-1} \preceq Z^1_{n-1}$ and $A_{n-1} - t_{n-1} \preceq Z^1_{n-1} - a_0^{n-1}$.

So $(Z^1_n - a^n_0 - a^n_1) - (A_n - l - (l + 1))$

$\succeq (P_{h-4} - P_{l-3}P_{h-l-1})A_{n-1} + x(P_{h-5} - P_{l-3}P_{h-l-2})(Z^1_{n-1} - a_0^{n-1})$

$-xP_{l-4}(P_{h-l-2} + xP_{h-l-3})(A_{n-1} - s_{n-1}) - x^2P_{l-4}P_{h-l-2}(A_{n-1} - s_{n-1} - t_{n-1})$

$= xP_{l-4}P_{h-l-2}[A_{n-1} - (A_{n-1} - s_{n-1}) - x(A_{n-1} - s_{n-1} - t_{n-1})]$

$+x^2P_{l-4}P_{h-l-3}[(Z^1_{n-1} - a_0^{n-1}) - (A_{n-1} - s_{n-1})] \succ 0$

Similarly, we can show that if $A_n \neq Z^2_n$, then $Z^2_n - b^n_1 - b^n_0 \prec A_n - l - (l + 1)$, where $l \in \{3, 4, \cdots, h\}$.

(c) We show that if $A_n \neq Z^1_n$, then $(A_n - l) + (A_n - (l + 1)) \prec (Z^1_n - a^n_0) + (Z^1_n - a^n_1)$.

$(Z^1_n - a^n_0) + (Z^1_n - a^n_1) - (A_n - l) - [A_n - (l + 1)]$

$= P_{h-3}Z^1_{n-1} + xP_{h-4}(Z^1_{n-1} - a_0^{n-1}) + P_{h-4}Z^1_{n-1} + xP_{h-4}(Z^1_{n-1} - a_1^{n-1}) + xP_{h-5}(Z^1_{n-1} - a_0^{n-1})$

$+x^2P_{h-5}(Z^1_{n-1} - a_0^{n-1} - a_1^{n-1}) - P_{l-3}P_{h-l}A_{n-1} - xP_{l-4}P_{h-l}(A_{n-1} - s_{n-1})$

$-xP_{l-3}P_{h-l-1}(A_{n-1} - t_{n-1}) - x^2P_{l-4}P_{h-l-1}(A_{n-1} - s_{n-1} - t_{n-1}) - P_{l-2}P_{h-l-1}A_{n-1}$

$-xP_{l-3}P_{h-l-1}(A_{n-1} - s_{n-1}) - xP_{l-2}P_{h-l-2}(A_{n-1} - t_{n-1})$

$-x^2P_{l-3}P_{h-l-2}(A_{n-1}-s_{n-1}-t_{n-1})$

(By the inductive hypotheses we have $A_{n-1}\preceq Z^1_{n-1}$ and $A_{n-1}-s_{n-1}-t_{n-1}\preceq Z^1_{n-1}-a^{n-1}_0-a^{n-1}_1$)

$\succeq (P_{h-3}+P_{h-4}-P_{l-3}P_{h-l}-P_{l-2}P_{h-l-1})A_{n-1}+xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)]$

$-xP_{l-3}P_{h-l-1}(A_{n-1}-s_{n-1})-xP_{l-2}P_{h-l-2}(A_{n-1}-t_{n-1})+xP_{h-5}(Z^1_{n-1}-a^{n-1}_0)$

$-xP_{l-4}P_{h-l}(A_{n-1}-s_{n-1})-xP_{l-3}P_{h-l-1}(A_{n-1}-t_{n-1})$

$+(x^2P_{h-5}-x^2P_{l-4}P_{h-l-1}-x^2P_{l-3}P_{h-l-2})(A_{n-1}-s_{n-1}-t_{n-1})$

(Where by (2) and (3), similar to (i) (c)),

$=xP_{l-4}P_{h-l-2}A_{n-1}+xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)-(A_{n-1}-s_{n-1})$

$-(A_{n-1}-t_{n-1})]+x^2P_{l-4}P_{h-l-2}(A_{n-1}-s_{n-1})+x^2P_{l-3}P_{h-l-3}(A_{n-1}-t_{n-1})$

$+xP_{h-5}(Z^1_{n-1}-a^{n-1}_0)-xP_{l-4}(P_{h-l-1}+xP_{h-l-2})(A_{n-1}-s_{n-1})$

$-xP_{l-3}(P_{h-l-2}+xP_{h-l-3})(A_{n-1}-t_{n-1})-x^2P_{l-4}P_{h-l-2}(A_{n-1}-s_{n-1}-t_{n-1})$

$=xP_{l-4}P_{h-l-2}A_{n-1}+xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)-(A_{n-1}-s_{n-1})-(A_{n-1}-t_{n-1})]$

$-xP_{l-4}P_{h-l-1}(A_{n-1}-s_{n-1})-xP_{l-3}P_{h-l-2}(A_{n-1}-t_{n-1})+xP_{h-5}(Z^1_{n-1}-a^{n-1}_0)$

$-x^2P_{l-4}P_{h-l-2}(A_{n-1}-s_{n-1}-t_{n-1})$

$=xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)-(A_{n-1}-s_{n-1})-(A_{n-1}-t_{n-1})]$

$+xP_{l-4}P_{h-l-2}A_{n-1}-xP_{l-4}(P_{h-l-2}+xP_{h-l-3})(A_{n-1}-s_{n-1})-xP_{l-3}P_{h-l-2}(A_{n-1}-t_{n-1})$

$+xP_{h-5}(Z^1_{n-1}-a^{n-1}_0)-x^2P_{l-4}P_{h-l-2}(A_{n-1}-s_{n-1}-t_{n-1})$

$=xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)-(A_{n-1}-s_{n-1})-(A_{n-1}-t_{n-1})]$

$+xP_{l-4}P_{h-l-2}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]$

$-x^2P_{l-4}P_{h-l-3}(A_{n-1}-s_{n-1})-xP_{l-3}P_{h-l-2}(A_{n-1}-t_{n-1})+xP_{h-5}(Z^1_{n-1}-a^{n-1}_0)$

(By inductive hypotheses, $A_{n-1}-s_{n-1}\preceq Z^1_{n-1}-a^{n-1}_0, A_{n-1}-t_{n-1}\preceq Z^1_{n-1}-a^{n-1}_0$)

$\succeq xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)-(A_{n-1}-s_{n-1})-(A_{n-1}-t_{n-1})]$

$+xP_{l-4}P_{h-l-2}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]$

$+(xP_{h-5}-xP_{l-3}P_{h-l-2}-x^2P_{l-4}P_{h-l-3})(Z^1_{n-1}-a^{n-1}_0)$

$=xP_{h-4}[(Z^1_{n-1}-a^{n-1}_0)+(Z^1_{n-1}-a^{n-1}_1)-(A_{n-1}-s_{n-1})-(A_{n-1}-t_{n-1})]$

$+xP_{l-4}P_{h-l-2}[A_{n-1}-(A_{n-1}-s_{n-1})-x(A_{n-1}-s_{n-1}-t_{n-1})]\succ 0$

(Where the coefficient of $Z^1_{n-1}-a^{n-1}_0=xP_{h-5}-xP_{l-3}P_{h-l-2}-x^2P_{l-4}P_{h-l-3}$

$=x^2P_{l-4}P_{h-l-3}-x^2P_{l-4}P_{h-l-3}=0$)

By inductive hypotheses and Claim 2.3, we get that

$$(A_n - l) + (A_n - (l+1)) \prec (Z_n^1 - a_0^n) + (Z_n^1 - a_1^n).$$

Similarly, we can show that if $A_n \neq Z_n^2$, then $(Z_n^2 - b_1^n) + (Z_n^2 - b_0^n) \prec (A_n - l) + (A_n - (l+1))$, where $l \in \{3, 4, \cdots, h\}$.

(d) We show that if $A_n \neq Z_n^1$, then $A_n \prec Z_n^1$. By (6), we get

$$A_n = P_{h-2}A_{n-1} + xP_{h-3}\{(A_{n-1} - s_{n-1}) + (A_{n-1} - t_{n-1})\}$$
$$+x^2P_{h-4}(A_{n-1} - s_{n-1} - t_{n-1}),$$
$$Z_n^1 = P_{h-2}Z_{n-1}^1 + xP_{h-3}\{(Z_{n-1}^1 - a_0^{n-1}) + (Z_{n-1}^1 - a_1^{n-1})\}$$
$$+x^2P_{h-4}(Z_{n-1}^1 - a_0^{n-1} - a_1^{n-1})$$

By the inductive hypotheses we have $A_{n-1} \preceq Z_{n-1}^1, (A_{n-1} - s_{n-1}) + (A_{n-1} - t_{n-1}) \preceq (Z_{n-1}^1 - a_0^{n-1}) + (Z_{n-1}^1 - a_1^{n-1})$, and $A_{n-1} - s_{n-1} - t_{n-1} \preceq Z_{n-1}^1 - a_0^{n-1} - a_1^{n-1}$. Since $A_n \neq Z_n^1$, either $A_{n-1} \neq Z_{n-1}^1$ or $\{s_{n-1}, t_{n-1}\} \neq \{a_0^{n-1}, a_1^{n-1}\}$, and hence, at least one of the three inequalities is strict. Therefore, we get that $A_n \prec Z_n^1$.

Similarly, we can show that if $A_n \neq Z_n^2$, then $Z_n^2 \prec A_n$.

The proof of Theorem 3.5 is complete.

For the Merrified-Simmons index, the parallel result can also be obtained. We will discuss it elsewhere.

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