Extremal polyphenyl chains concerning k-matchings and k-independent sets

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Abstract: Denote by $\mathcal{A}_n$ the set of the polyphenyl chains with n hexagons. For any $A_n \in \mathcal{A}_n$, let $m_k(A_n)$ and $i_k(A_n)$ be the numbers of k-matchings and k-independent sets of A_n, respectively. In the paper, we show that for any $A_n \in \mathcal{A}_n$ and for any $k \geq 0$, $m_k(M_n) \leq m_k(A_n) \leq m_k(O_n)$ and $i_k(M_n) \geq i_k(A_n) \geq i_k(O_n)$, with the equalities hold if $A_n = M_n$ or $A_n = O_n$, where M_n and O_n are the meta-chain and the ortho-chain, respectively. These generalize some related results in [1].

Key Words: polyphenyl chain; k-matching; k-independent set

1 Introduction

The molecular graphs (or more precisely, the graphs representing the carbon-atoms) of polyphenyls are called the polyphenyl system. This kind of macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives attracted the attention of chemists for many years [2-4]. The derivatives of polyphenyls are very important organic chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc. Biphenyl compounds also have extensive industrial applications. For example, 4,4-bis(chloromethyl)biphenyl can be used for the synthesis of brightening agents. Especially, polychlorinated biphenyls (PCBs) can be applied in print and dyeing extensively [5, 6]. On the other side, PCBs are dangerous organic pollutants, which lead to global pollution. Many years ago, a series

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of linear and branched polyphenyls and their derivatives were synthesized and some physical properties were discussed [7-12].

A polyphenyl system is said to be *tree-like* if each one of its vertices lies in a hexagon and the graph obtained by contracting every hexagon into a vertex in original molecular graphs is a tree. A hexagon H in a tree-like polyphenyl system has either one, two or three (at most six) neighboring hexagons. If H has only one neighboring hexagon, then it is said to be *terminal*. If it has three or more neighboring hexagons then it is said to be *branched*. A tree-like polyphenyl system without branched hexagons is called a *polyphenyl chain*.

The number of hexagons in a polyphenyl chain is called its *length*. Let G be a polyphenyl chain of length n. If $n > 1$ then G has two so called the *terminal hexagons*, each one of which contains a unique vertex of degree 3; while all other are the *internal hexagons*. If H is an internal hexagon, then its two vertices u and v are in *ortho-position* if they are adjacent, and in *meta-position* if they are separated by a path of length 2. An internal hexagon in G is called *ortho-hexagon* if its two vertices with degree 3 are in ortho-position. G is an *ortho-chain* if all its internal hexagons are ortho-hexagons. The meta-chain can also be analogously defined. Figure 1 (a) and (b) illustrate ortho-chain and meta-chain, respectively.

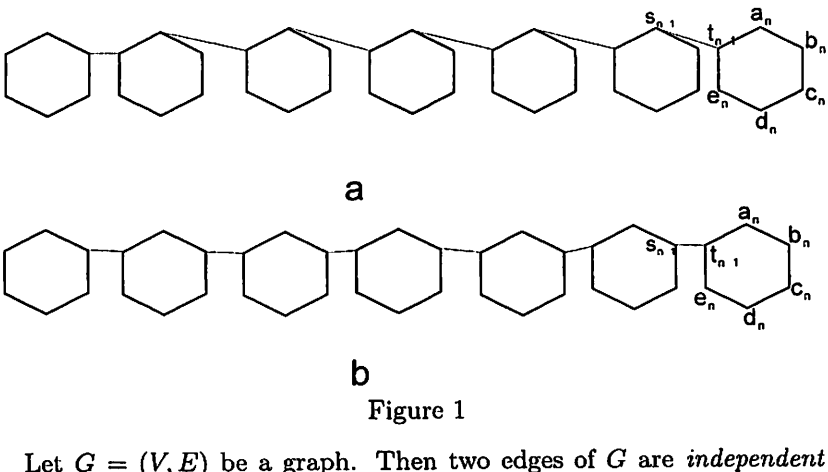

Figure 1

Let $G = (V, E)$ be a graph. Then two edges of G are *independent* if they are not incident. A subset M of E is called a *matching* of G if any two edges in M are independent. M is an *k-matching* if $| M |= k$. We denote by $m_k(G)$ the number of k-matchings of G.

Two vertices of G are *independent* if they are not adjacent. A subset I of V is called an *independent set* of G if any two vertices in I are independent. I is *k-independent* if $| I |= k$. We denote by $i_k(G)$ the number of k-independent sets of G.

In this paper, we show that *ortho*-polyphenyl chains and *meta*-polyphenyl chains are the extremal polyphenyl chains concerning k-matchings and k-independent sets. These generalize some related results in [1].

2 Some Preliminaries

The Z-polynomial (called Z-counting polynomial) was defined by Hosoya [13] as $Z(G) = \sum_k m_k(G)x^k$, which is a special case of the matching polynomial defined by Farrel, 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, $a_k \leq b_k$ $(0 \leq k \leq n)$; and $f(x) \prec g(x)$, if for each k, $a_k \leq b_k$ and there exists some k such that $a_k < b_k$ $(0 \leq k \leq n)$.

The following two lemmas are due to Farrell [14] and will be useful to the material which follows.

Lemma 1. *Suppose that G is a graph consisting of the components $G_1, G_2, \cdots, G_k$. Then*

(a) $Z(G) = Z(G_1) \cdot Z(G_2) \cdots Z(G_k)$,

(b) $Y(G) = Y(G_1) \cdot Y(G_2) \cdots Y(G_k)$.

Let $G = (V, E)$ be a graph and S be a subset of V. Then we denote by $G - S$ the subgraph of G obtained from G by removing all vertices of S. Specially, we write $G - u$ for $G - \{u\}$ if $S = \{u\}$. If $e \in E$ then we denote by $G - e$ the subgraph of G obtained from G by removing e.

Lemma 2. *Suppose that $e = vw$ is an edge of G and that N_u is the subset of $V(G)$ consisting of the vertex u and its neighbors. Then we have*

(a) $Z(G) = Z(G - e) + x \cdot Z(G - \{v, w\})$,

(b) $Y(G) = Y(G - u) + x \cdot Y(G - N_u)$.

3 Matchings in polyphenyl chains

Let $\mathcal{A}_n$ be a set consisting of all polyphenyl chains of length n. Then 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 hexagon H through an edge, as in Figure 2.

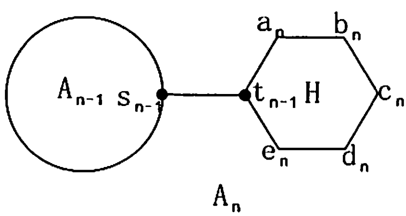

Figure 2

In this section, we will use the notation G for $Z(G)$ if no confusion arises. By (a) in Lemmas 1 and 2, we first obtain the following useful formulae.

$$A_n = HA_{n-1} + xP_5(A_{n-1} - s_{n-1}) \quad (1)$$

$$A_n - s = \begin{cases} P_5 A_{n-1} + xP_4(A_{n-1} - s_{n-1}) & \text{if } s = a_n, \\ P_5 A_{n-1} + xP_3(A_{n-1} - s_{n-1}) & \text{if } s = b_n, \\ P_5 A_{n-1} + x(1+x)^2(A_{n-1} - s_{n-1}) & \text{if } s = c_n. \end{cases} \tag{2}$$

By the formula (2), we can easily know

$$A_n - b_n \prec A_n - c_n \prec A_n - a_n \quad (n \geq 2). \tag{3}$$

We denote by O_n and M_n the ortho-chain and meta-chain, respectively. Now we use the known results to give the following theorem that contains the main results.

Theorem 3. *For any $A_n \in \mathcal{A}_n$ $(n \geq 3)$, we have*

(a) $M_n - b_n \preceq A_n - s \preceq O_n - a_n$ $(s \in \{a_n, b_n, c_n\})$;

(b) $M_n \preceq A_n \preceq O_n$.

Moreover, the above equalities hold if and only if $A_n = M_n$ and $s = b_n$, or $A_n = O_n$ and $s = a_n$.

Proof. If $A_n = M_n$ or $A_n = O_n$ then the results are obvious. So we below assume $A_n \neq M_n$ and $A_n \neq O_n$. We use the induction on n. Suppose $n = 3$. Then, by the formula (3), it suffices to show that $M_3 - b_3 \prec A_3 - b_3$ and $A_3 - a_3 \prec O_3 - a_3$ to prove (a). By the formula (2), we can obtain

$$M_3 - b_3 = P_5 M_2 + xP_3(M_2 - s_2) = P_5 M_2 + xP_3(M_2 - b_2)$$

$$A_3 - b_3 = P_5 A_2 + xP_3(A_2 - s_2) = P_5 M_2 + xP_3(M_2 - c_2)$$

This shows $M_3 - b_3 \prec A_3 - b_3$ by the formula (3). Similarly, we can show $A_3 - a_3 \prec O_3 - a_3$. By the formula (1), we have

$$M_3 = HM_2 + xP_5(M_2 - s_2) = HM_2 + xP_5(M_2 - b_2)$$

$$A_3 = HA_2 + xP_5(A_2 - s_2) = HA_2 + xP_5(A_2 - c_2) = HM_2 + xP_5(M_2 - c_2)$$

$$O_3 = HO_2 + xP_5(O_2 - s_2) = HO_2 + xP_5(O_2 - a_2) = HM_2 + xP_5(M_2 - a_2)$$

This shows $M_3 \prec L_3 \prec O_3$ by the formula (3).

Suppose next $n \geq 4$. By the formula (3), it suffices to show that $M_n - b_n \prec A_n - b_n$ and $A_n - a_n \prec O_n - a_n$ to prove (a). By the formula (2), we have

$$M_n - b_n = P_5 M_{n-1} + xP_3(M_{n-1} - s_{n-1}) = P_5 M_{n-1} + xP_3(M_{n-1} - b_{n-1})$$

$$A_n - b_n = P_5 A_{n-1} + xP_3(A_{n-1} - s_{n-1})$$

By the inductive hypotheses that $M_{n-1} \prec A_{n-1}$ and $M_{n-1} - b_{n-1} \prec A_{n-1} - s_{n-1}$, we have $M_n - b_n \prec A_n - b_n$. Similarly, we can also prove $A_n - a_n \prec O_n - a_n$.

By the formula (1), we get

$$M_n = HM_{n-1} + xP_5(M_{n-1} - s_{n-1}) = HM_{n-1} + xP_5(M_{n-1} - b_{n-1})$$
$$A_n = HA_{n-1} + xP_5(A_{n-1} - s_{n-1})$$
$$O_n = HO_{n-1} + xP_5(O_{n-1} - s_{n-1}) \prec HO_{n-1} + xP_5(O_{n-1} - a_{n-1})$$

By the inductive hypotheses that $M_{n-1} \prec A_{n-1} \prec O_{n-1}$ and $M_{n-1} - b_{n-1} \prec A_{n-1} - s_{n-1} \prec O_{n-1} - a_{n-1}$, we have $M_n \prec A_n \prec O_n$. □

As one consequence of Theorem 3, we have the following

Theorem 4. *For any $A_n \in \mathcal{A}_n$ $n \geq 3$,*

$$m_k(M_n) \leq m_k(A_n) \leq m_k(O_n).$$

Moreover, the above equality holds for each k if and only if $A_n = M_n$ or $A_n = O_n$.

Finally, we give the recurrences of matching polynomial on O_n and M_n. We first give the following basic results, that is

$$O_0 = M_0 = 1;$$
$$O_1 = M_1 = 1 + 6x + 9x^2 + 2x^3.$$

Theorem 5. *If $n \geq 2$, then we have*

(a) $O_n = (H + xP_4)O_{n-1} + x(P_5^2 - P_4H)O_{n-2}$,

(b) $M_n = (H + xP_3)M_{n-1} + x(P_5^2 - P_3H)M_{n-2}$.

Proof. We use the induction on n. Suppose that O_n is as in Figure 1. If $n = 2$ then (a) is clearly true. So we assume $n \geq 3$. Deleting the edge $s_{n-1}t_{n-1}$, by (a) in Lemmas 1 and 2, we have

$$\begin{aligned} O_n &= (O_n - s_{n-1}t_{n-1}) + x(O_n - s_{n-1} - t_{n-1}) \\ &= O_{n-1}H + xP_5(O_{n-1} - a_{n-1}) \end{aligned} \tag{2.1}$$

Note that

$$\begin{aligned} O_{n-1} - a_{n-1} &= (O_{n-1} - a_{n-1} - s_{n-2}t_{n-2}) + x(O_{n-1} - a_{n-1} - s_{n-2} - t_{n-2}) \\ &= P_5O_{n-2} + xP_4(O_{n-2} - a_{n-2}) \end{aligned} \tag{2.2}$$

The result follows from (2.1) and (2.2). Similarly, we can show that (b) is also true. □

4 Independent sets in polyphenyl chains

In this section, we will use the notation G for $Y(G)$ when it would lead to no confusion. By (b) in Lemmas 1 and 2, we first obtain the following useful formulae.

$$A_n = P_5A_{n-1} + xP_3(A_{n-1} - s_{n-1}) \tag{1'}$$

$$A_n - s = \begin{cases} (1+4x+3x^2)A_{n-1} + x(1+3x+x^2)(A_{n-1} - s_{n-1}) & \text{if } s = a_n, \\ (1+4x+4x^2+x^3)A_{n-1} + x(1+2x)(A_{n-1} - s_{n-1}) & \text{if } s = b_n, \\ (1+2x)^2 A_{n-1} + x(1+x)^2(A_{n-1} - s_{n-1}) & \text{if } s = c_n. \end{cases} \quad (2')$$

According to formula (2′), we can easily know

$$A_n - b_n \succ A_n - c_n \succ A_n - a_n. \quad (3')$$

Using formulae (2′) and (3′), we can prove the following Theorem 6 as in the proof of Theorem 3.

Theorem 6. *For any $A_n \in \mathcal{A}_n$ $(n \geq 3)$,*

(a) $M_n - b_n \succeq A_n - s \succeq O_n - a_n$, *where* $s \in \{a_n, b_n, c_n\}$;

(b) $M_n \succeq A_n \succeq O_n$.

Moreover, the above equalities hold if and only if $A_n = M_n$ and $s = b_n$ or $A_n = O_n$ and $s = a_n$.

The following result is an immediate consequence of Theorem 6.

Theorem 7. *For any $A_n \in \mathcal{A}_n$ and each $k \geq 0$,*

$$i_k(O_n) \leq i_k(A_n) \leq i_k(M_n)$$

Moreover, the above equalities hold for each k if and only if $A_n = O_n$ or $A_n = M_n$.

Similar to the matching polynomial, we also have the recurrences of polynomial of independent set on O_n and M_n.

$$O_0 = M_0 = 1;$$
$$O_1 = M_1 = 1 + 6x + 9x^2 + 2x^3.$$

Theorem 8. *If $n \geq 2$, then we have*

(a) $O_n = (P_5 + xP_3)O_{n-1} + xP_3(P_4 - P_5)O_{n-2}$;

(b) $M_n = (P_5 + xP_2)M_{n-1} + x(P_1P_3^2 - P_2P_5)M_{n-2}$.

Proof. Suppose that the chain O_n is as in Figure 1. If $n = 2$ then we can easily verify that (a) is true. So we next assume $n \geq 3$. Deleting t_{n-1}, by (b) in Lemmas 1 and 2, we have

$$\begin{aligned} O_n &= (O_n - t_{n-1}) + x(O_n - N_{t_{n-1}}) \\ &= P_5 O_{n-1} + xP_3(O_{n-1} - a_{n-1}) \end{aligned} \quad (2.1')$$

Note that

$$\begin{aligned} O_{n-1} - a_{n-1} &= (O_{n-1} - a_{n-1} - t_{n-2}) + x(O_{n-1} - a_{n-1} - N_{t_{n-2}}) \\ &= P_4 O_{n-2} + xP_3(O_{n-2} - a_{n-2}) \end{aligned} \quad (2.2')$$

The result follows from (2.1′) and (2.2′). Similarly, we can show that (b) is also true. □

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