On the Merrifield-Simmons index and Hosoya index of bicyclic graphs with a given girth

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Abstract. For a graph \( G \), the Merrifield-Simmons index \( i(G) \) and the Hosoya index \( z(G) \) are defined as the total number of independent sets and the total number of matchings of the graph \( G \), respectively. In this paper, we characterize the graphs with the maximal Merrifield-Simmons index and the minimal Hosoya index, respectively, among the bicyclic graphs on \( n \) vertices with a given girth \( g \).

Keywords: Merrifield-Simmons index; Hosoya index; bicyclic graph

AMS subject classification: 05C69, 05C05

1. Introduction

All graphs considered in this paper are finite, undirected and simple. Let \( G = (V, E) \) be a graph on \( n \) vertices and \( m \) edges. If \( m = n - 1 + c \), then \( G \) is called a \( c \)-cyclic graph. If \( c = 0, 1 \) and 2, then \( G \) is a tree, unicyclic graph, and bicyclic graph, respectively. An independent \( k \)-set is a set of \( k \) vertices, no two of which are adjacent. Denote by \( i(G, k) \) the number of \( k \)-independent sets of \( G \). It follows directly from definition that \( i(G, 0) = 1 \) for any graph \( G \). The Merrifield-Simmons index, denoted by \( i(G) \), is defined to be the total number of independent sets of \( G \), that is, \( i(G) = \sum_{k=0}^{n} i(G, k) \). A \( k \)-matching of \( G \) is a set of \( k \) mutually independent edges. Denote by \( Z(G, k) \) the number of \( k \)-matchings of \( G \). For convenience, we regard the empty edge set as a matching. Then \( Z(G, 0) = 1 \) for any graph \( G \). The Hosoya index, denoted by \( z(G) \), is defined to be the total number of matchings, namely, \( Z(G) = \sum_{k=1}^{\lfloor n/2 \rfloor} Z(G, k) \).

The Hosoya index was introduced by Hosoya [9] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical properties such as boiling point, entropy or heat of vaporization are well studied. Similar connections are known for Merrifield-Simmons index. For detailed information on the chemical applications, we refer to [7, 10, 15] and the references therein.

Since then, many authors have investigated these graphic invariants. An important direction is to determine the graphs with maximal or minimal...
indices in a given class of graphs. As for \(n\)-vertex trees, the star is the tree that maximizes the Merrifield-Simmons index, and that the path is the tree that minimizes it[7, 18]. The situation for the Hosoya index is absolutely analogous. The star minimizes the Hosoya index, while the path maximizes it[8]. Among all unicyclic graphs of order \(n\)[2, 16, 17, 19], the maximum of the Merrifield-Simmons index and the minimum of the Hosoya index are attained for the graph that results from attaching \(n - 3\) leaves to a triangle (the only exception being \(n = 4\), in which case the cycle \(C_4\) also maximizes the Merrifield-Simmons index). On the other hand, the maximum of the Hosoya index and the minimum of the Merrifield-Simmons index is attained for the cycle \(C_n\); in the case of the Merrifield-Simmons index, the graph that results from attaching a path to a triangle attains the maximum as well. The maximum of the Merrifield-Simmons index among all bicyclic graphs is \(5 \cdot 2^{n-4} + 1\), and it is attained for a graph that results from a star by connecting one of the leaves to two other leaves[6]. The same graph minimizes the Hosoya index (with a value of \(3n - 4\))[4]. On the other hand, the minimum of the Merrifield-Simmons is attained for a graph that consists of two 3-cycles, connected by a path of length \(n-5\) (the Merrifield-Simmons index of this graph is \(5F_{n-2}\))[5], while the graph that maximizes the Hosoya index results from identifying two edges of a cycle of length 4 and a cycle of length \(n - 2\) (its Hosoya index is \(F_{n+1} + F_{n-1} + 2F_{n-3}\))[3], respectively. For further details, we refer readers to survey papers [10, 11, 12, 22, 21], especially, a recent paper by S. Wagner and I. Gutman [21], which is a wonderful survey on this topic, and the cited references therein.

Let \(\mathcal{B}(n, g)\) be the class of bicyclic graph on \(n\) vertices with a given girth \(g\). In this paper, we characterize the graphs with the maximal Merrifield-Simmons index and the minimal Hosoya index, respectively, in \(\mathcal{B}(n, g)\).

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobáς [1]. If \(W \subset V(G)\), we denote by \(G - W\) the subgraph of \(G\) obtained by deleting the vertices of \(W\) and the edges incident with them. Similarly, if \(E \subset E(G)\), we denote by \(G - E\) the subgraph of \(G\) obtained by deleting the edges of \(E\). If \(W = \{v\}\) and \(E = \{xy\}\), we write \(G - v\) and \(G - xy\) instead of \(G - \{v\}\) and \(G - \{xy\}\), respectively. We denote by \(P_n\), \(C_n\) and \(S_n\) the path, the cycle and the star on \(n\) vertices, respectively. \(kP_1\) means \(k\) copies of \(P_1\). Let \(G, H\) be two connected graphs with \(V(G) \cap V(H) = \{v\}\), then let \(G \circ H\) be a graph defined by \(V(G \circ H) = V(G) \cup V(H)\) and \(E(G \circ H) = E(G) \cup E(H)\). In \(G \circ S_{k+1}\), for simplicity, let \(v\) be the center of \(S_{k+1}\). Set \(N(v) = \{u|uv \in E(G)\}\), \(N[v] = N(v) \cup \{v\}\).

Denote by \(F_n\) the \(n\)th Fibonacci number. Recall that \(F_0 = F_1 = 1\), \(F_{n+2} = F_{n+1} + F_n\), \(n \geq 2\) with initial conditions \(F_0 = F_1 = 1\). Then \(i(P_n) = F_{n+1}\), \(z(P_n) = F_{n+2}\). Note that \(F_{n+m} = F_nF_m + F_{n-1}F_{m-1}\). For convenience, we let \(F_n = 0\) for \(n < 0\).

Now we give some lemmas that will be used in the proof of our main results.

**Lemma 1.1** ([7]). Let \(G = (V, E)\) be a graph.

(i) If \(uv \in E(G)\), then \(i(G) = i(G - uv) - i(G - \{N[u] \cup N[v]\})\) and \(z(G) = z(G - uv) + z(G - \{u, v\})\);

(ii) If \(v \in V(G)\), then \(i(G) = i(G - v) + i(G - N[v])\) and \(z(G) = z(G - v) + \sum_{u \in N(v)} z(G - \{u, v\})\);
If \(G_1, G_2, \ldots, G_t\) are the components of the graph \(G\), then 
\[ i(G) = \prod_{j=1}^{t} i(G_j) \quad \text{and} \quad z(G) = \prod_{j=1}^{t} z(G_j). \]

**Lemma 1.2** ([13]). Let \(G\) be a connected graph and \(T_{l+1}\) be a tree of order \(l+1\) with \(V(G) \cap V(T_{l+1}) = \{v\}\). Then \(i(GvT_{l+1}) \leq i(GvS_{l+1})\) and \(z(GvT_{l+1}) \geq z(GvS_{l+1})\).

**Lemma 1.3** ([14]). Let \(H, X, Y\) be three connected graphs disjoint in pair. Suppose that \(u, v\) are two vertices of \(H\), \(v'\) is a vertex of \(X\), \(u'\) is a vertex of \(Y\). \(G\) be the graph obtained from \(H, X, Y\) by identifying \(v, v', u\) and \(u, v\) with \(u', v\), respectively. Let \(G_1^*\) be the graph obtained from \(H, X, Y\) by identifying vertices \(v, v', u, u'\) and \(G_2^*\) be the graph obtained from \(H, X, Y\) by identifying vertices \(u, v, v'\). Then
\[ (i) \ i(G_1^*) > i(G) \quad \text{or} \quad i(G_2^*) > i(G); \]
\[ (ii) \ z(G_1^*) < z(G) \quad \text{or} \quad z(G_2^*) < z(G). \]

2. **Bicyclic graphs with maximal Merrifield - Simmons index**

Let \(B\) be a bicyclic graph. The base of \(B\), denoted by \(\hat{B}\), is the minimal bicyclic subgraph of \(B\). Obviously, \(\hat{B}\) is the unique bicyclic subgraph of \(B\) containing no pendant vertex, and \(B\) can be obtained from \(\hat{B}\) by planting trees to some vertices of \(\hat{B}\).

![Figure 1: The bases of \(\mathcal{B}(n, g)\)](image)

It is well known that bicyclic graphs have the following three types of bases (as shown in Figure 1):

Let \(\hat{B}(p, q)\) be the bicyclic graph obtained from two vertex-disjoint cycles \(C_p\) and \(C_q\) by identifying vertices \(u\) of \(C_p\) and \(v\) of \(C_q\). For convenience, \(u\) in \(\hat{B}(p, q)\) is always the common vertex.

Let \(\hat{B}(p, l, q)\) be the graph obtained by joining a new path \(v_1v_2\cdots v_l\) between two vertex-disjoint cycles \(C_p\) and \(C_q\), where \(v_1 \in V(C_p)\) and \(v_l \in V(C_q)\).
Let \( P(p, q, r) \) be the bicyclic graph consisting of three pairwise internal disjoint paths \( P_{p+1}, P_{q+1}, P_{r+1} \) with common endpoints.

Now we can define the following three classes of bicyclic graphs on \( n \) vertices with a given girth \( g \):

\[ \mathcal{B}_1(n, g) = \{ B \in \mathcal{B}(n, g) \mid B = \tilde{B}(p, g) \text{ for some } p \geq g \geq 3 \}; \]
\[ \mathcal{B}_2(n, g) = \{ B \in \mathcal{B}(n, g) \mid B = \tilde{B}(p, l, g) \text{ for some } p \geq g \geq 3 \text{ and } l \geq 2 \}; \]
\[ \mathcal{B}_3(n, g) = \{ B \in \mathcal{B}(n, g) \mid B = P(p, q, r) \text{ for some } p \geq q \geq r \geq 1 \text{ and } q + r = g \geq 3 \}. \]

Then \( \mathcal{B}(n, g) = \mathcal{B}_1(n, g) \cup \mathcal{B}_2(n, g) \cup \mathcal{B}_3(n, g) \).

**Lemma 2.1.** For \( p \geq g \geq 3 \),

(i) \( i(\tilde{B}(p, g)uS_{n-p-g+2}) \leq i(\tilde{B}(g, g)uS_{n-2g+2}) \). The equality holds if and only if \( p = g \).

(ii) \( z(\tilde{B}(p, g)uS_{n-p-g+2}) \geq z(\tilde{B}(g, g)uS_{n-2g+2}) \). The equality holds if and only if \( p = g \).

*Proof.* (i) By Lemma 1.1, we have

\[
i(\tilde{B}(p, g)uS_{n-p-g+2}) = i(\tilde{B}(p, g)uS_{n-p-g+2} - u) + i(\tilde{B}(p, g)uS_{n-p-g+2} - N[u])
= i(P_{p-1} \cup P_{g-1} \cup (n - p - g + 1)P_1) + i(P_{p-3} \cup P_{g-3})
= 2^{n-p-g+1}F_pF_g + F_{p-2}F_{g-2}. \tag{2.1}
\]

Then

\[
i(\tilde{B}(p, g)uS_{n-p-g+2}) - i(\tilde{B}(p + 1, g)uS_{n-p-g+1})
= 2^{n-p-g+1}F_pF_g + F_{p-2}F_{g-2} - (2^{n-p-g}F_{p+1}F_g + F_{p-1}F_{g-2})
\geq F_{p-2}F_g - F_{p-3}F_{g-2} > 0,
\]

since \( p \geq g \geq 3 \). Hence

\[ i(\tilde{B}(p, g)uS_{n-2g+2}) > i(\tilde{B}(p + 1, g)uS_{n-2g+1}) > \cdots > i(\tilde{B}(p, g)uS_{n-p-g+2}). \]

So \( i(\tilde{B}(p, g)uS_{n-p-g+2}) \leq i(\tilde{B}(g, g)uS_{n-2g+2}) \). The equality holds if and only if \( p = g \).

(ii) Let \( v_1, \ldots, v_{n-p-g+1} \) be the pendant vertices of \( \tilde{B}(p, g)uS_{n-p-g+1} \).

By Lemma 1.1, we have

\[
z(\tilde{B}(p, g)uS_{n-p-g+2})
= z(\tilde{B}(p, g)uS_{n-p-g+2} - uv_1) + z(\tilde{B}(p, g)uS_{n-p-g+2} - \{u, v_1\})
= z(\tilde{B}(p, g)uS_{n-p-g+2} - uv_1) + F_{g-1}F_{p-1}
= \cdots
= z(\tilde{B}(p, g)) + (n - p - g + 1)F_{g-1}F_{p-1}
= z(\tilde{B}(p, g) - u) + \sum_{v \in N(u)} z(G - \{u, v\}) + (n - p - g + 1)F_{g-1}F_{p-1}
= (n - p - g + 2)F_{g-1}F_{p-1} + 2F_{g-2}F_{p-1} + 2F_{g-1}F_{p-2}. \tag{2.2}
\]
Then

\[
\begin{align*}
&z(\hat{B}(p+1, g)uS_{n-p-g+1}) - z(\hat{B}(p, g)uS_{n-p-g+2}) \\
&\quad = (n - p - g + 1)F_{g-1}F_p + 2F_{g-2}F_p + 2F_{g-3}F_{p-1} - \\
&\quad [(n - p - g + 2)F_{g-1}F_{p-1} + 2F_{g-2}F_{p-1} + 2F_{g-3}F_{p-2}] \\
&\quad = (n - p - g + 1)F_{g-1}F_p - F_{g-1}F_{p-1} + 2F_{g-2}F_{p-2} + 2F_{g-3}F_{p-3} \\
&\quad \geq -F_{g-1}F_{p-1} + 2F_{g-2}F_{p-2} + 2F_{g-3}F_{p-3} \\
&\quad = F_{g-1}F_{p-3} + F_{p-2}(F_{g-2} - F_{g-3}) > 0,
\end{align*}
\]

since \( p \geq g \geq 3 \). So

\[
z(\hat{B}(g, g)uS_{n-2g+2}) < z(\hat{B}(g+1, g)uS_{n-2g+1}) < \cdots < z(\hat{B}(p, g)uS_{n-p-g+2}).
\]

Hence \( z(\hat{B}(p, g)uS_{n-p-g+2}) \geq z(\hat{B}(g, g)uS_{n-2g+2}). \) The equality holds if and only if \( p = g \).

**Theorem 2.2.** For any graph \( G \in \mathcal{B}_1(n, g) \), we have

(i) \( i(G) \leq i(\hat{B}(g, g)uS_{n-2g+2}) \). The equality holds if and only if \( G \cong \hat{B}(g, g)uS_{n-2g+2} \).

(ii) \( z(G) \geq z(\hat{B}(g, g)uS_{n-2g+2}) \). The equality holds if and only if \( G \cong \hat{B}(g, g)uS_{n-2g+2} \).

**Proof.** For any graph \( G \in \mathcal{B}_1(n, g) \), it can be obtained from \( \hat{B}(p, g)(p \geq g) \) by planting some trees to some vertices of \( \hat{B}(p, g) \). Denote \( G_1 \) be the graph obtained from \( G \) by replacing each tree with a star with the same order.

(i) By Lemma 1.2, we have \( i(G) \leq i(G_1) \). Repeatedly by Lemma 1.3, we can move all stars to a vertex \( x \), which is a center of some star, and the Merrifield-Simmons index is increasing. Without loss of generality, let \( x \in V(C_p) \), denote by \( G_2 \) the graph obtained by identifying the center \( x \) of \( S_{n-p-g+2} \) with \( u \) or moving \( C_g \) to \( x \), obviously, \( G_2 \cong \hat{B}(p, g)uS_{n-p-g+2} \).

By Lemma 1.3, we have \( i(G_1) \leq i(G_2) \). Then \( i(G) \leq i(\hat{B}(p, g)uS_{n-p-g+2}) \). The equality holds if and only if \( G \cong G_1 \cong G_2 \). Furthermore, by Lemma 2.1, we can obtain our desired result.

Similar to the proof of (i), we can prove (ii).

By Lemma 1.3 and Theorem 2.2, we have

**Theorem 2.3.** For any graph \( G \in \mathcal{B}_2(n, g) \), we have

(i) \( i(G) < i(\hat{B}(g, g)uS_{n-2g+2}) \).

(ii) \( z(G) > z(\hat{B}(g, g)uS_{n-2g+2}) \).

By Lemma 1.1, we have

**Lemma 2.4.** For graph \( P(p, q, r)uS_{n-p-g+2} \), we have
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For $i \geq 0$, we have

\[ n \geq (p - 2) \sum_{j=1}^{p-2} (F_{2j} F_{2j+1} F_{2j+2} + F_{2j} F_{2j+1}^2 + F_{2j+1} F_{2j+2} F_{2j+3} + F_{2j+1}^2 F_{2j+2} + F_{2j+2} F_{2j+3} F_{2j+4} - 2F_{2j+1} F_{2j+2} F_{2j+3}) \]

Then

\[ F_{p-1} F_{p-2} F_{p-3} + \sum_{j=1}^{p-2} (F_{2j} F_{2j+1} F_{2j+2} + F_{2j} F_{2j+1}^2 + F_{2j+1} F_{2j+2} F_{2j+3} + F_{2j+1}^2 F_{2j+2} + F_{2j+2} F_{2j+3} F_{2j+4} - 2F_{2j+1} F_{2j+2} F_{2j+3}) \]

Hence $z(P(p, q, r) uS_{n-p+3}) > z(P(p, q, r) uS_{n-p+2})$.

**Lemma 2.6.** For $p \geq q \geq r$, we have

(i) $i(P(p, q, r) uS_{n-p+2}) \leq i(P(q, q, r) uS_{n-q+2})$. The equality holds if and only if $p = q$.

(ii) $z(P(p, q, r) uS_{n-p+2}) \geq z(P(q, q, r) uS_{n-q+2})$. The equality holds if and only if $p = q$.

**Proof.** Note that $r \geq 1, q \geq 2$. If $p = 2$, then $p = q = 2$ since $p \geq q \geq r$. If $p + r > q$, then $p > q$ since $q + r = g$, that is, $p \geq 3, q \geq 2$.

(i) By Lemma 2.4(i), we have

\[ i(P(p-1, q, r) uS_{n-p+3}) \]

Then

\[ i(P(p-1, q, r) uS_{n-p+3}) - i(P(p, q, r) uS_{n-p+2}) \]

So $i(P(p-1, q, r) uS_{n-p+3}) > i(P(p, q, r) uS_{n-p+2})$.

If $p - 1 = q$, we obtain our desired result.

If $p - 1 > q$, applying the above procedures repeatedly, we can also obtain our desired result.

(ii) By Lemma 2.4(ii), we have

\[ z(P(p-1, q, r) uS_{n-p+3}) \]

Then

\[ z(P(p, q, r) uS_{n-p+2}) - z(P(p-1, q, r) uS_{n-p+3}) \]

\[ 7 \]
\[(F_q + F_{q-2})F_{p-1} + 2F_{q-1}F_{p-2} + F_{p-3}F_{q-1}F_{r-1} + (n - p - g + 1)(F_q - 1)F_{p-1} + F_{p-2}F_{q-1}F_{r-1} - [F_q + F_{q-2})F_{p-2} + 2F_{q-1}F_{p-3} + F_{p-4}F_{q-1}F_{r-1} + (n - p - g + 2)(F_{q-1}F_{p-2} + F_{p-3}F_{q-1}F_{r-1})] \geq 2F_{q-2}F_{p-3} > 0.\]

So \(z(P_{n-p+2}) > z(P_{n-p+3})\).

Applying the above procedures repeatedly, we can obtain our desirable result. □

Let
\[
\begin{align*}
f(q, r) &= 2^{n-q-g+1}(F_q F_q F_r + F_{q-1}F_{q-1}F_{r-1}) + F_{q-1}F_{q-1}F_{r-1} + F_{q-2}F_{q-2}F_{r-2} \\
h(q, r) &= (F_q + F_{q-2})F_{q-1} + 2F_{q-1}F_{q-2} + F_{q-3}F_{q-1}F_{r-1} + (n - q - g + 1)(F_{q-1}F_{q-1} + F_{q-2}F_{q-1}F_{r-1})
\end{align*}
\]

(2.3)

**Lemma 2.7.** If \(q + r \geq 2\),

(i) \(f(q-1, r + 1) > f(q, r)\).

(ii) \(h(q-1, r + 1) < h(q, r)\).

**Proof.** Since \(q + r \geq 2 \text{ and } r \geq 1\), then \(q \geq 3\).

(i) By (2.3), we have
\[
f(q-1, r + 1) = 2^{n-q-g+1}(F_{q-1}F_{q-1}F_{r+1} + F_{q-2}F_{q-2}F_r) + F_{q-2}F_{q-2}F_r + F_{q-3}F_{q-3}F_{r-1}.
\]

Then
\[
f(q-1, r + 1) - f(q, r)
= 2^{n-q-g+2}(F_{q-1}F_{q-1}F_{r+1} + F_{q-2}F_{q-2}F_r) + F_{q-2}F_{q-2}F_r
+ F_{q-3}F_{q-3}F_{r-1} - [2^{n-q-g+1}(F_q F_q F_r + F_{q-1}F_{q-1}F_{r-1})
+ F_{q-1}F_{q-1}F_{r-1} + F_{q-2}F_{q-2}F_{r-2}]
= 2^{n-q-g+1}(2F_{q-1}F_{r+1} + 2F_{q-2}F_r - F_{q-1}F_{r-1} + F_{q-2}F_r
- F_{q-3}F_{r-1} + F_{q-3}F_{r-1} - F_{q-2}F_{r-2}
\geq 2F_{q-1}F_{r+1} + 2F_{q-2}F_r - F_{q-1}F_{r-1} + F_{q-2}F_r - F_{q-1}F_{r-1}
+ F_{q-3}F_{r-1} - F_{q-2}F_{r-2}
= (F_{q-1}F_{r+1} + F_{q-2}F_r + 2F_{q-2}F_r - F_{q-1}F_{r-1}) + F_{q-2}F_r - F_{q-1}F_{r-1}
+ F_{q-3}F_{r-1} - F_{q-2}F_{r-2}
= F_{q-1}F_r + F_{q-1}F_{r-1} + F_{q-2}F_{r-2} + 2F_{q-2}F_r - F_{q-1}F_{r-1}
+ F_{q-3}F_{r-1}
= 2F_{q-1}F_r + 2F_{q-2}F_r - F_{q-1}F_{r-1} + F_{q-3}F_{r-1}
\]

8
\[
(2F_{q-1}^2 + F_{q-2}^2 - F_q^2)F_r + F_{q-2}^2F_{r-1} + F_{q-3}^2Fr-1 \\
(\frac{F_q - F_{q-2}}{2}F_r + F_{q-2}^2F_{r-1} + F_{q-3}^2Fr-1 \\
\geq F_{q-2}^2Fr-1 > 0.
\]

(ii) By (2.4), we have
\[
h(q-1,r+1) = (F_g + F_{g-2})F_{q-2} + 2F_{g-1}F_{q-3} + F_{q-4}F_{q-2}Fr. \\
+(n-q-g+1)(F_{g-1}F_{q-2} + F_{q-3}F_{q-2}Fr).
\]

Then
\[
h(q,r) - h(q-1,r+1) \\
=(F_g + F_{g-2})F_{q-1} + 2F_{g-1}F_{q-2} + F_{q-3}F_{q-1}Fr-1 \\
+(n-q-g+1)(F_{g-1}F_{q-1} + F_{q-2}F_{q-1}Fr-1) - [(F_g + F_{g-2})F_{q-2} \\
+2F_{g-1}F_{q-3} + F_{q-4}F_{q-2}Fr + (n-q-g+1)(F_{g-1}F_{q-2} \\
+ F_{q-3}F_{q-2}Fr)] \\
\geq F_{q-3}F_{q-1}Fr-1 > 0.
\]

As desired. \(\Box\)

**Theorem 2.8.** For any graph \(G \in B_3(n,g)\), we have

(i) \(i(G) \leq i(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{\lfloor \frac{g}{2} \rfloor}{2} \rfloor)uS_n-\lfloor \frac{g}{2} \rfloor - g+2)\). The equality holds if and only if

\[G \cong P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{\lfloor \frac{g}{2} \rfloor}{2} \rfloor)uS_n-\lfloor \frac{g}{2} \rfloor - g+2\.

(ii) \(z(G) \geq z(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{\lfloor \frac{g}{2} \rfloor}{2} \rfloor)uS_n-\lfloor \frac{g}{2} \rfloor - g+2)\). The equality holds if and only if

\[G \cong P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{\lfloor \frac{g}{2} \rfloor}{2} \rfloor)uS_n-\lfloor \frac{g}{2} \rfloor - g+2\.

**Proof.** For any graph \(G \in B_3(n,g)\), it can be obtained from \(P(p,q,r)\) by planting some trees to some vertices of \(P(p,q,r)\).

(i) Using Lemma 1.2 and 1.3 repeatedly, we can obtain that

\[i(G) \leq i(P(p,q,r)xs_{n-p-g+2})\]

where \(x \in V(P(p,q,r))\). By Lemma 2.5 and 2.6, we have

\[i(G) \leq i(P(q,g,r)us_{n-q-g+2})\]

Repeated applying Lemma 2.7, we have \(0 \leq q-r \leq 1\). Since \(q \geq r, q+r = g\), then \(q = \lfloor \frac{g}{2} \rfloor\) and \(r = \lfloor \frac{\lfloor g \rfloor}{2} \rfloor\). Hence

\[i(G) \leq i(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{\lfloor g \rfloor}{2} \rfloor)uS_n-\lfloor \frac{g}{2} \rfloor - g+2)\]

The equality holds if and only if \(G \cong P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{\lfloor g \rfloor}{2} \rfloor)uS_n-\lfloor \frac{g}{2} \rfloor - g+2\).

Similarly, we can prove (ii). \(\Box\)
By induction, it is easy to prove Lemma 2.9.

**Lemma 2.9.** For any integer \( n \), then (i) \( F_n \geq n \) if \( n \geq 0 \); (ii) \( 2^n \geq F_{n+2} \) if \( n \geq 3 \).

**Theorem 2.10.** For any graph \( G \in \mathcal{B}(n, g) \), we have

(i) \( i(G) \leq i(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor))uS_{n-\lfloor \frac{g}{2} \rfloor-2g+2} \). The equality holds if and only if

\[
G \cong P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor)uS_{n-\lfloor \frac{g}{2} \rfloor-2g+2}.
\]

(ii) \( z(G) \geq z(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor))uS_{n-\lfloor \frac{g}{2} \rfloor-2g+2} \). The equality holds if and only if

\[
G \cong P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor)uS_{n-\lfloor \frac{g}{2} \rfloor-2g+2}.
\]

**Proof.** (i) By Theorem 2.2, 2.3 and 2.8, we have

\[
i(G) \leq \max\{i(\tilde{B}(g, g))uS_{n-2g+2}, i(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor))uS_{n-\lfloor \frac{g}{2} \rfloor-2g+2}\}.
\]

By (2.1) and Lemma 2.4, we have

\[
i(\tilde{B}(g, g))uS_{n-2g+2} = 2^{n-2g+1}F_g^2 + F_{g-2}^2\quad (2.4)
\]

\[
i(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor))uS_{n-\lfloor \frac{g}{2} \rfloor-2} = 2^{n-\lfloor \frac{g}{2} \rfloor+1}F_{\lfloor \frac{g}{2} \rfloor}^2F_{\lfloor \frac{g}{2} \rfloor-1} + F_{\lfloor \frac{g}{2} \rfloor-1}F_{\lfloor \frac{g}{2} \rfloor-2} + F_{\lfloor \frac{g}{2} \rfloor-1}^2\quad (2.5)
\]

Case 1. \( g \) is even. By (2.5) and (2.6), we have

\[
i(P(\lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor, \lfloor \frac{g}{2} \rfloor))uS_{n-2g+2} - i(\tilde{B}(g, g))uS_{n-2g+2}\]

\[
= 2^{n-\lfloor \frac{g}{2} \rfloor+1}(F_{\lfloor \frac{g}{2} \rfloor}^3 + F_{\lfloor \frac{g}{2} \rfloor}^3 + F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-1}^3 - 2^{n-2g+1}F_g^2 + F_{g-2}^2)
\]

\[
= 2^{n-\lfloor \frac{g}{2} \rfloor+1}(2F_{\lfloor \frac{g}{2} \rfloor}^3 + 2F_{\lfloor \frac{g}{2} \rfloor-1}^3 - F_{\lfloor \frac{g}{2} \rfloor}^2) + F_{\lfloor \frac{g}{2} \rfloor-1}^2 + F_{\lfloor \frac{g}{2} \rfloor-2}^2 - F_{\lfloor \frac{g}{2} \rfloor-2}^2
\]

\[
\geq 2^{n-\lfloor \frac{g}{2} \rfloor+1}(2F_{\lfloor \frac{g}{2} \rfloor}^3 + 2F_{\lfloor \frac{g}{2} \rfloor-1}^3 - F_{\lfloor \frac{g}{2} \rfloor}^2) + F_{\lfloor \frac{g}{2} \rfloor-1}^2 + F_{\lfloor \frac{g}{2} \rfloor-2}^2 - F_{\lfloor \frac{g}{2} \rfloor-2}^2 \quad \text{(by Lemma 2.9)}
\]

\[
= (F_{\lfloor \frac{g}{2} \rfloor-1}^3 + 2F_{\lfloor \frac{g}{2} \rfloor-1}^3 + (F_{\lfloor \frac{g}{2} \rfloor-1} + 2F_{\lfloor \frac{g}{2} \rfloor})F_{\lfloor \frac{g}{2} \rfloor-1} - (F_{\lfloor \frac{g}{2} \rfloor}^2 + F_{\lfloor \frac{g}{2} \rfloor-1}^2)^2 + F_{\lfloor \frac{g}{2} \rfloor-1}^3
\]

\[
+ 2F_{\lfloor \frac{g}{2} \rfloor-1}^2 - F_{\lfloor \frac{g}{2} \rfloor-2}^2
\]

\[
= (F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-2}^3)^4 + F_{\lfloor \frac{g}{2} \rfloor-1}^3F_{\lfloor \frac{g}{2} \rfloor}^3 + 2F_{\lfloor \frac{g}{2} \rfloor}^3F_{\lfloor \frac{g}{2} \rfloor-1}^3 - 2F_{\lfloor \frac{g}{2} \rfloor}^2F_{\lfloor \frac{g}{2} \rfloor-1}^2 + F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-2}^2
\]

\[
- (F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-2}^3)^2
\]

\[
= (F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-2}^3)^2 + 2F_{\lfloor \frac{g}{2} \rfloor-1}^3F_{\lfloor \frac{g}{2} \rfloor-2}^2 + F_{\lfloor \frac{g}{2} \rfloor-1}^3 + 2F_{\lfloor \frac{g}{2} \rfloor}^3F_{\lfloor \frac{g}{2} \rfloor-1}^2 - 2F_{\lfloor \frac{g}{2} \rfloor}^2F_{\lfloor \frac{g}{2} \rfloor-1}^2
\]

\[
+ F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-2}^3 - (F_{\lfloor \frac{g}{2} \rfloor-1}^3 + F_{\lfloor \frac{g}{2} \rfloor-2}^3)^2
\]
By (2.2) and Lemma 2.4, we have

\[
\begin{align*}
F &= \frac{n}{2} - 1 + \frac{F_2}{2} - 2 + 4F_2 - 1F_2 - 2(F_2^2 - 1 + F_2 - 2) + 4F_2^2 - 1F_2^2 - 2 \\
F_3^2 - 1 + \frac{F_2}{2} - 2 + 2F_2 - 1(F_2 - 1) - F_2^2 \\
+ \frac{F_3}{2} - 1 + \frac{F_2}{2} - 2 - (F_2^2 - 1 + F_2 - 2)^2 \\
&= 4F_2 - 1F_2^2 - 2 + 4F_2 - 1F_2^2 - 2 + 4F_2 - 1F_2^2 - 2 + F_2^2 - 1F_3^2 - 2 \\
&- 2F_2^2 F_2^2 - 1F_2^2 - 2 + F_3^2 - 2 \\
&= -2F_2^2 F_2^2 + (2F_2 - 1 - F_2) + 4F_2^2 - 1F_2^2 - 2 + 4F_2^2 - 1F_2^2 - 2 + F_2^2 - 1F_3^2 \\
&+ 2F_2^3 F_2 - 1 + F_3^2 - 2 \\
&= 2F_2 - 1F_2^2 - 2F_2 - 3 + 4F_2 - 1F_2^2 - 2 + 4F_2^2 - 1F_2^2 - 2 + F_2^2 - 1F_3^2 \\
&+ 2F_2^3 F_2 - 1 + F_3^2 - 2 \\
&> F_3^2 - 1 > 0
\end{align*}
\]

Case 2. \( g \) is odd. Similar to case 1, we have

\[
i(P(g, g)uS_n) = i(\hat{B}(g, g)uS_n - 2g)
\]

\[
= 2^{-n - 2g} + 1(F_2^2 F_2^2 - 1 + F_2^2 F_2^2 - 1 + F_2^2 F_2^2) \\
+ F_2^2 F_2^2 - 2 - F_2^2 \\
\geq F_2^2 F_2^2 - 1 + F_2^2 F_2^2 - 1 + F_2^2 F_2^2 - 1 + F_2^2 F_2^2 - 1 - (F_2^2 F_2^2 - 1 + F_2^2 F_2^2 - 1)^2 \\
- (F_2^2 F_2^2 - 1 + F_2^2 F_2^2 - 1)^2 \\
+ F_2^2 F_2^2 F_2^2 \\
= (F_2^2 F_2^2 - 1 - F_2^2 F_2^2) + (F_2^2 F_2^2 + F_2^2 F_2^2 - 2F_2^2 F_2^2 F_2^2) \\
+ F_2^2 F_2^2 F_2^2 \\
\geq F_2^2 F_2^2 - 1.
\]

Then \( i(\hat{B}(g, g)uS_n - 2g) > i(\hat{B}(g, g)uS_n - 2g) \).

By Theorem 2.2, 2.3 and 2.8 and Lemma 2.9, we have

\[
z(G) \geq \min\{z(\hat{B}(g, g)uS_n - 2g), z(P(\frac{g}{2}, \frac{g}{2}, \frac{g}{2})), uS_n - 2g\}.
\]

By (2.2) and Lemma 2.4, we have

\[
z(\hat{B}(g, g)uS_n - 2g) = (n - 2g + 2)F_{g-1}F_{g-1} + 4F_{g-1}F_{g-2} \quad (2.6)
\]
\[ z(P(\frac{g}{2}, \frac{g}{2}, \frac{g}{2})_n) \rightarrow z(P(\frac{g}{2}, \frac{g}{2}, \frac{g}{2})_n) \]

\[ = (F_g + F_{g-2})F_{\frac{g}{2}-1} + 2F_{g-1}F_{\frac{g}{2}-2} + F_{\frac{g}{2} - 3}F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 1} + (n - \lceil \frac{g}{2} \rceil + 1)(F_{g-1}F_{\frac{g}{2} - 1} - 2F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 1}) \quad (2.7) \]

Case 1. \( g \) is even. By (2.7) and (2.8), we have

\[ z(\hat{B}(g, g)_nS_{n-2}) = z(P(\frac{g}{2}, \frac{g}{2}, \frac{g}{2})_n) \]

\[ = [(n - 2g + 2)F_{g-1}F_{g-1} + 4F_{g-1}F_{g-2}] - [(F_g + F_{g-2})F_{\frac{g}{2}} - 1]
\]

\[ + 2F_{g-1}F_{\frac{g}{2} - 2} + F_{\frac{g}{2} - 3}F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 1} + (n - \frac{3g}{2} + 1)(F_{g-1}F_{\frac{g}{2} - 1} + F_{\frac{g}{2} - 2}F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 1}) \]

\[ = (n - 2g + 2)F_{g-1}F_{\frac{g}{2} - 1} + 4F_{g-1}F_{\frac{g}{2} - 2} + 4F_{g-1}F_{\frac{g}{2} - 2} - F_{g-1}F_{\frac{g}{2} - 1}
\]

\[ - 2F_{g-2}F_{\frac{g}{2} - 1} - 2F_{g-1}F_{\frac{g}{2} - 2} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 3} \]

\[ - (n - \frac{3g}{2} + 1)F_{g-1}F_{\frac{g}{2} - 1} - (n - \frac{3g}{2} + 1)F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} \]

\[ > F_{g-1}(F_{\frac{g}{2} - 1}(n - 2g + 2)F_{\frac{g}{2} - 1} + (n - 2g + 2)F_0 + 4F_{\frac{g}{2} - 1} -
\]

\[ (n - \frac{3g}{2} + 2)] - 2F_{g-2}F_{\frac{g}{2} - 1} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 3} - (n - \frac{3g}{2} + 1)F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} \]

\[ = (n - 2g + 2)F_{g-1}F_{\frac{g}{2} - 1} + 4F_{g-1}F_{\frac{g}{2} - 2} - \frac{g}{2}F_{g-1}F_{\frac{g}{2} - 1}
\]

\[ - 2F_{g-2}F_{\frac{g}{2} - 1} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 3} - (n - \frac{3g}{2} + 1)F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} \]

\[ = F_{\frac{g}{2} - 1}(n - 2g + 2)F_{g-1}F_{\frac{g}{2} - 1} + 4F_{g-1}F_{\frac{g}{2} - 1} - \frac{g}{2}F_{g-1}F_{\frac{g}{2} - 1}
\]

\[ - 2F_{g-2} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 3} - (n - \frac{3g}{2} + 1)F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} \]

\[ = F_{\frac{g}{2} - 1}(n - 2g + 2)F_{g-1}F_{\frac{g}{2} - 1} + 4F_{g-1}F_{\frac{g}{2} - 1} - \frac{g}{2}(F_{g}F_{\frac{g}{2} - 1}
\]

\[ + F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} - 2F_{g-2} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 3} - (n - \frac{3g}{2} + 1)F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} \]

\[ > F_{\frac{g}{2} - 1}(F_{g-1}F_{\frac{g}{2} - 1} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2}) + 4F_{g-1}F_{\frac{g}{2} - 1} - \frac{g}{2}F_{\frac{g}{2} - 1}
\]

\[ - 2F_{g-2} - F_{\frac{g}{2} - 1} \]

\[ = F_{\frac{g}{2} - 1}(F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 1} + F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} - F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} + 4F_{\frac{g}{2} - 1}
\]

\[ + 4F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 2} - \frac{g}{2}F_{\frac{g}{2} - 1}F_{\frac{g}{2} - 1} - 2F_{\frac{g}{2} - 1} - 2F_{\frac{g}{2} - 1} \]
\[ F_{\frac{g}{2} - 1} = F_{\frac{g}{2}} F_{\frac{g}{2} - 1} (F_{\frac{g}{2}} - \frac{g}{2}) + F_{\frac{g}{2} - 2} (F_{\frac{g}{2}} - 1) + F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} (F_{\frac{g}{2}} - 1) + F_{\frac{g}{2} - 1} (4 F_{\frac{g}{2}} - 3) + 2 F_{\frac{g}{2} - 2} (2 F_{\frac{g}{2} - 1} - F_{\frac{g}{2} - 2}) > 0. \]

Case 2. If \( g \) is odd. If \( g = 3, \)

\[ z(\hat{B}(g,g)uS_{n-2g+2}) - z(P(\frac{g+1}{2}, \frac{g+1}{2}, \frac{g-1}{2})uS_{n-\lceil \frac{g+1}{2} \rceil + 2}) = n - 4 > 0, \]

since \( n \geq 2g - 1 \). If \( g \geq 5 \), we have

\[ z(\hat{B}(g,g)uS_{n-2g+2}) - z(P(\frac{g+1}{2}, \frac{g+1}{2}, \frac{g-1}{2})uS_{n-\lceil \frac{g+1}{2} \rceil + 2}) \]

\[ = (n - 2g + 2)[F_{\frac{g}{2} - 1} - F_{\frac{g}{2} - 1} (F_{\frac{g}{2} - 1} - 1) + F_{\frac{g}{2} - 2} (F_{\frac{g}{2} - 1} - 1) + F_{\frac{g}{2} - 1} (4 F_{\frac{g}{2}} - 3) + 2 F_{\frac{g}{2} - 2} (2 F_{\frac{g}{2} - 1} - F_{\frac{g}{2} - 2}) + F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} - (F_{\frac{g}{2}} + F_{\frac{g}{2} - 2}) F_{\frac{g}{2} - 1} - 2 F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1} - (F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} + F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1}) F_{\frac{g}{2} - 1} - (F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} + F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1}) F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} + F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1}] \]

\[ \geq F_{\frac{g}{2} - 1} + 4 F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1} - (F_{\frac{g}{2}} + F_{\frac{g}{2} - 2}) F_{\frac{g}{2} - 1} - 2 F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1} \]

\[ = (3 F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} - 3 F_{\frac{g}{2} - 1}) + (4 F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1} - 4 F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1}) + (F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} - F_{\frac{g}{2} - 1} F_{\frac{g}{2} - 2} F_{\frac{g}{2} - 1}) + F_{\frac{g}{2} - 1} \]

\[ \geq F_{\frac{g}{2} - 1} > 0. \]

Then \( z(\hat{B}(g,g)uS_{n-2g+2}) > z(P(\lceil \frac{g}{2} \rceil, \lceil \frac{g}{2} \rceil, \lceil \frac{g}{2} \rceil)uS_{n-g-\lceil \frac{g}{2} \rceil + 2}). \]

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References


