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Extremal polyomino chains on k-matchings and k-independent sets*

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Denote by $\mathcal{T}_n$ the set of polyomino chains with n squares. For any $T_n \in \mathcal{T}_n$, let $m_k(T_n)$ and $i_k(T_n)$ be the number of k-matchings and k-independent sets of T_n, respectively. In this paper, we show that for any polyomino chain $T_n \in \mathcal{T}_n$ and any $k \geqslant 0$, $m_k(L_n) \geqslant m_k(T_n) \geqslant m_k(Z_n)$ and $i_k(L_n) \leqslant i_k(T_n) \leqslant i_k(Z_n)$, with the left equalities holding for all k only if $T_n = L_n$, and the right equalities holding for all k only if $T_n = Z_n$, where L_n and Z_n are the linear chain and the zig-zag chain, respectively.

KEY WORDS: polyomino chain, square lattice, graph invariant, Z-polynomial, Y-polynomial, k-matching, k-independent set, total π-electron energy

1. Introduction

Ordering of graphs with respect to their number of matchings, especially finding the graphs extremal with regard to this invariant, has been the topic of several earlier works [1–4]. These results have chemical applications. The same problem has been considered for many other invariants such as the total π-electron energy and the number of independent sets [5–9]. In statistical mechanics, the enumeration of independent sets of $m \times n$ square lattices and $m \times n$ hexagonal lattices are known as hard square problem and hard hexagon problem, respectively. In recent years there has interest amongst physicists and combinatorialists [10–15]. In this paper we will consider some extremal problems concerning k-matchings and k-independent sets of a special kind of square lattice, the polyomino chain.

Let us recall some basic concepts. A hexagonal system is a finite 2-connected plane graph such that each interior face is surrounded by a regular hexagon of length one. A hexagonal chain is a hexagonal system with the properties that it has no vertex belonging to three hexagons and it has no hexagon adjacent to more than two hexagons [5].

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Similarly, A polyomino system is a finite 2-connected plane graph such that each interior face (say a cell) is surrounded by a regular square of length one. A polyomino chain is a polyomino system, in which the joining of the centers of its adjacent regular squares forms a path $c_1c_2\cdots c_n(\forall_n \in N)$, where c_i is the center of the ith square $(i = 1, 2, \ldots, n)$.

In [5], Zhang and one of the present authors determined the extremal hexagonal chains concerning their k-matchings and k-independent sets. In [16, 17], Wang and Li and one of the present authors determined the extremal hexagonal chains concerning the total π-electron energy.

But how about the polyomino chain? In this paper we will determine the extremal polyomino chains concerning their k-matchings and k-independent sets. Note that the problem is not so easy at our first glance. There is some essential difference between the hexagonal chain and the polyomino chain. In fact each hexagonal chain or polyomino chain can be formed inductively. And in each step we need to attach a new cell to the previous one. It's clear that for the hexagonal chain, successive attached edges are disjoint. This property makes the mathematical induction easily to be carried out. But in the case of polyomino chain, successive attached edges need not to be disjoint (cf. the zig-zag chain showing in figure 1(b)). This fact brings about some trouble for the inductive approach. In order to overcome the difficulty, in this paper we introduce a "double" labelling for the attached edges of T_n which will be explained later in this section. In next section we introduce some materials very useful to our paper. In sections 3 and 4 we deal with the extremal problems of polyomino chain concerning their k-matchings and k-independent sets, respectively. Finally we will point out that to determine the extremal polyomino chain concerning their total π-electron energy we will face more serious difficulty which we can not overcome now.

Denote by $\mathcal{T}_n$ the set of polyomino chains with n squares. Let $T_n \in \mathcal{T}_n$. Similarly to [5] we have definitions as follows. If the subgraph of T_n induced by the vertices with degree 3 is a graph with exactly n–2 squares, then T_n is called a linear chain and denoted by L_n. If the subgraph of T_n induced by the vertices with degree bigger than two is a path with n–1 edges, then T_n is called a zig-zag chain and denoted by Z_n. figure 1(a) and (b) illustrate L_n and Z_n, respectively.

Let G be a graph without loops and multiple edges. For k being a positive integer, $m_k(G)$ denotes the number of k-matchings in G, that is, the number of k-element sets of independent edges of G. In addition, it is consistent to define $m_0(G) = 1$ for all graphs G, as well as $m_k(G) = 0$ for all $k < 0$ [1]. Similarly $i_k(G)$ denotes the number of k-independent sets of G. Consistently we define $i_0(G) = 1$ for all graphs G, as well as $i_k(G) = 0$ for all $k < 0$.

Given a $T_n \in \mathcal{T}_n$, the squares in T_n are fixed by the path $c_1c_2\cdots c_n$ mentioned above. What's more, $T_i(i = 1, \ldots, n-1)$ denotes the part of T_n with the first i squares. From the definition of polyomino chain we see that any element T_i of $\mathcal{T}_i$ can be obtained from an appropriately chosen graph $T_{i-1} \in \mathcal{T}_{i-1}$ by attaching to it a new cell t_i (cf. figure 2(a)), which denotes the ith square. Note

that there are two ways to attach an edge of t_i to an edge e of the end square in T_{i-1}; either e is incident with two vertices of degree two in T_{i-1}, which we denote as $T_i^{(1)}$ (cf. figure 2(b)); or e is incident with a vertex of degree two and the other vertex of degree three in T_{i-1}, which we denote as $T_i^{(2)}$ (cf. figure 2(c)). To unify $T_n^{(1)}$ and $T_n^{(2)}$, we introduce a "double" labelling as follows. For any polyomino chain $T_n \in \mathcal{T}_n$ and for each $i \in \{1, \dots, n-1\}$, $\{x_i, y_i\}$ denotes the common edge of the ith and the $(i+1)$th squares; $x^{(i+1)}$ and $y^{(i+1)}$ denote the vertices of degree two in the $(i+1)$th end square of T_{i+1} (cf. figure 2). What's more, we designate $x^{(i+1)}$ as the vertex adjacent to x_i in T_{i+1} while we designate $y^{(i+1)}$ as the vertex adjacent to y_i in T_{i+1}. It's consistent to define $x^{(1)} = x_1, y^{(1)} = y_1$. For convenience, let x_i to be always of degree two in T_i. That's to say, the vertex x_i always belongs to only one square – the ith end square t_i in T_i. For example in figure 1(b), for each $i \in \{1, 2, \dots, n-1\}$, $x_i = u_i$, $y_i = u_{i-1}$. We would like to emphasize that in our case one vertex can attain two labels and each one represents the same vertex. In fact only use this "double" labelling can we get the recurrence relations of $Z(Z_n), Z(T_n), Z(L_n), Y(Z_n), Y(T_n), Y(L_n)$, respectively. Moreover, it's knowable that $\mathcal{T}_1 = \{L_1\} = \{Z_1\}$,$\mathcal{T}_2 = \{L_2\} = \{Z_2\}$, and $\mathcal{T}_3 = \{L_3, Z_3\}$, and clearly a_i and $b_i (i = 0, 1, 2, \dots, n)$ can be interchanged simultaneously in any subgraph of L_n , such as $L_n - a_n = L_n - b_n$, $L_n - a_n - b_{n-1} = L_n - b_n - a_{n-1}$ (figure 1(a)).
Now we may state our main results.

Theorem 1. For any polyomino chain $T_n \in \mathcal{T}_n$ and for each $k \geqslant 0$,

$$m_k(L_n) \geqslant m_k(T_n) \geqslant m_k(Z_n).$$

Moreover, the equality of the left-hand side holds for each k only if $T_n = L_n$; and the equality of the right-hand side holds for each k only if $T_n = Z_n$.

Theorem 2. For any polyomino chain $T_n \in \mathcal{T}_n$ and for each $k \geqslant 0$,

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

Moreover, the equality of the left-hand side holds for each k only if $T_n = L_n$; and the equality of the right-hand side holds for each k only if $T_n = Z_n$.

In order to prove theorems 1 and 2, we consider the following two polynomials.

The Z-polynomial (Z-counting polynomial) was defined by Hosoya [18] as

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

which is a special case of the matching polynomial defined by Farrell [19], and has essentially the same combinatorial contents as the matching polynomial.

According to the independent sets, Y-polynomial is defined as [5]

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

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 $a_k < b_k$ [5].

As $\mathcal{T}_1 = \{L_1\} = \{Z_1\}$,$\mathcal{T}_2 = \{L_2\} = \{Z_2\}$, we will prove the following two theorems, which are equivalent to theorems 1 and 2, respectively.

Theorem 3. For any $n \geqslant 3$ and for any polyomino chain $T_n \in \mathcal{T}_n$,

(a) if $T_n \neq L_n$, then $Z(T_n) \prec Z(L_n)$,

(b) if $T_n \neq Z_n$, then $Z(T_n) \succ Z(Z_n)$.

Theorem 4. For any $n \geqslant 3$ and for any polyomino chain $T_n \in \mathcal{T}_n$,

(a) if $T_n \neq L_n$, then $Y(T_n) \succ Y(L_n)$,

(b) if $T_n \neq Z_n$, then $Y(T_n) \prec Y(Z_n)$.

2. Some preliminaries

Now let's recall some results[18–21] useful to this paper.

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 $\mathcal{N}_u$ be the subset of V(G) containing the vertex u and its neighbors. Then $Y(G) = Y(G - u) + xY(G - \mathcal{N}_u)$.

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) (b) hold only if v is the unique neighbor of u.

3. The proof of theorem 3

Without confusion in this section we write $Z(G)$ in G for convenience.

Referring to figures 1 and 2, by claims 1(a) and 2(a), we get

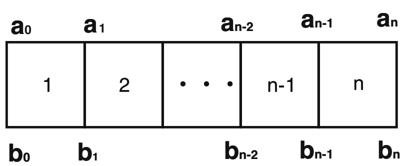
(1) $T_n = (1+x)T_{n-1} + x[(T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})] + x^2(T_{n-1} - x_{n-1} - y_{n-1})$,

(2) $T_n - x^{(n)} = T_{n-1} + x(T_{n-1} - y_{n-1})$
$T_n - y^{(n)} = T_{n-1} + x(T_{n-1} - x_{n-1})$
$T_n - x_{n-1} = (1+x)(T_{n-1} - x_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$
$T_n - y_{n-1} = (1+x)(T_{n-1} - y_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$
$L_n - a_n = (L_{n-1} - a_{n-1}) + x(L_{n-1} - b_{n-1}) + x(L_{n-1} - a_{n-1} - b_{n-1})$
$\quad + x(L_{n-1} - a_{n-1} - a_{n-2})$,

(3) $T_n - x_{n-1} - x^{(n)} = (T_{n-1} - x_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$
$T_n - x^{(n)} - y^{(n)} = (T_{n-1} - x_{n-1}y_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$,

(4) $Z_n - u_{n-1} = Z_{n-1} + x^2(Z_{n-2} - u_{n-3})$
$Z_n - u_n = Z_{n-1} + x^2(Z_{n-2} - u_{n-2}) + x(Z_{n-2} - u_{n-2}) + x^2(Z_{n-2} - u_{n-2} - u_{n-3})$,

(5) $L_n - a_n - a_{n-1} = (L_{n-1} - a_{n-1}) + x(L_{n-1} - a_{n-1} - b_{n-1})$
$L_{n-1} = (L_{n-1} - a_{n-1}) + x(L_{n-1} - a_{n-1} - b_{n-1}) + x(L_{n-1} - a_{n-1} - a_{n-2})$.



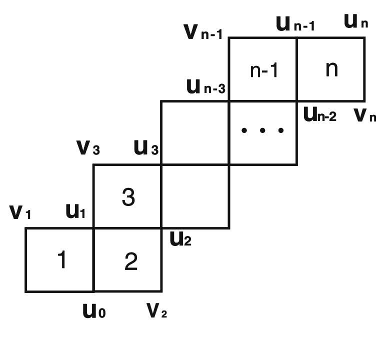


Figure 1. (a) The subgraph of the polyomino chain induced by the vertices with degree 3 is a graph with exactly $n-2$ squares, we call it the linear chain L_n. Denote by $a_0, a_1, \ldots, a_n$ the $n+1$ vertices in one side of the path $c_1c_2\cdots c_n$ and $b_0, b_1, \cdots, b_n$ the $n+1$ vertices in the other side of the path $c_1c_2\ldots c_n$, respectively. What's more, $a_ib_i (i = 1, \ldots, n-1)$ is the common edge of the ith and the $(i+1)$th squares, while a_0b_0 belongs to the first square and a_nb_n belongs to the nth end square, respectively. (b) The subgraph of the polyomino chain induced by the vertices with degree bigger than two is a path with n–1 edges, we call it the zig-zag chain Z_n. Here the path is labelled by $u_0u_1\cdots u_{n-1}$, where u_0 is a vertex of the first square. Consistently denote by u_n the unlabelled vertex adjacent to u_{n-1} in the nth end square. Denote by $v_i (i = 1, \ldots, n)$ the unlabeled vertex adjacent to u_i in the ith square.

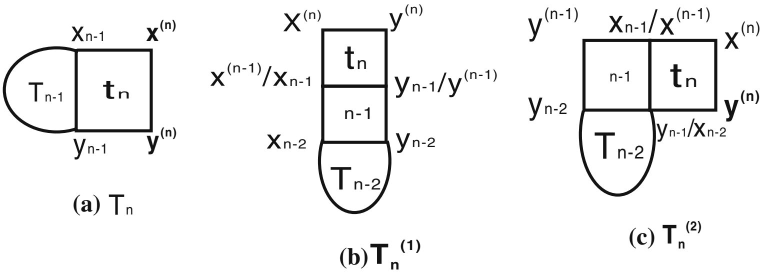


Figure 2. (a) T_n is a polyomino chain with n squares, which is obtained from $T_{n-1} \in \mathcal{T}_{n-1}$ by attaching to it a new cell t_n. $\{x_{n-1}, y_{n-1}\}$ denotes the common edge of the $(n-1)$th and the nth squares, while $x^{(n)}$, $y^{(n)}$ denotes the other two vertices of degree two in the nth end square in T_n. And $x^{(n)}$ is adjacent to x_{n-1} in the nth end square, while $y^{(n)}$ is adjacent to y_{n-1} in the nth end square. Note that it may not be a unique labelling. (b) The labelling is based on that of figure 2(a). And the edge $\{x_{n-1}, y_{n-1}\}$ is incident with two vertices of degree two in T_{n-1}, which is denoted by $T_n^{(1)}$. $\{x_{n-2}, y_{n-2}\}$ denotes the common edge of the $(n-2)$th and the $(n-1)$th squares, while $x^{(n-1)}$, $y^{(n-1)}$ denotes the other two vertices of degree two in the $(n-1)$th end square in T_{n-1}. And $x^{(n-1)}$ is adjacent to x_{n-2} in the $(n-1)$th square, while $y^{(n-1)}$ is adjacent to y_{n-2} in the $(n-1)$th square. Note that it's not a unique labelling. In figure 2(c), the labelling is based on that of figure 2(a). And the edge $\{x_{n-1}, y_{n-1}\}$ is incident with a vertex of degree two and the other vertex of degree three in T_{n-1}, which is denoted by $T_n^{(2)}$. $\{x_{n-2}, y_{n-2}\}$ denotes the common edge of the $(n-2)$th and the $(n-1)$th squares, while $x^{(n-1)}$, $y^{(y-1)}$ denotes the vertices with degree two in the $(n-1)$th end square in T_{n-1}. And $x^{(n-1)}$ is adjacent to x_{n-2} in the $(n-1)$th square, while $y^{(n-1)}$ is adjacent to y_{n-2} in the $(n-1)$th square. What's more, we designate x_i to be always of degree two in $T_i (i = n-2, n-1)$. Note that it may not be a unique labelling.

Lemma 1. For any integer $n \geqslant 2$, we have

(a) $(L_n - b_n) = (L_n - a_n) \succ (L_n - a_{n-1}) = (L_n - b_{n-1})$,

(b) $L_{n-1} = (L_n - a_n - b_n) \succ (L_n - a_n - a_{n-1}) = (L_n - b_n - b_{n-1})$,

(c) $(Z_n - u_n) \succ (Z_n - u_{n-1})$,

(d) $(Z_n - v_n) \succ (Z_n - u_n) (n \geqslant 3)$,

(e) $(T_n - x^{(n)} - y^{(n)}) \succ (T_n - x^{(n)} - x_{n-1})$.

Proof.

(a) Referring to figure 1(a), clearly $(L_1 - a_1) = (L_1 - a_0)$. For $n \geqslant 2$, since $(L_{n-1} - a_{n-1}) = (L_{n-1} - b_{n-1})$, by (2), it's easy to get $(L_n - a_n) - (L_n - a_{n-1}) = x(L_{n-1} - a_{n-1} - a_{n-2}) \succ 0$. The result follows.

(b) Obviously $(L_1 - a_1 - b_1) = (L_1 - a_1 - a_0)$. For $n \geqslant 2$, by (5), $L_{n-1} - (L_n - a_n - a_{n-1}) = x(L_{n-1} - a_{n-1} - a_{n-2}) \succ 0$. The result follows.

(c) By induction. First by (4),
$(Z_n - u_n) = Z_{n-1} + x^2(Z_{n-2} - u_{n-2}) + x(Z_{n-2} - u_{n-2}) + x^2(Z_{n-2} - u_{n-2} - u_{n-3})$,
$(Z_n - u_{n-1}) = Z_{n-1} + x^2(Z_{n-2} - u_{n-3})$.

For $n = 2$, by lemma 1(a), $(Z_2 - u_2) = (L_2 - a_2) \succ (L_2 - a_1) = (Z_2 - u_1)$.
For $n = 3$, since $(Z_1 - u_1) = (Z_1 - u_0)$, then $(Z_3 - u_3) - (Z_3 - u_2) = x(Z_1 - u_1) + x^2(Z_1 - u_1 - u_0) \succ 0$.
Suppose (c) holds for all zig-zag chains with fewer than n ($n \geqslant 4$) squares. Then by the inductive hypotheses, $(Z_{n-2} - u_{n-2}) \succ (Z_{n-2} - u_{n-3})$.
Thus $(Z_n - u_n) \succ (Z_n - u_{n-1})$.

(d) For $n \geqslant 3$, by (2), $(Z_n - v_n) = Z_{n-1} + x(Z_{n-1} - u_{n-1})$, $(Z_n - u_n) = Z_{n-1} + x(Z_{n-1} - u_{n-2})$. By lemma 1(c), $(Z_{n-1} - u_{n-1}) \succ (Z_{n-1} - u_{n-2}) (n - 1 \geqslant 2)$.
Therefore $(Z_n - v_n) \succ (Z_n - u_n) (n \geqslant 3)$.

(e) For $n \geqslant 2$, by (3), $(T_n - x^{(n)} - y^{(n)}) = (T_{n-1} - x_{n-1} y_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$. $(T_n - x^{(n)} - x_{n-1}) = (T_{n-1} - x_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$.
Whence by claim 2(a), we have $(T_{n-1} - x_{n-1} y_{n-1}) \succ (T_{n-1} - x_{n-1})$.
Therefore $(T_n - x^{(n)} - y^{(n)}) \succ (T_n - x^{(n)} - x_{n-1})$.

The proof of lemma 1 is completed.

In order to use induction to prove theorem 3, we will prove the following theorem which contains more contents than that of theorem 3.

Theorem 5. For any integer $n \geqslant 3$ and any polyomino chain $T_n \in \mathcal{T}_n$,

(a) $(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1}) \succeq (T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1}) \succeq (Z_{n-1} - u_{n-1}) + (Z_{n-1} - u_{n-2})$,

(b) $(L_{n-1} - a_{n-1} - b_{n-1}) \succeq (T_{n-1} - x_{n-1} - y_{n-1}) \succeq (Z_{n-1} - u_{n-1} - u_{n-2})$,

(c) $(T_n - x^{(n)}) \succeq (Z_n - u_n)$, $(T_n - y^{(n)}) \succ (Z_n - u_n)$,

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

Moreover, the equalities of the left-hand side of (a)(d) hold only if $T_n = L_n$; the equalities of (c) and the right-hand side of (a)(b)(d) hold only if $T_n = Z_n$. For the left-hand side of (b), $T_n = L_n$ is just a sufficient condition.

Proof. First it's easy to see that if $T_n = L_n$ then the left-hand side of (a)(b)(d) hold; if $T_n = Z_n$ then (c) (by lemma 1(d)) and the right-hand side of (a)(b)(d) hold. Consequently, when we prove the left-hand side of (a)(b)(d) we may assume that $T_n \neq L_n$; when we prove (c) and the right-hand side of (a)(b)(d) we may assume that $T_n \neq Z_n$.

Now let's prove theorem 5 by induction.

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

(a) By our assumption we need only to prove
$(L_2 - a_2) + (L_2 - b_2) \succ (Z_2 - u_2) + (Z_2 - u_1) = (L_2 - a_2) + (L_2 - a_1)$.
And this is supported by lemma 1(a).

(b) By our assumption we need only to prove
$(L_2 - a_2 - b_2) \succ (Z_2 - u_2 - u_1) = (L_2 - a_2 - a_1)$.
And this is supported by lemma 1(b).

(c) Clearly $Z_2 = L_2$. If $T_3 \neq Z_3$, then $T_3 = L_3$. By (2),
$(L_3 - a_3) = L_3 - b_3 = L_2 + x(L_2 - a_2)$, $(Z_3 - u_3) = Z_2 + x(Z_2 - u_1) = L_2 + x(L_2 - a_1)$.
By lemma, 1(a) $(L_2 - a_2) \succ (L_2 - a_1)$.
Therefore $L_3 - a_3 \succ Z_3 - u_3$.

(d) By our assumptions we need only to prove $L_3 > Z_3$. By (1),
$L_3 = (1 + x)L_2 + x[(L_2 - a_2) + (L_2 - b_2)] + x^2(L_2 - a_2 - b_2)$.
$Z_3 = (1 + x)Z_2 + x[(Z_2 - u_2) + (Z_2 - u_1)] + x^2(Z_2 - u_2 - u_1)$,
Since $L_2 = Z_2$, by (a)(b) proved just now we get that $L_3 \succ Z_3$.

Hence theorem 5 holds when $n = 3$.

(ii) Suppose the theorem holds for all polyomino chains with fewer than $n (n \geqslant 4)$ squares. Let T_n be a polyomino chain with n squares ($n \geqslant 4$), which is obtained from $T_{n-1} \in \mathcal{T}_{n-1}$ by attaching to it a new cell t_n (figure 2(a)). In the following we mostly consider $T_n^{(1)}$, $T_n^{(2)}$ instead of T_n by convenience.

(a) By (2) and claim 3(a),
In $T_n^{(1)}$, $(T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1}) = 2T_{n-2} + x[(T_{n-2} - x_{n-2}) + (T_{n-2} - y_{n-2})]$.
Especially $(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1}) = 2L_{n-2} + x[(L_{n-2} - a_{n-2}) + (L_{n-2} - b_{n-2})]$.
In $T_n^{(2)}$, $(T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1}) = (T_{n-1} - x^{(n-1)}) + (T_{n-1} - x_{n-2})$
$= T_{n-2} + x[(T_{n-2} - x_{n-2}) + (T_{n-2} - y_{n-2})] + (T_{n-2} - x_{n-2}) + x(T_{n-2} - x_{n-2} - y_{n-2})$
$\prec 2T_{n-2} + x[(T_{n-2} - x_{n-2}) + (T_{n-2} - y_{n-2})]$.
Especially $(Z_{n-1} - u_{n-1}) + (Z_{n-1} - u_{n-2})$
$= Z_{n-2} + x[(Z_{n-2} - u_{n-2}) + (Z_{n-2} - u_{n-3})] + (Z_{n-2} - u_{n-2}) + x(Z_{n-2} - u_{n-2} - u_{n-3})$
$\prec 2Z_{n-2} + x[(Z_{n-2} - u_{n-2}) + (Z_{n-2} - u_{n-3})]$.
For the left-hand side, by the inductive hypotheses,
$L_{n-2} \succeq T_{n-2}$, $(L_{n-2} - a_{n-2}) + (L_{n-2} - b_{n-2}) \succeq (T_{n-2} - x_{n-2}) + (T_{n-2} - y_{n-2})$.
Therefore in $T_n^{(2)}$, $(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1}) \succ (T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})$.
Since $T_n^{(2)} \neq L_n$, $T_{n-1} \neq L_{n-1}$ at least one of the two inequalities must be strict.

Whence $(L_{n-1}-a_{n-1})+(L_{n-1}-b_{n-1}) \succ (T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1})$.
For the right-hand side, by the inductive hypotheses,
$T_{n-2} \succeq Z_{n-2}, (T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2}) \succeq (Z_{n-2}-u_{n-2})+(Z_{n-2}-u_{n-3})$.
Therefore In $T_n^{(1)}, (T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1}) \succ (Z_{n-1}-u_{n-1})+(Z_{n-1}-u_{n-2})$.
In $T_n^{(2)}$, since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses,
$T_{n-2} \succeq Z_{n-2}, (T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2}) \succeq (Z_{n-2}-u_{n-2})+(Z_{n-2}-u_{n-3}), (T_{n-2}-x_{n-2}) \succeq (Z_{n-2}-u_{n-2}), (T_{n-2}-x_{n-2}-y_{n-2}) \succeq (Z_{n-2}-u_{n-2}-u_{n-3})$.
Since $T_n^{(2)} \neq Z_n$, $T_{n-1} \neq Z_{n-1}$, at least one of the inequalities must be strict.
Whence $(T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1}) \succ (Z_{n-1}-u_{n-1})+(Z_{n-1}-u_{n-2})$.

(b) For the left-hand side, in $T_n^{(1)}$, by inductive hypothesis,
$(L_{n-1}-a_{n-1}-b_{n-1}) = L_{n-2} \succeq T_{n-2} = (T_{n-1}-x_{n-1}-y_{n-1})$.
In $T_n^{(2)}$, by lemma 1(e) and the inductive hypothesis, $(T_{n-1}-x_{n-1}-y_{n-1}) = (T_{n-1}-x^{(n-1)}-x_{n-2})$
$\prec (T_{n-1}-x^{(n-1)}-y^{(n-1)}) = T_{n-2} \preceq L_{n-2} = (L_{n-1}-a_{n-1}-b_{n-1})$.
In a word, if $T_n \neq L_n$, $(L_{n-1}-a_{n-1}-b_{n-1}) \succeq (T_{n-1}-x_{n-1}-y_{n-1})$.
For the right-hand side, in $T_n^{(1)}$, by lemma 1(e) and the inductive hypotheses,
$(T_{n-1}-x_{n-1}-y_{n-1}) = T_{n-2} \succeq Z_{n-2} = (Z_{n-1}-u_{n-1}-v_{n-1}) \succ (Z_{n-1}-u_{n-1}-u_{n-2})$.
That is $(T_{n-1}-x_{n-1}-y_{n-1}) \succ (Z_{n-1}-u_{n-1}-u_{n-2})$.
In $T_n^{(2)}$, by (3), $(T_{n-1}-x_{n-1}-y_{n-1}) = (T_{n-1}-x^{(n-1)}-x_{n-2})$
$= (T_{n-2}-x_{n-2})+x(T_{n-2}-x_{n-2}-y_{n-2})$.
Especially $(Z_{n-1}-u_{n-1}-u_{n-2}) = (Z_{n-2}-u_{n-2})+x(Z_{n-2}-u_{n-2}-u_{n-3})$.
Since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses,
$(T_{n-2}-x_{n-2}) \succeq (Z_{n-2}-u_{n-2})$, $(T_{n-2}-x_{n-2}-y_{n-2}) \succeq (Z_{n-2}-u_{n-2}-u_{n-3})$.
Since $T_n^{(2)} \neq Z_n$, $T_{n-1} \neq Z_{n-1}$, at least one of the inequalities must be strict.
Therefore $(T_{n-1}-x_{n-1}-y_{n-1}) \succ (Z_{n-1}-u_{n-1}-u_{n-2})$.

(c) By (2), $(T_n-x^{(n)}) = T_{n-1}+x(T_{n-1}-y_{n-1})$, $(T_n-y^{(n)}) = T_{n-1}+x(T_{n-1}-x_{n-1})$. Especially $(Z_n-u_n) = Z_{n-1}+x(Z_{n-1}-u_{n-2})$.
In $T_n^{(1)}$, since $y_{n-1} \in \{x^{(n-1)}, y^{(n-1)}\}$, then by lemma 1(c) and the inductive hypotheses,
$T_{n-1} \succeq Z_{n-1}$, $(T_{n-1}-y_{n-1}) \succeq (Z_{n-1}-u_{n-1}) \succ (Z_{n-1}-u_{n-2})$.

Hence $(T_n^{(1)} - x^{(n)}) \succ (Z_n - u_n)$.
Similarly we can show that $(T_n^{(1)} - y^{(n)}) \succ (Z_n - u_n)$.
In $T_n^{(2)}$, by (2), lemma 1(c) and the inductive hypotheses,
$(Z_n - u_n) = Z_{n-1} + x(Z_{n-1} - u_{n-2}) \prec Z_{n-1} + x(Z_{n-1} - u_{n-1})$
$\preceq T_{n-1} + x(T_{n-1} - x^{(n-1)}) = T_{n-1} + x(T_{n-1} - x_{n-1}) = T_n^{(2)} - y^{(n)}$,
$(T_n^{(2)} - x^{(n)}) = T_{n-1} + x(T_{n-1} - x_{n-2})$, $Z_n - u_n = Z_{n-1} + x(Z_{n-1} - u_{n-2})$.
And then $(T_{n-1} - x_{n-2}) = (1+x)(T_{n-2} - x_{n-2}) + x(T_{n-2} - x_{n-2} - y_{n-2})$.
Especially $(Z_{n-1} - u_{n-2}) = (1+x)(Z_{n-2} - u_{n-2}) + x(Z_{n-2} - u_{n-2} - u_{n-3})$.
Since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses, (1) $T_{n-1} \succeq Z_{n-1}$, $(T_{n-2} - x_{n-2}) \succeq (Z_{n-2} - u_{n-2})$, $(T_{n-2} - x_{n-2} - y_{n-2}) \succeq (Z_{n-2} - u_{n-2} - u_{n-3})$.
Since $T_n^{(2)} \neq Z_n$, $T_{n-1} \neq Z_{n-1}$, at least one of the inequalities must be strict.
Whence $(T_n^{(2)} - x^{(n)}) \succ (Z_n - u_n)$.
Therefore if $T_n \neq Z_n$, then $(T_n - x^{(n)}) \succ (Z_n - u_n)$, $(T_n - y^{(n)}) \succ (Z_n - u_n)$.

(d) By (1),
$L_n = (1+x)L_{n-1} + x[(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1})] + x^2(L_{n-1} - a_{n-1} - b_{n-1})$,
$T_n = (1+x)T_{n-1} + x[(T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})] + x^2(T_{n-1} - x_{n-1} - y_{n-1})$.
By the inductive hypotheses, $L_{n-1} \succeq T_{n-1}$, $(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1}) \succeq (T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})$, $(L_{n-1} - a_{n-1} - b_{n-1}) \succeq (T_{n-1} - x_{n-1} - y_{n-1})$.
Since $T_n \neq L_n$, at least one of the three inequalities must be strict.
Therefore $L_n \succ T_n$.

Similarly we can show that if $T_n \neq Z_n$, then $T_n \succ Z_n$.

The proof of theorem 5 is completed.

4. The proof of theorem 4

Without confusion in this section we write $Y(G)$ in G for convenience.

Referring to figures 1 and 2, by claims 1(b) and 2(b), we get

(1′) $T_n = T_{n-1} + x[(T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})]$,

(2′) $(T_n - x^{(n)}) = T_{n-1} + x(T_{n-1} - y_{n-1})$
$(T_n - y^{(n)}) = T_{n-1} + x(T_{n-1} - x_{n-1})$

$(T_n - x_{n-1}) = (1 + x)(T_{n-1} - x_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$
$(T_n - y_{n-1}) = (1 + x)(T_{n-1} - y_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$,

(3′) $(T_n - x^{(n)} - x_{n-1}) = (T_{n-1} - x_{n-1}) + x(T_{n-1} - x_{n-1} - y_{n-1})$
$(L_n - a_n - a_{n-1}) = L_{n-2} + xL_{n-2} + x(L_{n-2} - b_{n-2})$,

(4′) $(Z_n - u_n) = (Z_n - u_n - u_{n-1}) + x(Z_{n-2} - u_{n-2}) + x^2(Z_{n-2} - u_{n-2})$
$(Z_n - u_{n-1}) = (Z_n - u_n - u_{n-1}) + xZ_{n-2} + x^2(Z_{n-2} - u_{n-3})$.

Lemma 2. For any integer $n \geqslant 2$,

(a) $(L_n - a_n) \prec (L_n - a_{n-1})$,

(b) $(L_n - a_n - b_n) \prec (L_n - a_n - a_{n-1})$,

(c) $(Z_n - u_n) \prec (Z_n - u_{n-1})$,

(d) $(Z_n - v_n) \prec (Z_n - u_n)(n \geqslant 3)$.

Proof.

(a) For $n \geqslant 2$, by (2′) and claim 2(b),
$(L_n - a_n) = L_{n-1} + x(L_{n-1} - b_{n-1}) = (L_{n-1} - a_{n-1}) + x(L_{n-1} - a_{n-1} - b_{n-1} - a_{n-2}) + x(L_{n-1} - b_{n-1})$,
$(L_n - a_{n-1}) = (L_{n-1} - a_{n-1}) + x(L_{n-1} - a_{n-1} - b_{n-1}) + x(L_{n-1} - a_{n-1})$.
Since $(L_{n-1} - a_{n-1}) = (L_{n-1} - b_{n-1})$, and by claim 2(b) we get
$(L_{n-1} - a_{n-1} - b_{n-1} - a_{n-2}) \prec (L_{n-1} - a_{n-1} - b_{n-1})$.
Thus $(L_n - a_n) \prec (L_n - a_{n-1})$.

(b) For $n \geqslant 2$, by (1′) and (3′),
$(L_n - a_n - b_n) = L_{n-1} = L_{n-2} + x(L_{n-2} - a_{n-2}) + x(L_{n-2} - b_{n-2})$,
$(L_n - a_n - a_{n-1}) = L_{n-2} + xL_{n-2} + x(L_{n-2} - b_{n-2})$.
Then by claim 2(b) we can get that $(L_n - a_n - b_n) \prec (L_n - a_n - a_{n-1})$.

(c) By induction. First by (4′), we can easily get that
$(Z_n - u_n) - (Z_n - u_{n-1}) = x[(Z_{n-2} - u_{n-2}) - Z_{n-2}] + x^2[(Z_{n-2} - u_{n-2}) - (Z_{n-2} - u_{n-3})]$.
For n=2, by lemma 2(a), $(Z_2 - u_2) = (L_2 - a_2) \prec (L_2 - a_1) = (Z_2 - u_1)$.
For n=3, since $(Z_1 - u_1) = (Z_1 - u_0)$, by claim 2(b) we get
$(Z_3 - u_3) - (Z_3 - u_2) = x[(Z_1 - u_1) - Z_1] + x^2[(Z_1 - u_1) - (Z_1 - u_0)] \prec 0$.
Suppose (c) holds for all zig-zag chains with fewer than $n(n \geqslant 4)$ squares. Then by claim 2(b) and the inductive hypotheses,
$(Z_{n-2} - u_{n-2}) \prec Z_{n-2}$, $(Z_{n-2} - u_{n-2}) \prec (Z_{n-2} - u_{n-3})$.
Therefore $(Z_n - u_n) \prec (Z_n - u_{n-1})$.

(d) By (2′), $(Z_n - v_n) = Z_{n-1} + x(Z_{n-1} - u_{n-1})$, $Z_n - u_n = Z_{n-1} + x(Z_{n-1} - u_{n-2})$.
By lemma 2(c), $(Z_{n-1} - u_{n-1}) \prec (Z_{n-1} - u_{n-2})(n - 1 \geqslant 2)$.
Therefore $(Z_n - v_n) \prec (Z_n - u_n)(n \geqslant 3)$.

The proof of lemma 2 is completed.

In order to use induction to prove theorem 4, we will prove the following theorem which contains more contents than that of theorem 4.

Theorem 6. For any integer $n \geqslant 3$ and any polyomino chain $T_n \in \mathcal{T}_n$,

(a) $(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1}) \preceq (T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1}) \preceq (Z_{n-1} - u_{n-1}) + (Z_{n-1} - u_{n-2})$,

(b) $(T_{n-1} - x_{n-1} - y_{n-1}) \preceq (Z_{n-1} - u_{n-1} - u_{n-2})$,

(c) $(T_n - x^{(n)}) \preceq (Z_n - u_n)$, $(T_n - y^{(n)}) \prec (Z_n - u_n)$,

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

Moreover, the equalities of the left-hand side of (a)(d) hold only if $T_n = L_n$; the equalities of (b)(c) and the right-hand side of (a)(d) hold only if $T_n = Z_n$.

Proof. First it's easy to see that if $T_n = L_n$, then the left-hand side of (a)(d)hold; if $T_n = Z_n$, (b)(c)(by lemma 2(c) and (d)) and the right-hand side of (a)(d) hold. Consequently, when we prove the left-hand side of (a)(d) we may assume that $T_n \neq L_n$; when we prove (b)(c) and the right-hand side of (a)(d) we may assume that $T_n \neq Z_n$.

Now let's prove theorem 6 by induction.

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

(a) By our assumptions we need only to prove $(L_2 - a_2) + (L_2 - b_2) \prec (Z_2 - u_2) + (Z_2 - u_1) = (L_2 - a_2) + (L_2 - a_1)$. And this is supported by lemma 2(a) and the fact that $(L_2 - a_2) = (L_2 - b_2)$.

(b) It is equivalent to prove $(L_2 - a_2 - b_2) \prec (Z_2 - u_2 - u_1)$. By lemma 2(b), $(L_2 - a_2 - b_2) \prec (L_2 - a_2 - a_1) = (Z_2 - u_2 - u_1)$. The result follows.

(c) Since $(L_3 - a_3) = (L_3 - b_3)$, we need only to prove $(L_3 - b_3) \prec (Z_3 - u_3)$.
By $(2')$, $(L_3 - b_3) = L_2 + x(L_2 - a_2)$, $(Z_3 - u_3) = Z_2 + x(Z_2 - u_1) = L_2 + x(L_2 - a_1)$.
By lemma 2(a), $(L_2 - a_2) \prec (L_2 - a_1)$.
Whence $(L_3 - b_3) \prec (Z_3 - u_3)$.

(d) By our assumptions we need only to prove $L_3 \prec Z_3$. By $(1')$, $L_3 = L_2 + x[(L_2 - a_2) + (L_2 - b_2)]$, $Z_3 = Z_2 + x[(Z_2 - u_2) + (Z_2 - u_1)]$. Then by (a) proved just now and the fact that $Z_2 = L_2$, we get that $L_3 \prec Z_3$.

Hence theorem 6 holds when $n = 3$.

(ii) Suppose the theorem holds for all polyomino chains with fewer than n ($n \geqslant 4$) squares. Let T_n be a polyomino chain with n squares ($n \geqslant 4$), which is obtained from $T_{n-1} \in \mathcal{T}_{n-1}$ by attaching to it a new cell t_n (figure 2(a)).
In the following we mostly consider $T_n^{(1)}, T_n^{(2)}$ instead of T_n.

(a) In $T_n^{(1)}$, by (2′), $(T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1}) = 2T_{n-2}+x[(T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2})]$.
Especially $(L_{n-1}-a_{n-1})+(L_{n-1}-b_{n-1}) = 2L_{n-2}+x[(L_{n-2}-a_{n-2})+(L_{n-2}-b_{n-2})]$.
In $T_n^{(2)}$, by (2′), claims 1(b), 2(b) and 3(b),
$(T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1}) = (T_{n-1}-x^{(n-1)})+(T_{n-1}-x_{n-2})$
$= T_{n-2}+x(T_{n-2}-y_{n-2})+(T_{n-1}-x_{n-2}-y^{(n-1)})+x(T_{n-1}-x_{n-2}-y^{(n-1)}-x^{(n-1)}-y_{n-2})$
$= T_{n-2}+x[(T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2})]+(T_{n-2}-x_{n-2})+x(T_{n-2}-x_{n-2}-y_{n-2})$
$\succ 2T_{n-2}+x[(T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2})]$.
Especially $(Z_{n-1}-u_{n-1})+(Z_{n-1}-u_{n-2})$
$= Z_{n-2}+x[(Z_{n-2}-u_{n-2})+(Z_{n-2}-u_{n-3})]+(Z_{n-2}-u_{n-2})+x(Z_{n-2}-u_{n-2}-u_{n-3})$
$\succ 2Z_{n-2}+x[(Z_{n-2}-u_{n-2})+(Z_{n-2}-u_{n-3})]$.
For the left-hand side, by the inductive hypotheses,
$L_{n-2} \preceq T_{n-2}, (L_{n-2}-a_{n-2})+(L_{n-2}-b_{n-2}) \preceq (T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2})$.
Whence in $T_n^{(2)}$, $(L_{n-1}-a_{n-1})+(L_{n-1}-b_{n-1}) \prec (T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1})$.
Since $T_n^{(1)} \neq L_n$, $T_{n-1} \neq L_{n-1}$, at least one of the inequalities must be strict. Whence
$(L_{n-1}-a_{n-1})+(L_{n-1}-b_{n-1}) \prec (T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1})$.
For the right-hand side, by the inductive hypotheses,
$T_{n-2} \preceq Z_{n-2}, (T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2}) \preceq (Z_{n-2}-u_{n-2})+(Z_{n-2}-u_{n-3})$.
Hence in $T_n^{(1)}$,$(T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1}) \prec (Z_{n-1}-u_{n-1})+(Z_{n-1}-u_{n-2})$.
In $T_n^{(2)}$, since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses, $T_{n-2} \preceq Z_{n-2}, (T_{n-2}-x_{n-2})+(T_{n-2}-y_{n-2}) \preceq (Z_{n-2}-u_{n-2})+(Z_{n-2}-u_{n-3}), (T_{n-2}-x_{n-2}) \preceq (Z_{n-2}-u_{n-2}),\quad (T_{n-2}-x_{n-2}-y_{n-2}) \preceq (Z_{n-2}-u_{n-2}-u_{n-3})$.
Since $T_n^{(2)} \neq Z_n$, $T_{n-1} \neq Z_{n-1}$, at least one of the inequalities must be strict. Therefore
$(T_{n-1}-x_{n-1})+(T_{n-1}-y_{n-1}) \prec (Z_{n-1}-u_{n-1})+(Z_{n-1}-u_{n-2})$.

(b) By (3′), $(Z_{n-1}-u_{n-1}-u_{n-2}) = (Z_{n-2}-u_{n-2})+x(Z_{n-2}-u_{n-2}-u_{n-3})$.

When $n \geqslant 4$, x_{n-2} must have another neighbor except y_{n-2} in T_{n-2}. Thus in $T_n^{(1)}$, by claims 2(b) and 3(b),
$(T_{n-1}-x_{n-1}-y_{n-1}) = T_{n-2} \prec (T_{n-2}-x_{n-2})+x(T_{n-2}-x_{n-2}-y_{n-2})$.
Since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses,
$(T_{n-2} - x_{n-2}) \preceq (Z_{n-2} - u_{n-2}), (T_{n-2} - x_{n-2} - y_{n-2}) \preceq (Z_{n-2} - u_{n-2} - u_{n-3})$.
It follows that $(T_{n-1} - x_{n-1} - y_{n-1}) \prec (Z_{n-1} - u_{n-1} - u_{n-2})$.
In $T_n^{(2)}$, by (3′), $(T_{n-1} - x_{n-1} - y_{n-1}) = (T_{n-1} - x^{(n-1)} - x_{n-2}) = (T_{n-2} - x_{n-2}) + x(T_{n-2} - x_{n-2} - y_{n-2})$
Since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses,
$(T_{n-2} - x_{n-2}) \preceq (Z_{n-2} - u_{n-2}), (T_{n-2} - x_{n-2} - y_{n-2}) \preceq (Z_{n-2} - u_{n-2} - u_{n-3})$.
Since $T_n^{(2)} \neq Z_n$, $T_{n-1} \neq Z_{n-1}$, at least one of the inequalities must be strict.
Therefore $(T_{n-1} - x_{n-1} - y_{n-1}) \prec (Z_{n-1} - u_{n-1} - u_{n-2})$.

(c) In $T_n^{(1)}$, by (2′) and lemma 2(c), $(T_n - x^{(n)}) = T_{n-1} + x(T_{n-1} - y_{n-1})$,
$(Z_n - u_n) = Z_{n-1} + x(Z_{n-1} - u_{n-2}) \succ Z_{n-1} + x(Z_{n-1} - u_{n-1})$.
Since $y_{n-1} \in \{x^{(n-1)}, y^{(n-1)}\}$, by the inductive hypotheses,
$Z_{n-1} \succeq T_{n-1}$, $(Z_{n-1} - u_{n-1}) \succeq (T_{n-1} - y_{n-1})$.
Whence $(T_n - x^{(n)}) \prec (Z_n - u_n)$.
Similarly we can show that $(T_n - y^{(n)}) \prec (Z_n - u_n)$.
In $T_n^{(2)}$, since $T_n^{(2)} \neq Z_n$, $T_{n-1} \neq Z_{n-1}$, by (2)
lemma 2(c) and the inductive hypotheses,
$(T_n - y^{(n)}) = T_{n-1} + x(T_{n-1} - x_{n-1}) = T_{n-1} + x(T_{n-1} - x^{(n-1)})$
$\prec Z_{n-1} + x(Z_{n-1} - u_{n-1}) \prec Z_{n-1} + x(Z_{n-1} - u_{n-2}) = Z_n - u_n$,
$(T_n - x^{(n)}) = T_{n-1} + x(T_{n-1} - y_{n-1}) = T_{n-1} + x(T_{n-1} - x_{n-2})$
$= T_{n-1} + x[(1 + x)(T_{n-2} - x_{n-2}) + x(T_{n-2} - x_{n-2} - y_{n-2})]$.
Especially $(Z_n - u_n) = Z_{n-1} + x[(1 + x)(Z_{n-2} - u_{n-2}) + x(Z_{n-2} - u_{n-2} - u_{n-3})]$.
Since $x_{n-2} \in \{x^{(n-2)}, y^{(n-2)}\}$, by the inductive hypotheses, $T_{n-1} \prec Z_{n-1}$, $(T_{n-2} - x_{n-2} - y_{n-2}) \preceq (Z_{n-2} - u_{n-2} - u_{n-3})$, $(T_{n-2} - x_{n-2}) \preceq (Z_{n-2} - u_{n-2})$.
It follows that if $T_n^{(2)} \neq Z_n$, then $(T_n - x^{(n)}) \prec (Z_n - u_n)$, $(T_n - y^{(n)}) \prec (Z_n - u_n)$.

(d) By (1′), $L_n = L_{n-1} + x[(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1})]$,
$T_n = T_{n-1} + x[(T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})]$.
By the inductive hypotheses, $L_{n-1} \preceq T_{n-1}$,
$(L_{n-1} - a_{n-1}) + (L_{n-1} - b_{n-1}) \preceq (T_{n-1} - x_{n-1}) + (T_{n-1} - y_{n-1})$.
Since $T_n \neq L_n$, at least one of the inequalities must be strict.
Whence $L_n \prec T_n$.

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

The proof of theorem 6 is completed.

Remark. Clearly our results imply the results of the extremal polymino chains with respective to their Hosoya index (the number of matchings) [18] and Merrifield-Simmons index (the number of independent sets) [22].

A further problem is to determine the extremal polyomino chain with respect to their total π-electron energy. The basic approach to compare the total π-electron energy is to compare the coefficients of their characteristic polynomials.

Let G be a bipartite graph with n vertices, its characteristic polynomial can be written as

$$\Phi(G) = |xI - A| = \Sigma_{k=0}^{\llcorner n/2 \lrcorner}(-1)^k b(G,k) x^{n-2k}, \quad (\triangle)$$

where A is the adjacency matrix of G. Note that $b(G,0) = 1$, $b(G,k) \geqslant 0$ for $0 \leqslant k \leqslant \llcorner n/2 \lrcorner$. For the other k, we assume $b(G,k) = 0$ for convenience. Let G be a molecular graph. The total π-electron energy of G is defined to be the sum of the absolute values of the roots of $\Phi(G)$. We denote it as

$$E(G) = \Sigma_{j=1}^{n} |\lambda_j|.$$

If for two bipartite graphs G_1 and G_2 whose characteristic polynomials are in the form $(\triangle)$, $b(G_1,k) \geqslant b(G_2,k)$ holds for all $k \geqslant 0$, we say that G_1 is not less than G_2, written as $G_1 \succeq G_2$. Moreover if $G_1 \succeq G_2$ and there exists some k such that $b(G_1,k) > b(G_2,k)$, then we write $G_1 \succ G_2$. It's well known that for two bipartite graphs G_1 and G_2, if $G_1 \succeq G_2$, then $E(G_1) \geqslant E(G_2)$. If $G_1 \succ G_2$, then $E(G_1) > E(G_2)$ [17]. We may compute the characteristic polynomial of a graph G by Mathematica. For example, we have computed that

$$\Phi(L_3) = |xI - L_3| = 1 - 10x^2 + 23x^4 - 10x^6 + x^8,$$
$$\Phi(Z_3) = |xI - Z_3| = 0 - 12x^2 + 22x^4 - 10x^6 + x^8,$$

where L_3 and Z_3 represent the linear chain and zig-zag chain of order 8, respectively. It's easy to see that $b(L_3,2) = 23 > 22 = b(Z_3,2)$ while $b(L_3,3) = 10 < 12 = b(Z_3,3)$. Therefore in order to determine the extremal polyomino chains with respect to their total π-electron energy, we need to find some new approach.

Another such kind of example on the octagonal chain has been found in [23] (example 3.7).

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