Extremal Polyphenyl Spiders Concerning k-matchings and k-independent Sets*

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Abstract. Denote by $\mathscr{S}(n_1, n_2, n_3)$ the set of all polyphenyl spiders with three legs of lengths n_1, n_2 and n_3. Let $S^j(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)(j \in \{1, 2, 3\})$ be three non-isomorphic polyphenyl spiders with three legs of lengths n_1, n_2 and n_3, and let $m_k(G)$ and $i_k(G)$ be the numbers of k-matchings and k-independent sets of a graph G, respectively. In this paper, we show that for any $S^j(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)(j \in \{1, 2, 3\})$, we have $m_k(S^3_M(n_1, n_2, n_3)) \leq m_k(S^j(n_1, n_2, n_3)) \leq m_k(S^1_O(n_1, n_2, n_3))$ and $i_k(S^1_O(n_1, n_2, n_3)) \leq i_k(S^j(n_1, n_2, n_3)) \leq i_k(S^3_M(n_1, n_2, n_3))$, with the equalities if and only if $S^j(n_1, n_2, n_3) = S^3_M(n_1, n_2, n_3)$ or $S^j(n_1, n_2, n_3) = S^1_O(n_1, n_2, n_3)$, where $S^1_O(n_1, n_2, n_3)$ and $S^3_M(n_1, n_2, n_3)$ are respectively an ortho-polyphenyl spider and a meta-polyphenyl spider.
Key words: Polyphenyl spider; k-matching; k-independent set

1 Introduction

Let $G = (V, E)$ be a graph. For $x \in V$ and $e \in E$, we use $G - x$ and $G - e$ to denote the graphs obtained from G by deleting x (and all its adjacent edges) and by deleting e, respectively. More generally, for $S \subseteq V$ or $S \subseteq E$, we denote by $G - S$ the graph obtained from G by deleting all the elements of S. The open neighborhood of a vertex u is denoted by $N(u)$ and the closed neighborhood of u is denoted by $N[u] = N(u) \cup \{u\}$. Our standard reference for graph theoretical terminology is [3].

A set $M \subseteq E$ is called a matching of G if any two edges of M are independent in G. A matching M is called a k-matching if $|M| = k$. We denote by $m(G)$ and $m_k(G)$ the numbers of matchings and k-matchings of G, respectively. Obviously, $m(G) = \sum_k m_k(G)$.

A set $I \subseteq V$ is called an independent set of G if any two vertices of I are independent in G. An independent set I is said to be a k-independent set if $|I| = k$. We denote by $i(G)$ and $i_k(G)$ the numbers of independent sets and k-independent sets of G, respectively. Obviously, $i(G) = \sum_k i_k(G)$.

It is well known that the graph invariants $m(G)$ and $i(G)$, called "Hosoya index" [10] and "Merrifield-Simmons index" [14] respectively, are important ones in structural chemistry. For chemical applications of these two indices we refer to [8], [9], [11], [14] and [16]. In recent years, quite a lot of

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works have been done on the extremal problems for these two indices, i.e., the problems of determining the graphs within certain prescribed classes which maximize or minimize the indices values (see, e.g. [1], [13], [15] and [17]).

Note that there are some works on the extremal problems pertaining to k-matchings and k-independent sets which imply the results of extremal problems of "Hosoya index" and "Merrifield-Simmons index" In 2000, Zhang and Zhang[19] obtained extremal hexagonal chains concerning k-matchings and k-independent sets. In 2007, Zeng and Zhang [18] obtained extremal polyomino chains on k-matchings and k-independent sets. In 2010, Li, Bian, Zhang and Wang [12] obtained extremal polyphenyl chains concerning k-matchings and k-independent sets. For more mathematical and mathematico-chemical results on polyphenyl chains see, for example, [2], [4], [5], [7] and the references cited therein.

In the remainder of the section, we give the definitions of some chemical graphs and fix symbols and terminology.

A polyphenyl system is said to be tree-like if each 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 C in a tree-like polyphenyl system could have one to at most six neighboring hexagons. If C has only one neighboring hexagon, then it is said to be terminal, and if C has at least three neighboring hexagons, then it is called branched hexagon. A tree-like polyphenyl system without branched hexagons is called a polyphenyl chain.

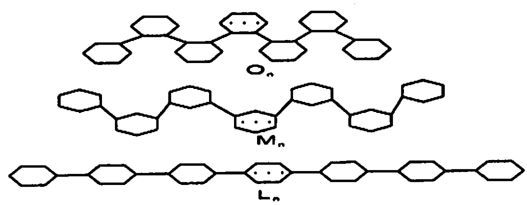


Fig. 1: ortho-polyphenyl, meta-polyphenyl and para-polyphenyl chain (O_n, M_n, L_n).

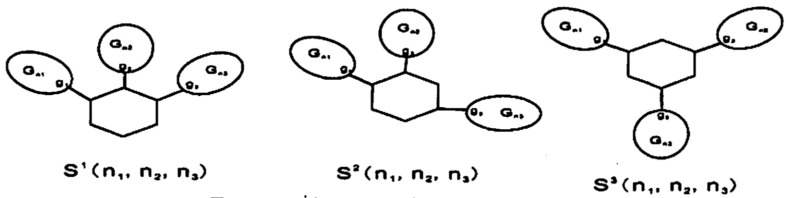
The number of hexagons in a polyphenyl chain is called its length. Let G be a polyphenyl chain of length n. If $n > 1$, then G has two terminal hexagons, each of which contains a unique vertex of degree 3, while all others are the internal hexagons. If C is an internal hexagon, then its two vertices of degree 3 are in ortho-position if they are adjacent, in meta-position if they are connected by a path of length 2, and in para-position if they are connected by a path of length 3. An internal hexagon in G is called an ortho-hexagon if its two vertices of degree 3 are in ortho-position. G is an ortho-chain if all its internal hexagons are ortho-hexagons. The meta-chain and para-chain can be analogously defined. Denote by $\mathscr{A}_n$ the set of polyphenyl chains with n hexagons. Figure.1 illustrates an ortho-polyphenyl chain, a meta-polyphenyl chain and a para-polyphenyl chain.

A graph G is called a spider (or spider graph) if it is a tree and contains only one vertex of degree greater than 2. Such vertex is called the center of the spider. A polyphenyl system H is called a polyphenyl spider if its tree-like graph is a spider with maximum degree 3, (i.e., the degree of the center vertex of the tree-like graph of H is 3).

Suppose S is a polyphenyl spider. Let C be the center hexagon of S. Then $S-C$ consists of three components, each of which is called a leg of S.

Let S_C be the tree-like graph of S. The polyphenyl chains corresponding to the legs of S_C are called the legs of S. The number of hexagons contained in a leg is called the length of the leg.

For positive integers n_1, n_2, n_3, we denote by $\mathscr{S}(n_1, n_2, n_3)$ the set of all polyphenyl spiders with three legs of lengths n_1, n_2, n_3, and by $S^j(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)$ the non-isomorphic polyphenyl spiders with three legs of lengths n_1, n_2 and n_3, $j \in \{1, 2, 3\}$. Let G_{n_1}, G_{n_2} and G_{n_3} denote the three legs of $S^j(n_1, n_2, n_3)$ for $j \in \{1, 2, 3\}$, see Figure 2.



$S^1(n_1, n_2, n_3)$ $S^2(n_1, n_2, n_3)$ $S^3(n_1, n_2, n_3)$

Fig. 2: $S^j(n_1, n_2, n_3)$ for $j \in \{1, 2, 3\}$.

If the three legs of a polyphenyl spider $S^j(n_1, n_2, n_3)$ are all ortho-polyphenyl chain (or meta-polyphenyl chain, para-polyphenyl chain, respectively), then such a graph is denoted by $S_O^j(n_1, n_2, n_3)$(or $S_M^j(n_1, n_2, n_3)$, $S_N^j(n_1, n_2, n_3)$, respectively) for $j \in \{1, 2, 3\}$.

Shiu [15] gives the extremal Hosoya index and Merrifield-Simmons index of the hexagonal spiders. Here, we consider the extremal polypnenyl spiders concerning k-matchings and k-independent sets. We show that for any $S^j(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)$, $j \in \{1, 2, 3\}$, we have $m_k(S_M^3(n_1, n_2, n_3)) \leq m_k(S^j(n_1, n_2, n_3)) \leq m_k(S_O^1(n_1, n_2, n_3))$ and $i_k(S_O^1(n_1, n_2, n_3)) \leq i_k(S^j(n_1, n_2, n_3)) \leq i_k(S_M^3(n_1, n_2, n_3))$, with the equalities if and only if $S^j(n_1, n_2, n_3) = S_M^3(n_1, n_2, n_3)$ or $S^j(n_1, n_2, n_3) = S_O^1(n_1, n_2, n_3)$.

2 Preliminaries

The Z-polynomial (also called Z-counting polynomial) was defined by Hosoya [10] as $Z(G) = \sum_k m_k x^k$, which is a special case of the matching polynomial defined by Farrell [6] and has essentially the same combinatorial contents as the matching polynomial. The Y-polynomial, related to independent sets of a graph G, is defined as $Y(G) = \sum_k i_k x^k$.

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 in x. We say $f(x) \preceq g(x)$ if $a_k \leq b_k$ $(0 \leq k \leq n)$, and $f(x) \prec g(x)$ if $f(x) \preceq g(x)$ and there exists an l $(0 \leq l \leq n)$ such that $a_l < b_l$.

The following two lemmas are due to Farrell [6] and will be used.

Lemma 2.1 *Let G be a graph with the components $G_1, G_2, \ldots, G_k$. Then* (a) $Z(G)=Z(G_1) \cdot Z(G_2) \cdots Z(G_k)$; (b) $Y(G)=Y(G_1) \cdot Y(G_2) \cdots Y(G_k)$.

Lemma 2.2 *Suppose that $e = vw$ is an edge of G and $N(u)$ is the neighborhood of u in G. Then we have*
(a) $Z(G)=Z(G-e)+x \cdot Z(G-\{v, w\})$; (b) $Y(G)=Y(G-u)+x \cdot Y(G-N(u))$.

Among polyphenyl chains with extremal topological indices, O_n and M_n play important roles. We conclude this section by listing some known results on k-matchings and k-independent sets of polyphenyl chains.

Theorem 2.1 *([12])For any $A_n \in \mathscr{A}_n$, $n \geq 3$*

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

Moreover, the equality of the left-hand side (right-hand side, respectively) holds for each k only if $A_n = M_n$ ($A_n = O_n$, respectively).

Theorem 2.2 *([12])For any $A_n \in \mathscr{A}_n$, and each $k \geq 0$*

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

Moreover, the equality of the left-hand side (right-hand side, respectively) holds for each k only if $A_n = O_n$ ($A_n = M_n$, respectively).

3 Matchings in polyphenyl spiders

Recall that $\mathscr{A}_n$ is the set of all polyphenyl chains of length n. Let P_n denote a path of order n. Any element A_n of $\mathscr{A}_n$ can be obtained from an appropriately chosen graph $A_{n-1} \in \mathscr{A}_{n-1}$ by attaching a new hexagon C through an edge, as shown in Figure 3.

Employing Lemma 2.1(a) and Lemma 2.2(a), we can obtain the following two useful formulae:

$$Z(A_n) = Z(C) \cdot Z(A_{n-1}) + x \cdot Z(P_5) \cdot Z(A_{n-1} - s_{n-1}), \qquad (1)$$

where $Z(C) = 1 + 6x + 9x^2 + 2x^3$, $Z(P_5) = 1 + 4x + 2x^2$.

$$Z(A_n - s) = \begin{cases} Z(P_5) \cdot Z(A_{n-1}) + x \cdot Z(P_4) \cdot Z(A_{n-1} - s_{n-1}) \text{ if } s = a_n; \\ Z(P_5) \cdot Z(A_{n-1}) + x \cdot Z(P_3) \cdot Z(A_{n-1} - s_{n-1}) \text{ if } s = b_n; \\ Z(P_5) \cdot Z(A_{n-1}) + x \cdot (1+x)^2 \cdot Z(A_{n-1} - s_{n-1}) \text{ if } s = c_n, \end{cases} \qquad (2)$$

where $Z(P_4) = 1 + 3x + x^2$, $Z(P_3) = 1 + 2x$.

By formulae (1) and (2), we can easily know that

$$Z(A_n - s) \preceq Z(A_n), \qquad (s \in \{a_n, b_n, c_n\}). \qquad (3)$$

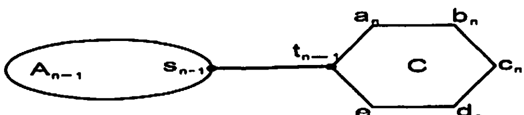


Fig. 3: A_n.

Lemma 3.1*For $S^1(n_1,n_2,n_3), S^2(n_1,n_2,n_3), S^3(n_1,n_2,n_3) \in \mathscr{S}(n_1,n_2,n_3)$, we have $Z(S^3(n_1,n_2,n_3)) \preceq Z(S^2(n_1,n_2,n_3)) \preceq Z(S^1(n_1,n_2,n_3))$.*

Proof. Let $S^j(n_1,n_2,n_3) \in \mathscr{S}(n_1,n_2,n_3)$ $j \in \{1,2,3\}$, and let g_1, g_2 and g_3 be the three vertices given in Figure 2. Then by Lemmas 2.1(a) and 2.2(a), we can obtain the following formulae:

$Z(S^1(n_1,n_2,n_3))$
$= Z(C) \cdot Z(G_{n_1}) \cdot Z(G_{n_2}) \cdot Z(G_{n_3}) + x \cdot Z(P_5) \cdot Z(G_{n_1}) \cdot Z(G_{n_2} - g_2) \cdot Z(G_{n_3})$
$+ x \cdot Z(P_5) \cdot Z(G_{n_1} - g_1) \cdot Z(G_{n_2}) \cdot Z(G_{n_3}) + x^2 \cdot Z(P_4) \cdot Z(G_{n_1} - g_1) \cdot Z(G_{n_2} -$

$g_2)\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3)+ x^2\cdot Z(P_4)\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3) + x^2\cdot Z(P_3)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3) + x^3\cdot Z(P_3)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3);$

$Z(S^2(n_1,n_2,n_3))$
$= Z(C)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}) + x^2\cdot Z(P_4)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3)+ x^2\cdot Z(P_3)\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3) + x^2\cdot Z^2(P_2)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3) + x^3\cdot Z(P_2)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3);$

$Z(S^3(n_1,n_2,n_3))$
$= Z(C)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}) + x^2\cdot Z(P_3)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}) + x\cdot Z(P_5)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3)+ x^2\cdot Z(P_3)\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3) + x^2\cdot Z(P_3)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3) + x^3\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3).$

By formula (3), we have
$Z(S^2(n_1,n_2,n_3)) - Z(S^1(n_1,n_2,n_3))$
$=(x^2\cdot Z(P_3) - x^2\cdot Z(P_4))\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3) + (x^2\cdot Z^2(P_2) - x^2\cdot Z(P_3))\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3) + (x^3\cdot Z(P_2) - x^3\cdot Z(P_3))\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3)$
$= (-x^3 - x^4)\cdot Z(G_{n_1})\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3) + x^4\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2})\cdot Z(G_{n_3}-g_3) + (-x^4)\cdot Z(G_{n_1}-g_1)\cdot Z(G_{n_2}-g_2)\cdot Z(G_{n_3}-g_3)$
$\preceq (-x^3 - x^4)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}) + x^4\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}) + (-x^4)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3})$
$= (-x^3 - x^4)\cdot Z(G_{n_1})\cdot Z(G_{n_2})\cdot Z(G_{n_3}) \preceq 0,$
so $Z(S^2(n_1,n_2,n_3)) \preceq Z(S^1(n_1,n_2,n_3))$.

Similarly, we can show that $Z(S^3(n_1,n_2,n_3)) \preceq Z(S^2(n_1,n_2,n_3))$. Hence $Z(S^3(n_1,n_2,n_3)) \preceq Z(S^2(n_1,n_2,n_3)) \preceq Z(S^1(n_1,n_2,n_3))$.

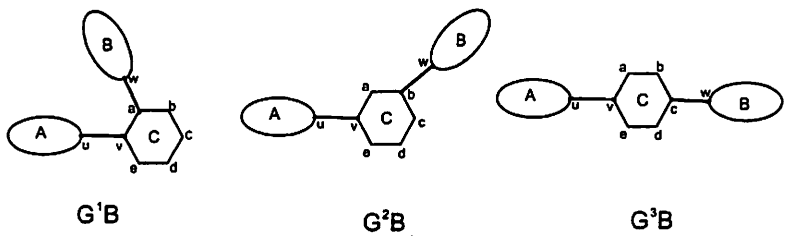


Fig. 4: G^1B, G^2B and G^3B.

Lemma 3.2 *([12]) For any $A_n \in \mathscr{A}_n$ $(n \geq 3)$. We have*

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

Suppose A is a graph and $C = abcdeva$ is a hexagon. Let G be a graph obtained from A and C by joining u and v, where $u \in V(A)$. The graph G obtained in this way will be denoted by $G = A \oplus_v^u C$.

Let $G = A \oplus_v^u C$, and B be any graph with $w \in V(B)$. Denote by G^1B the graph obtained from G and B with add-on edge defined by joining a to w, by G^2B from G and B with add-on edge defined by joining b to w, by G^3B from G and B with add-on edge defined by joining c to w, see Fig. 4.

Lemma 3.3 *Let G^1B, G^2B and G^3B be three graphs as shown in Fig.4. Then $Z(G^2B) \preceq Z(G^3B) \preceq Z(G^1B)$.*

Proof. By Lemmas 2.1(a) and 2.2(a)

$Z(G^1B)=Z(C)\cdot Z(A)\cdot Z(B) + x\cdot Z(P_5)\cdot Z(A)\cdot Z(B-w)+ x\cdot Z(P_5)\cdot Z(A-u)\cdot Z(B) + x^2\cdot Z(P_4)\cdot Z(A-u)\cdot Z(B-w)$;

$Z(G^2B)=Z(C)\cdot Z(A)\cdot Z(B) + x\cdot Z(P_5)\cdot Z(A)\cdot Z(B-w) + x\cdot Z(P_5)\cdot Z(A-u)\cdot Z(B) + x^2\cdot Z(P_3)\cdot Z(A-u)\cdot Z(B-w)$;

$Z(G^3B)=Z(C)\cdot Z(A)\cdot Z(B) + x\cdot Z(P_5)\cdot Z(A)\cdot Z(B-w) + x\cdot Z(P_5)\cdot Z(A-u)\cdot Z(B) + x^2\cdot Z^2(P_2)\cdot Z(A-u)\cdot Z(B-w)$,

where $Z(P_4) = 1+3x+x^2$, $Z(P_3) = 1+2x$, $Z(P_2) = 1+x$. So $Z(G^2B) \preceq Z(G^3B) \preceq Z(G^1B)$.

Theorem 3.1 *If $S^1(n_1,n_2,n_3) \in \mathscr{S}(n_1,n_2,n_3)$ has the maximum k-matchings among all the polyphenyl spiders in $\mathscr{S}(n_1,n_2,n_3)$, then $S^1(n_1,n_2,n_3)$ is an orhto-polyphenyl spider $S_O^1(n_1,n_2,n_3)$.*

Proof. Suppose the contrary, that $S^1(n_1,n_2,n_3)$ has the maximum k-matchings and one of its legs together with the central hexagon C is not an ortho-polyphenyl chain. Without loss of generality, we may assume that this chain is $B = CC_1C_2\cdots C_{n_1}$, i.e., there exist two adjacent hexagons which are not in ortho-position. In this case $n_1 \geq 2$. Let k be the least integer such that C_k, C_{k+1} form a non-ortho-polyphenyl chain for some k with $2 \leq k \leq n_1 - 1$.

Let $K{=}S^1(n_1,n_2,n_3) - (C_1 \cup C_2 \cup \cdots \cup C_k)$ and O_k be an ortho-polyphenyl chain with k hexagons. Then O_k^tK is a polyphenyl spider of type $S^1(n_1,n_2,n_3)$ for $t \in \{1,2,3\}$. By Lemma 3.1 and 3.3 we have $Z(S^1(n_1,n_2,n_3)) \prec Z(O_k^1K)$, since $O_k^1K \in \mathscr{S}(n_1,n_2,n_3)$, a contradiction.

By using Lemmas 3.1, 3.3 and a similar argument as that in the proof of Theorem 3.1, we have the following two theorems.

Theorem 3.2 *If $S^3(n_1,n_2,n_3) \in \mathscr{S}(n_1,n_2,n_3)$ has the minimum k-matchings among all the polyphenyl spiders in $\mathscr{S}(n_1,n_2,n_3)$, then $S^3(n_1,n_2,n_3)$ is a meta-polyphenyl spider $S_M^3(n_1,n_2,n_3)$.*

Theorem 3.3 *For $S^j(n_1,n_2,n_3) \in \mathscr{S}(n_1,n_2,n_3)$ $j \in \{1,2,3\}$, we have $m_k(S_M^3(n_1,n_2,n_3)) \leq m_k(S^j(n_1,n_2,n_3)) \leq m_k(S_O^1(n_1,n_2,n_3))$, with the equalities if and only if $S^j(n_1,n_2,n_3) = S_M^3(n_1,n_2,n_3)$ or $S^j(n_1,n_2,n_3) = S_O^1(n_1,n_2,n_3)$.*

Corollary 3.1 *For $S^j(n_1,n_2,n_3) \in \mathscr{S}(n_1,n_2,n_3)$ $j \in \{1,2,3\}$, we have $m(S_M^3(n_1,n_2,n_3)) \leq m(S^j(n_1,n_2,n_3)) \leq m(S_O^1(n_1,n_2,n_3))$, with the equalities if and only if $S^j(n_1,n_2,n_3) = S_M^3(n_1,n_2,n_3)$ or $S^j(n_1,n_2,n_3) = S_O^1(n_1,n_2,n_3)$.*

4 Independent sets in polyphenyl spiders

By Lemmas 2.1(b) and 2.2(b), we first obtain the following useful formulae.

$$Y(A_n) = Y(P_5)\cdot Y(A_{n-1}) + x\cdot Y(P_3)\cdot Y(A_{n-1}-s_{n-1}), \qquad (4)$$

where $Y(P_5) = 1+5x+6x^2+x^3$ and $Y(P_3) = 1+3x+x^2$.

$$Y(A_n - s) = \begin{cases} (1+4x+3x^2)\cdot Y(A_{n-1}) + x(1+3x+x^2)\cdot Y(A_{n-1}-s_{n-1}) & \text{if } s = a_n; \\ (1+4x+4x^2+x^3)\cdot Y(A_{n-1}) + x(1+2x)\cdot Y(A_{n-1}-s_{n-1}) & \text{if } s = b_n; \\ (1+2x)^2\cdot Y(A_{n-1}) + x\cdot(1+x)^2\cdot Y(A_{n-1}-s_{n-1}) & \text{if } s = c_n. \end{cases} \qquad (5)$$

By formulae (4) and (5), one can see that

$$Y(A_n - s) \preceq Y(A_n), \qquad (s\in\{a_n, b_n, c_n\}) \qquad (6)$$

Lemma 4.1*For $S^1(n_1,n_2,n_3)$,$S^2(n_1,n_2,n_3)$, $S^3(n_1,n_2,n_3)\in\mathscr{S}(n_1,n_2,n_3)$, we have $Y(S^1(n_1,n_2,n_3))\preceq Y(S^2(n_1,n_2,n_3))\preceq Y(S^3(n_1,n_2,n_3))$.*

Proof. For $S^j(n_1,n_2,n_3)\in\mathscr{S}(n_1,n_2,n_3)$, by Lemmas 2.1($b$) and 2.2($b$), we can see that

$Y(S^1(n_1,n_2,n_3)) = Y(P_3)\cdot Y(G_{n_1})\cdot Y(G_{n_2})\cdot Y(G_{n_3}) + x\cdot Y(P_3)\cdot Y(G_{n_1})\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}) + x\cdot Y(P_2)\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2})\cdot Y(G_{n_3}) + x\cdot Y(P_2)\cdot Y(G_{n_1})\cdot Y(G_{n_2})\cdot Y(G_{n_3}-g_3) + x^2\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2})\cdot Y(G_{n_3}-g_3)$;

$Y(S^2(n_1,n_2,n_3)) = Y(P_2)\cdot Y(G_{n_1})\cdot Y(G_{n_2})\cdot Y(G_{n_3}) + x\cdot Y(P_2)\cdot Y(G_{n_1})\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}) + x\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2})\cdot Y(G_{n_3}) + x\cdot Y(G_{n_1})\cdot Y(G_{n_2})\cdot Y(G_{n_3}-g_3) + x^2\cdot Y(G_{n_1})\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}-g_3) + x^2\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2})\cdot Y(G_{n_3}-g_3)$;

$Y(S^3(n_1,n_2,n_3)) = Y(G_{n_1})\cdot Y(G_{n_2})\cdot Y(G_{n_3}) + x\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2})\cdot Y(G_{n_3}) + x\cdot Y(G_{n_1})\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}) + x^2\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}) + x\cdot Y(G_{n_1})\cdot Y(G_{n_2})\cdot Y(G_{n_3}-g_3) + x^2\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2})\cdot Y(G_{n_3}-g_3) + x^2\cdot Y(G_{n_1})\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}-g_3) + x^3\cdot Y(G_{n_1}-g_1)\cdot Y(G_{n_2}-g_2)\cdot Y(G_{n_3}-g_3)$.

Using a similar argument as that of the proof of Lemma 3.1, we can show that $Y(S^1(n_1,n_2,n_3))\preceq Y(S^2(n_1,n_2,n_3))\preceq Y(S^3(n_1,n_2,n_3))$.

Lemma 4.2 *([12]) For any $A_n\in\mathscr{A}$ $(n\geq 3)$, $Y(O_n)\preceq Y(A_n)\preceq Y(M_n)$.*

Lemma 4.3 *Let A, B, $G{=}A\oplus_v^u C$, G^1B, G^2B and G^3B be the graphs given in Fig.4. Then $Y(G^1B)\preceq Y(G^3B)\preceq Y(G^2B)$.*

Proof. By Lemmas 2.1(b) and 2.2(b)

$$\begin{aligned} Y(G^1B) &= Y(P_4)\cdot Y(A)\cdot Y(B) + x\cdot Y(P_3)\cdot Y(A)\cdot Y(B-w) \\ &\quad + x\cdot Y(P_3)\cdot Y(A-u)\cdot Y(B); \\ Y(G^2B) &= Y(P_3)\cdot Y(A)\cdot Y(B) + x\cdot Y(P_2)\cdot Y(A)\cdot Y(B-w) \\ &\quad + x\cdot Y(P_2)\cdot Y(A-u)\cdot Y(B) + x^2\cdot Y(A-u)\cdot Y(B-w); \\ Y(G^3B) &= Y^2(P_2)\cdot Y(A)\cdot Y(B) + x\cdot Y(A)\cdot Y(B-w) \\ &\quad + x\cdot Y(A-u)\cdot Y(B) + x^2\cdot Y(A-u)\cdot Y(B-w), \end{aligned}$$

where $Y(P_4) = 1 + 4x + 3x^2$, $Y(P_3) = 1 + 3x + x^2$, $Y(P_2) = 1 + 2x$. So $Y(G^1B) \preceq Y(G^3B) \preceq Y(G^2B)$.

Using the lemmas established in this section and a similar argument as that of the proof of Theorem 3.1, it is not difficult to prove the following three theorems, here we omit the proofs.

Theorem 4.1 *If $S^3(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)$ has the maximum k-independent sets among all the polyphenyl spiders in $\mathscr{S}(n_1, n_2, n_3)$, then $S^3(n_1, n_2, n_3)$ is a meta-polyphenyl spider $S_M^3(n_1, n_2, n_3)$.*

Theorem 4.2 *If $S^1(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)$ has the minimum k-independent sets among all the polyphenyl spiders in $\mathscr{S}(n_1, n_2, n_3)$, then $S^1(n_1, n_2, n_3)$ is an orhto-polyphenyl spider $S_O^1(n_1, n_2, n_3)$.*

Theorem 4.3 *For $S^j(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)$ $j \in \{1, 2, 3\}$, we have $i_k(S_O^1(n_1, n_2, n_3)) \leq i_k(S^j(n_1, n_2, n_3)) \leq i_k(S_M^3(n_1, n_2, n_3))$, with the equalities if and only if $S^j(n_1, n_2, n_3) = S_O^1(n_1, n_2, n_3)$ or $S^j(n_1, n_2, n_3) = S_M^3(n_1, n_2, n_3)$.*

Corollary 4.1 *For $S^j(n_1, n_2, n_3) \in \mathscr{S}(n_1, n_2, n_3)$ $j \in \{1, 2, 3\}$, we have $i(S_O^1(n_1, n_2, n_3)) \leq i(S^j(n_1, n_2, n_3)) \leq i(S_M^3(n_1, n_2, n_3))$, with the equalities if and only if $S^j(n_1, n_2, n_3) = S_O^1(n_1, n_2, n_3)$ or $S^j(n_1, n_2, n_3) = S_M^3(n_1, n_2, n_3)$.*

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