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Extremal Bicyclic Graph with Perfect Matching for Different Indices

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Abstract. Let $\mathscr{B}(2m,m)$ be the set of all bicyclic graphs on $2m(m \geq 2)$ vertices with perfect matchings. In this paper, we characterize the bicyclic graphs with minimal number of matchings and maximal number of independent sets in $\mathscr{B}(2m,m)$.

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1. Introduction

Let $G = (V,E)$ be a simple connected graph. Two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. Denote by $z(G)$ the total number of matchings in a graph G, that is, $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G,k)$, where $z(G,k)$ is the number of k-matchings of G for $k \geq 1$ and $z(G,0) = 1$. Two vertices of G are said to be independent if they are not adjacent in G. An independent k-set is a set of k vertices, no two of which are adjacent. Let $i(G)$ be the total number of independent sets of G, then $i(G) = \sum_{k=0}^{n} i(G,k)$, where $i(G,k)$ is the number of k-independent sets of G for $k \geq 1$ and $i(G,0) = 1$.

The index $z(G)$ (resp. $i(G)$) is also called *Hosoya index*(resp. *Merrifield-Simmons index*) in graphic chemistry. 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 [8, 20]. Up to now, many researchers have investigated these graphic invariants. An important direction is to determine the graphs with maximal or minimal number of matchings (or independent sets, resp.) in a given class of graphs. For instance, it was observed in [9, 15] that the star S_n has the minimal number of matchings (or the maximal number of independent sets, resp.) and the path P_n has the maximal number of matchings (or the minimal number of independent sets, resp.) amongst all trees with n vertices, respectively. In [17], Liu *et al.* studied trees with a prescribed diameter with respect to the number of matchings and independent sets, respectively. Hou [12] characterized the trees with a given size of matching and having minimal and second minimal number of matchings, respectively. In [3], Deng and Chen gave the sharp lower bound

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on the number of matchings of unicyclic graphs. Ou [16] characterized extremal unicyclic molecular graphs with maximal number of matchings. In [14], Li and one of the present authors studied the number of independent sets in unicyclic graphs with a given diameter. Wang and Hua [22] characterized the extremal (maximal and minimal) number of independent sets of unicyclic graphs with a given girth. Xu and Xu [27] determined all the unicyclic graphs of order n and with given maximum degree maximizing the number of matchings and minimizing the number of independent sets, respectively. Also n-vertex bicyclic graphs have been the object of study of a series of articles by Deng and coauthors [4, 5, 6, 7]. In particular, Yu and Tian [28] characterized the extremal graphs with minimal number of matchings and maximal number of independent sets, respectively, among all the connected graphs of order n and size $n+t-1$ with $0 \leq t \leq m-1$, where m is the matching number. For further details, we refer readers to survey papers [10, 11, 19, 21, 23, 25, 26, 29, 30], especially, a recent paper by S. Wagner and I. Gutman [24], which is a wonderful survey on this topic, and the cited references therein.

Let $\mathscr{B}(2m,m)$ be the set of all bicyclic graphs on $2m(m \geq 2)$ vertices with perfect matchings. In this paper, we consider the bicyclic graphs with minimal number of matchings and maximal number of independent sets, respectively, in $\mathscr{B}(2m,m)$.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [1]. For a vertex v of G, denote the degree of v by $d_G(v)$. Set $N_G(v) = \{u|uv \in E(G)\}$, $N_G[v] = N_G(v) \cup \{v\}$. 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. Denote by F_n the nth Fibonacci number. Recall that $F_n = F_{n-1}+F_{n-2}, n \geq 2$ with initial conditions $F_0 = F_1 = 1$. Then $i(P_n) = F_{n+1}, z(P_n) = F_n$.

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

Lemma 1.1. [9] *Let $G = (V,E)$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G-uv)+z(G-\{u,v\})$;*
(ii) *If $v \in V(G)$, then $z(G) = z(G-v)+\sum_{u \in N_G(v)} z(G-\{u,v\})$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

Lemma 1.2. [9] *Let $G = (V,E)$ be a graph.*

(i) *If $uv \in E(G)$, then $i(G) = i(G-uv) - i(G-N_G[u] \cup N_G[v])$;*
(ii) *If $v \in V(G)$, then $i(G) = i(G-v)+i(G-N_G[v])$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $i(G) = \prod_{j=1}^{t} i(G_j)$.*

Lemma 1.3. [18] *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. Let G be the graph obtained from H,X,Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H,X,Y by identifying vertices v,v',u' and G_2^* be the graph obtained from H,X,Y by identifying vertices u,v',u'. Then*

(i) $z(G_1^*) < z(G)$ *or* $z(G_2^*) < z(G)$;
(ii) $i(G_1^*) > i(G)$ *or* $i(G_2^*) > i(G)$.

Let G consist of connected graph G_1 and a pendent tree T, where $G_1 \cap T = r$. Vertex r is called the root of T on G_1 and T is named the attaching tree to G_1 rooted at r. Denote by $|V(T)|$ the order of T not including the root r of T.

Lemma 1.4. [2] *Let G be a connected graph with perfect matchings which consists of a connected subgraph H and a tree T such that T is attached to a root-vertex r of H. If $|V(T)| \geq 2$ and $v \in V(T)$ is a vertex furthest from the root r. Then v is a pendent vertex and adjacent to a vertex u of degree 2.*

2. Preliminaries

Hoffman and Smith [13] define an *internal path* of G as a walk $u_0u_1 \dots u_s (s \geq 1)$ such that the vertices $u_0, u_1, \dots, u_{s-1}$ are distinct, $d(u_0) > 2, d(u_s) > 2$, and $d(u_i) = 2$, whenever $0 < i < s$. An internal path is closed if $u_0 = u_s$.

Transformation A Let $G \in \mathscr{B}(2m,m)$, $P = v_0v_1 \dots v_s$ be an internal path of G. If $s = 2$ and $v_0v_2 \notin E(G)$, joining v_0 and v_2 by an edge in $G - v_1$, the resulting graph is denoted by H'; Then, attaching a pendent edge v_0v_1 to v_0 in H' if v_0v_1 belongs to the perfect matchings of G, and a pendent edge v_2v_1 to v_2 if v_1v_2 belongs to the perfect matchings of G. The resulting graph is denoted by H''. If $s \geq 3$, $v_0 \neq v_3$ and $v_0v_3 \notin E(G)$, joining v_0 and v_3 by an edge in $G - \{v_1, v_2\}$, the resulting graph is denoted by G'; Then, attaching a path of length 2 to v_0 in G', denote the path by $v_0v_1v_2$. The resulting graph is denoted by G''.

Lemma 2.1. *Let $G \in \mathscr{B}(2m,m)$, $P = v_0v_1 \dots v_s$ be an internal path of G. H'', G'' be graphs as described in Transformation A.*

(i) *If $s = 2$ and $v_0v_2 \notin E(G)$, $z(G) > z(H'')$ and $i(G) < i(H'')$;*
(ii) *If $s \geq 3$, $v_0 \neq v_3$ and $v_0v_3 \notin E(G)$, $z(G) > z(G'')$ and $i(G) < i(G'')$.*

Proof. (i) Without loss of generality, let v_0v_1 belong to the perfect matchings of G. By Lemma 1.1 and Lemma 1.2, we have

$$z(G) = z(G - v_1v_2) + z(G - \{v_1, v_2\}),$$
$$z(H'') = z(H'' - v_0v_2) + z(H'' - v_0 - v_2) = z(H'' - v_0v_2) + z(H'' - \{v_0, v_1, v_2\});$$
$$i(G) = i(G - v_0) + i(G - N_G[v_0]),$$
$$i(H'') = i(H'' - v_0) + i(H'' - N_{H''}[v_0]).$$

Note that

$$G - v_1v_2 \cong H'' - v_0v_2, \quad H'' - \{v_0, v_1, v_2\} \subset G - \{v_1, v_2\},$$
$$G - v_0 \cong H'' - v_0, \qquad H'' - N_{H''}[v_0] \subset G - N_G[v_0].$$

Note that $H'' - N_{H''}[v_0]$ and $G - N_G[v_0]$ have the same order. Then

$$z(G - v_1v_2) = z(H'' - v_0v_2), \quad z(G - \{v_1, v_2\}) > z(H'' - \{v_0, v_1, v_2\}),$$
$$i(G - v_0) = i(H'' - v_0), \qquad i(G - N_G[v_0]) < i(H'' - N_{H''}[v_0]).$$

Hence $z(G) > z(H'')$ and $i(G) < i(H'')$.

(ii) By Lemma 1.1 and Lemma 1.2, we have

$$z(G) = z(G - v_2v_3) + z(G - \{v_2, v_3\}) = z(G - v_2v_3) + z(G - \{v_1, v_2, v_3\}) + z(G - \{v_0, v_1, v_2, v_3\}),$$
$$z(G'') = z(G'' - v_0v_3) + z(G'' - v_0 - v_3) = z(G'' - v_0v_3) + 2z(G'' - \{v_0, v_1, v_2, v_3\});$$
$$i(G) = i(G - v_3) + i(G - N_G[v_3]) = i(G - v_3) + i(G - N_G[v_3] \cup N_G[v_0])$$

$$+2i(G-N_G[v_3]\cup\{v_0,v_1\})$$

$$i(G'')=i(G''-v_3)+i(G''-N_{G''}[v_3])=i(G''-v_3)+3i(G''-N_{G''}[v_3]\cup\{v_1,v_2\}).$$

Note that

$$G-v_2v_3\cong G''-v_0v_3, G-\{v_0,v_1,v_2,v_3\}\cong G''-\{v_0,v_1,v_2,v_3\},$$
$$G''-\{v_0,v_1,v_2,v_3\}\subset G-\{v_1,v_2,v_3\};$$
$$G-v_3\cong G''-v_3, G-N_G[v_3]\cup\{v_0,v_1\}\cong G''-N_{G''}[v_3]\cup\{v_1,v_2\},$$
$$G-N_G[v_3]\cup N_G[v_0]\subset G''-N_{G''}[v_3]\cup\{v_1,v_2\}$$

Hence $z(G)>z(G''), i(G)<i(G'')$. ∎

Let $\hat{G}$ be a graph on m vertices, attach a pendent edge at each vertex of $\hat{G}$, denote the resulted graph by $C(\hat{G})$. Obviously, $C(\hat{G})$ has an unique perfect matchings which consists of all pendent edges. Contracting each edge of the matching in $C(\hat{G})$ yields the graph $\hat{G}$ on m vertices. We call the graph $\hat{G}$ the contracted graph of the graph $C(\hat{G})$.

Lemma 2.2. *Let $\hat{G}$ be the contracted graph of G, if there exists either an internal path of length no less than 2 or a closed internal path of length no less than 4 in $\hat{G}$, then there exists a connected graph G' with a path of length 2 attached such that $G'=C(\hat{G}')$ for some $\hat{G}'$ and $z(G)>z(G'), i(G)<i(G')$.*

Proof. Let $P=v_0v_1\ldots v_s$ be an internal path of length no less than 2 or a closed internal path of length no less than 4 in $\hat{G}$, and $v_0',v_1',\ldots,v_s'$ the pendent vertices corresponding to $v_0,v_1,\ldots,v_s$ in G, respectively. Denote by H the graph obtained from $G-v_1v_2$ by joining v_0,v_2 with an edge.

Case 1. If $P=v_0v_1\ldots v_s$ is a closed internal path of length no less than 4 in $\hat{G}$. By Lemma 1.1, we have

$$\begin{aligned}
z(G)&=z(G-v_1v_2)+z(G-\{v_1,v_2\})\\
&=z(G-v_1v_2)+z(G-\{v_0',v_1,v_2\})+z(G-\{v_0,v_0',v_1,v_2\})\\
&=z(G-v_1v_2)+z((G-\{v_0',v_1,v_1',v_2,v_2'\})\cup 2P_1)+z((G-\{v_0,v_0',v_1,v_1',v_2,v_2'\})\cup 2P_1)\\
&=z(G-v_1v_2)+z(G-\{v_0',v_1,v_1',v_2,v_2'\})+z(G-\{v_0,v_0',v_1,v_1',v_2,v_2'\}),\\
z(H)&=z(H-v_0v_2)+z(H-\{v_0,v_2\})\\
&=z(H-v_0v_2)+z(H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}\cup 2P_1\cup P_2)\\
&=z(H-v_0v_2)+2z(H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}),
\end{aligned}$$

and

$$G-v_1v_2\cong H-v_0v_2, G-\{v_0,v_0',v_1,v_1',v_2,v_2'\}\cong H-\{v_0,v_0',v_1,v_1',v_2,v_2'\},$$
$$H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}\subset G-\{v_0',v_1,v_1',v_2,v_2'\},$$

so

$$z(G-v_1v_2)=z(H-v_0v_2), z(G-\{v_0,v_0',v_1,v_1',v_2,v_2'\})=z(H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}),$$
$$z(G-\{v_0',v_1,v_1',v_2,v_2'\})>z(H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}).$$

Hence $z(G)>z(H)$.

By Lemma 1.2, we have

$$\begin{aligned} i(G) &= i(G-v_2)+i(G-N_G[v_2]) \\ &= i(G-v_2)+i((G-\{v_1,v_1',v_2,v_2',v_3,v_3'\})\cup 2P_1) \\ &= i(G-v_2)+4i(G-\{v_1,v_1',v_2,v_2',v_3,v_3'\}) \\ &= i(G-v_2)+4[i(G-\{v_0',v_1,v_1',v_2,v_2',v_3,v_3'\})+i(G-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\})] \\ &= i(G-v_2)+4[i(G-\{v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}\cup N_G[v_0]) \\ &\quad +2i(G-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\})], \\ i(H) &= i(H-v_2)+i(H-N_H[v_2]) \\ &= i(H-v_2)+i((H-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\})\cup 2P_1\cup P_2) \\ &= i(H-v_2)+12i(H-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}). \end{aligned}$$

Note that

$$\begin{aligned} &G-v_2\cong H-v_2, G-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}\cong H-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}, \\ &G-\{v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}\cup N_G[v_0]\subset H-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}, \end{aligned}$$

then

$$\begin{aligned} &i(G-v_2\cong H-v_2, i(G-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\})=i(H-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}), \\ &i(G-\{v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}\cup N_G[v_0])<i(H-\{v_0,v_0',v_1,v_1',v_2,v_2',v_3,v_3'\}. \end{aligned}$$

Hence $i(G)<i(H)$.

Case 2. If $P=v_0v_1\dots v_s$ is an internal path of length no less than 2 in $\hat{G}$. By Lemma 1.1 and Lemma 1.2, we have

$$\begin{aligned} z(G) &= z(G-v_1v_2)+z(G-\{v_1,v_2\})=z(G-v_1v_2)+z(G-\{v_1,v_1',v_2,v_2'\}) \\ &= z(G-v_1v_2)+z(G-\{v_0',v_1,v_1',v_2,v_2'\})+z(G-\{v_0,v_0',v_1,v_1',v_2,v_2'\}), \\ z(H) &= z(H-v_0v_2)+z(H-\{v_0,v_2\})=z(H-v_0v_2)+2z(H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}); \\ i(G) &= i(G-v_2)+i(G-N_G[v_2])=i(G-v_2)+2i(G-N_G[v_2]\cup\{v_1'\}) \\ &= i(G-v_2)+2i(G-N_G[v_2]\cup\{v_0',v_1'\})+2i(G-N_G[v_2]\cup\{v_0,v_0',v_1'\}) \\ &= i(G-v_2)+2i(G-N_G[v_2]\cup N_G[v_0]\cup\{v_1'\})+4i(G-N_G[v_2]\cup\{v_0,v_0',v_1'\}), \\ i(H) &= i(H-v_2)+i(H-N_H[v_2])=i(H-v_2)+6i(H-N_H[v_2]\cup\{v_0',v_1,v_1'\}). \end{aligned}$$

Note that

$$\begin{aligned} &G-v_1v_2\cong H-v_0v_2, G-\{v_0',v_1,v_1',v_2,v_2'\}\cong H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}, \\ &H-\{v_0,v_0',v_1,v_1',v_2,v_2'\}\subset G-\{v_0',v_1,v_1',v_2,v_2'\}; \\ &G-v_2\cong H-v_2, G-N_G[v_2]\cup\{v_0,v_0',v_1'\}\cong H-N_H[v_2]\cup\{v_0',v_1,v_1'\}, \\ &G-N_G[v_2]\cup N_G[v_0]\cup\{v_1'\}\subset H-N_H[v_2]\cup\{v_0',v_1,v_1'\}. \end{aligned}$$

Then $z(G)>z(H), i(G)<i(H)$.

Select $H=G'$, then we obtain our desirable results. ∎

3. Main results

Let G be a bicyclic graph. The base of G, denoted by $B(G)$, is the minimal bicyclic subgraph of G. Obviously, $B(G)$ is the unique bicyclic subgraph of G containing no pendant vertex, and G can be obtained from $B(G)$ by planting trees to some vertices of $B(G)$. It is well known that bicyclic graphs have the following two types of bases: $B(p,l,q)$ and $P(p,q,r)$, where $B(p,l,q)$ is the graph obtained by joining a new path $u_1u_2\dots u_l$ between two cycles C_p and C_q with $u_1 \in V(C_p), u_l \in V(C_q)$, and $P(p,q,r)$ is the bicyclic graph consisting of three pairwise internal disjoint paths $P_{p+1}, P_{q+1}, P_{r+1}$ with common endpoints u, v. Let $B_1(2m) = \{G \in \mathscr{B}(2m,m) | B(G) = B(p,l,q), p \le q\}; B_2(2m) = \{G \in \mathscr{B}(2m,m) | B(G) = P(p,q,r)\}$. Then $\mathscr{B}(2m,m) = B_1(2m) \cup B_2(2m)$.

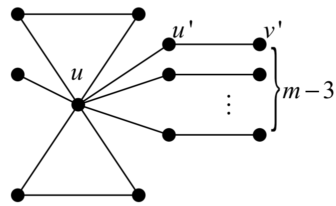

Figure 1. The graph B_{2m}.

Lemma 3.1. *Let B_{2m} be graph of the form in Figure 1. Then $z(B_{2m}) = 4 \cdot 2^{m-1} + (m-3) \cdot 2^{m-2}$ and $i(B_{2m}) = 2 \cdot 3^{m-1} + 2^{m-3}$.*

Proof. By Lemma 1.1 and Lemma 1.2, we have

$$\begin{aligned} z(B_{2m}) &= z(B_{2m} - u) + \sum_{v \in N_{B_{2m}}(u)} z(B_{2m} - \{u,v\}) \\ &= z((m-1)P_2 \cup P_1) + z((m-1)P_2) + 4z((m-2)P_2 \cup 2P_1) + (m-3)z((m-2)P_2 \cup 2P_1) \\ &= 4 \cdot 2^{m-1} + (m-3) \cdot 2^{m-2}, \\ i(B_{2m}) &= i(B_{2m} - u) + i(B_{2m} - N_{B_{2m}}[u]) = i((m-1)P_2 \cup P_1) + i((m-3)P_1) \\ &= 2 \cdot 3^{m-1} + 2^{m-3}. \end{aligned}$$

∎

Let $G_1, G_2, \dots, G_{14}$ be graphs of the form in Figure 2, by direct calculation, we have

$$\begin{aligned} &z(G_1) = 20, z(G_2) = 16, z(G_3) = 38, z(G_4) = 52, z(G_5) = 20; \\ &z(G_6) = 45, z(G_7) = 46, z(G_8) = 42, z(G_9) = 250, z(G_{10}) = 40; \\ &z(G_{11}) = 94, z(G_{12}) = 99, z(G_{13}) = 142, z(G_{14}) = 143. \end{aligned} \tag{3.1}$$

And

$$\begin{aligned} &i(G_1) = 17, i(G_2) = 19, i(G_3) = 52, i(G_4) = 48, i(G_5) = 15; \\ &i(G_6) = 45, i(G_7) = 44, i(G_8) = 47, i(G_9) = 384, i(G_{10}) = 48; \\ &i(G_{11}) = 136, i(G_{12}) = 132, i(G_{13}) = 128, i(G_{14}) = 132. \end{aligned} \tag{3.2}$$

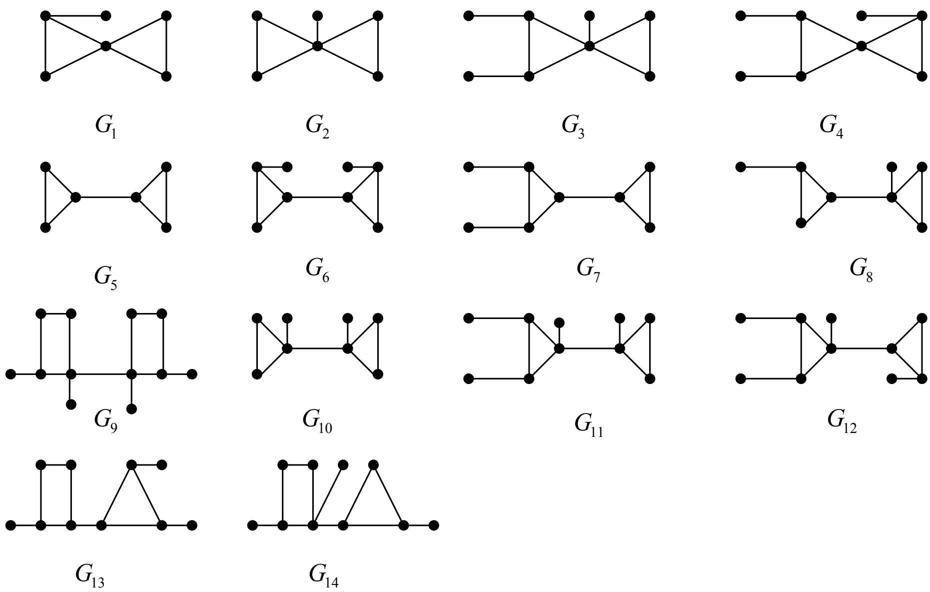

Figure 2. The graphs $G_1, G_2, \ldots, G_{14}$.

Theorem 3.1. *Let G be a graph in $B_1(2m), m \geq 3$. Then $z(G) \geq z(B_{2m})$ and $i(G) \leq i(B_{2m})$, the equalities hold if and only if $G \cong B_{2m}$.*

Proof. When $m = 3$, $B_1(2m) = \{G_1, G_2, G_5, \widehat{B}(3,1,4)\}$. By direct calculation, $z(\widehat{B}(3,1,4)) = 20$, $i(\widehat{B}(3,1,4)) = 17$, combining (3.1) and (3.2), we have $z(G) \geq z(G_2) = z(B_{2m})$, $i(G) \leq i(G_2) = i(B_{2m})$.

Now we suppose $m \geq 4$. Let $G \in B_1(2m)$.

Case 1. If G has a pendent vertex v' with its adjacent vertex u' of degree 2. Let $N_G(u') = \{v', r\}$. By Lemmas 1.1 and 1.2, we have

$$\begin{aligned}
z(G) &= z(G - v') + z(G - \{v', u'\}) = z(G - \{v', u', r\}) + 2z(G - \{v', u'\}),\\
z(B_{2m}) &= z(B_{2m} - v') + z(B_{2m} - \{v', u'\}) = z(B_{2m} - \{v', u', u\}) + 2z(B_{2m} - \{v', u'\})\\
&= z(K_1 \cup (m-2)K_2) + 2z(B_{2m} - \{v', u'\});\\
i(G) &= i(G - v') + i(G - \{v', u'\}) = i(G - \{v', u', r\}) + 2i(G - \{v', u'\}),\\
i(B_{2m}) &= i(B_{2m} - v') + i(B_{2m} - \{v', u'\}) = i(B_{2m} - \{v', u', u\}) + 2i(B_{2m} - \{v', u'\})\\
&= i(K_1 \cup (m-2)K_2) + 2i(B_{2m} - \{v', u'\}).
\end{aligned}$$

Since $G - \{v', u', r\}$ is a graph on $2m-3$ vertices with $(m-2)$-matching, $K_1 \cup (m-2)K_2$ is a spanning subgraph of $G - \{v', u', r\}$ when $G \ncong B_{2m}$, then $z(G - \{v', u', r\}) > z(K_1 \cup (m-2)K_2)$, $i(G - \{v', u', r\}) < i(K_1 \cup (m-2)K_2)$. Since $G - \{v', u'\}$ is a graph on $2m-2$ vertices with perfect matching, by induction hypothesis, we have $z(G - \{v', u'\}) > z(B_{2m} - \{v', u'\})$, $i(G - \{v', u'\}) < i(B_{2m} - \{v', u'\})$.

Then $z(G) \geq z(B_{2m})$, $i(G) \leq i(B_{2m})$.

Case 2. If G has not a pendent vertex v' with its adjacent vertex u' of degree 2. Then G can be obtained from $B(p,l,q)$ by attaching some pendent edges at some vertices of $B(p,l,q)$. In fact, if there is a vertex $u \in V(B(p,l,q))$ attaching a tree T with $|V(T)| \geq 2$, by Lemma 1.4, it is contradict to the choice of G. Let $P = v_0v_1 \dots v_s$ be the longest internal path in G.

Subcase 2.1. $s = 1$.

When $d(u_1) \geq 4$, then $G \cong C(B(p,l,q))$. If there exists either an internal path of length no less than 2 or a closed internal path of length no less than 4 in $B(p,l,q)$, by Lemma 2.2 and Case 1, we have the desired results. Otherwise, $B(p,l,q) \cong B(3,1,3)$ or $B(3,2,3)$, then

$$G \in \{C(B(3,1,3)), C(B(3,2,3))\}.$$

By direct calculation, we have

$$z(C(B(3,1,3))) = 90, z(C(B(3,2,3))) = 221; i(C(B(3,1,3))) = 144, i(C(B(3,2,3))) = 224.$$

By Lemma 3.1,

$$z(B_{10}) = 52, z(B_{12}) = 76; i(B_{10}) = 166, i(B_{12}) = 494. \tag{3.3}$$

Hence, we also have the desired results.

When $d(u_1) = 3$, then $l = 2$ and $d(u) = 3$ for any $u \in V(B(G))$. Let G' be the graph obtained form $G - u_1u_2$ by identifying u_1 with u_2 and adding a pendent edge at u_1, obviously, $G' \in B_1(2m)$ and $G' \cong C(B(p,l-1,q))$. By Lemma 1.3, we have $z(G) > z(G')$ and $i(G) < i(G')$, as above discussion, we have $z(G') > z(B_{2m})$ and $i(G') < i(B_{2m})$. Then we obtain the desired results.

Subcase 2.2. $s = 2$, then at least one of v_0, v_2 must be in $\{u_1, u_l\}$. Otherwise, v_1 must be an unmatched vertex, a contradiction. Then there are at most two internal paths of length 2.

Subcase 2.2.1. G has only one internal path of length 2.

When $v_0v_2 \notin E(G)$, by Lemma 2.1, we can obtain a connected graph G' such that $G' \cong C(B(p,l',q))$, where $l' \leq l$. By *Subcase 2.1.*, we have the desired results.

When $v_0v_2 \in E(G)$, then $B(G) \cong B(3,l,q)$. Without loss of generality, let $v_0 = u_1$. If $l \geq 3$, let G' be the graph obtained from G by deleting u_2u_3 and adding u_1u_3. Set $G - u_2u_3 = A \cup D$, where $u_2 \in V(A), u_3 \in V(D)$. By Lemmas 1.1 and 1.2, we have

$$\begin{aligned}
z(G) &= z(G - u_2u_3) + z(G - \{u_2,u_3\}) = z(A \cup D) + z((A - u_2) \cup (D - u_3)) \\
&= z(A \cup D) + 6z(D - u_3), \\
z(G') &= z(G' - u_1u_3) + z(G' - \{u_1,u_3\}) = z(A \cup D) + z((A - u_1) \cup (D - u_3)) \\
&= z(A \cup D) + 3z(D - u_3); \\
i(G) &= i(G - u_3) + i(G - N_G[u_3]) = i(A \cup (D - u_3)) + i((A - u_2) \cup (D - N_D[u_3])) \\
&= i(A \cup (D - u_3)) + 14i(D - N_D[u_3]),
\end{aligned}$$

$$i(G') = i(A \cup (D - u_3)) + 15i(D - N_D[u_3]). \tag{3.4}$$

Then $z(G) > z(G')$ and $i(G) < i(G')$ and there is a pendent vertex v' with its adjacent vertex u_2 of degree 2 in G'. Similarly, if $q \geq 4$, we also can find a graph G' which satisfy $z(G) > z(G')$ and $i(G) < i(G')$ and there is a pendent vertex v' with its adjacent vertex u' of degree 2 in G'. By Case 1, $z(G') > z(B_{2m})$ and $i(G') < i(B_{2m})$. Then we obtain the desired results. If $l \leq 2$ and $q = 3$, then $G \in \{G_4, G_{12}\}$. By (3.1), (3.2) and Lemma 3.1, we have the desired results.

Subcase 2.2.2. G have two internal paths of length 2, let $P = v_0v_1v_2$ and $P' = v'_0v'_1v'_2$ be the two paths.

When at least one of $v_0v_2, v'_0v'_2 \notin E(G)$, by Lemma 2.1, we can obtain a graph G' such that $z(G) > z(G')$ and $i(G) < i(G')$, and G' has one internal path of length 2, by *Subcase 2.2.1.*, we have the desired results.

When all of $v_0v_2, v'_0v'_2 \in E(G)$, then $B(G) \cong B(3,l,3)$. If $l \geq 3$, similar to *Subcase 2.2.1.*, we can obtain the desired results. If $l \leq 2$, then $G \cong G_6$. By (3.1), (3.2) and Lemma 3.1, we have the desired results.

Subcase 2.3. $s = 3$.

If there exists an internal path $P = v_0v_1v_2v_3$ with $v_0v_3 \notin E(G), v_0 \neq v_3$. By *Transformation A* and Lemma 2.1, we can find a graph G' such that $z(G) > z(G'), i(G) < i(G')$, and there is a pendent vertex v' with its adjacent vertex u' of degree 2 in G'. By Case 1, we have $z(G') \geq z(B_{2m}), i(G') \leq i(B_{2m})$, as desired. Otherwise, any internal path $P = v_0v_1v_2v_3$ in G, it has either $v_0v_3 \in E(G)$ or $v_0 = v_3$.

Subcase 2.3.1. Any internal path $P = v_0v_1v_2v_3$ in G, it has $v_0v_3 \in E(G)$. Obviously, there are at most two such internal paths.

When there are two such internal paths in G, then $B(G) \cong B(4,l,4)$. Further $l \geq 2$, otherwise $G \notin B_1(2m)$. If $d(u_1) = 3$, then u_1u_2 must be an matching edge and $d(u_2) = 2, d(u_3) \geq 3$. Let G' be the graph obtained from G by deleting u_2u_3 and adding u_1u_3. Similar to the procedure of (3.4), we have $z(G) > z(G')$ and $i(G) < i(G')$. To find the extremal graph, we can set $d(u_1), d(u_l) \geq 4$. Then we have $d(u_i) = 3$ for $i = 2, \ldots, l-1$, otherwise, it must have another internal path $P' = v'_0v'_1v'_2v'_3$ with $v'_0v'_3 \notin E(G)$, a contradiction. If $l \geq 3$, similar to the discussion of *Subcase 2.2.1.*, we have the desired results. For $l = 2$, $G \cong G_9$, by (3.1-3.3), we have the desired results.

When there is only one such internal path in G, then $B(G) \cong B(4,l,q)$. If $l \geq 3$ or $q \geq 4$, similar to the discussion of *Subcase 2.2.1.*, we have the desired results. If $l \leq 2$ and $q = 3$, $G \in \{G_{13}, G_{14}\}$, by (3.1-3.3), we have the desired results.

Subcase 2.3.2. Any internal path $P = v_0v_1v_2v_3$ in G, it has $v_0 = v_3$. Obviously, there are at most two such internal paths.

When there are two such internal paths in G, then $B(G) \cong B(3,l,3)$. If $l \geq 3$, similar to the discussion of *Subcase 2.2.1.*, we have the desired results. If $l \leq 2$, $G \in \{G_2, G_5, G_{10}\}$, by (3.1–3.3), we have the desired results.

When there is only one such internal path in G, then $B(G) \cong B(3,l,q)$. If $l \geq 3$ or $q \geq 4$, similar to the discussion of *Subcase 2.2.1.*, we have the desired results. If $l \leq 2$ and $q = 3$, $G \in \{G_1, G_3, G_7, G_8, G_{11}\}$, by (3.1–3.3), we have the desired results.

Subcase 2.4. $s \geq 4$. By *Translation A*, Lemma 2.1 and *Case 1*, we have the desired results.

This completes the proof. ∎

Let $W_1, W_2, \ldots, W_{12}$ be graphs of the form in Figure 3, by direct calculation, we have

$$\begin{aligned} &z(W_1) = 22, z(W_2) = 20, z(W_3) = 20, z(W_4) = 19, z(W_5) = 24, z(W_6) = 18, \\ &z(W_7) = 19, z(W_8) = 26, z(W_9) = 21, z(W_{10}) = 46, z(W_{11}) = 108, z(W_{12}) = 44. \end{aligned} \tag{3.5}$$

And

$$\begin{aligned} &i(W_1) = 17, i(W_2) = 18, i(W_3) = 16, i(W_4) = 12, i(W_5) = 17, i(W_6) = 18, \\ &i(W_7) = 17, i(W_8) = 17, i(W_9) = 16, i(W_{10}) = 52, i(W_{11}) = 136, i(W_{12}) = 48. \end{aligned} \tag{3.6}$$

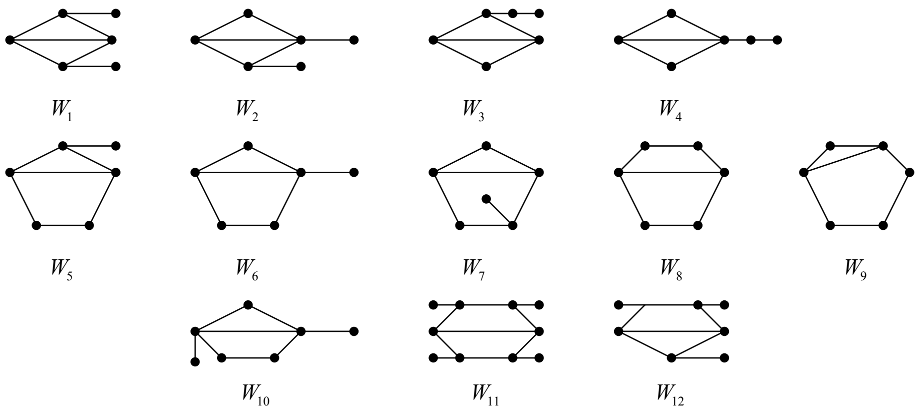

Figure 3. The graphs $W_1, W_2, \ldots, W_{12}$.

Theorem 3.2. *Let G be a graph in $B_2(2m), m \geq 3$. Then $z(G) > z(B_{2m})$ and $i(G) < i(B_{2m})$.*

Proof. When $m = 3$, $B_1(2m) = \{G_1, G_2, G_5, \widehat{B}(3,1,4)\}$, $B_2(2m) = \{W_1, W_2, \ldots, W_9\}$. By (3.5), (3.6), Lemma 3.1 and Theorem 3.2, we have $z(G) > z(B_{2m}), i(G) < i(B_{2m})$.

We now suppose $m \geq 4$. For any graph $G \in B_2(2m)$, $B(G) \cong P(p,q,r)$. For convenience, let $q \leq r \leq p$.

Case 1. G has a pendent vertex v' with its adjacent vertex u' of degree 2. Similar to the proof of *Case 1* in Theorem 3.2, we have the desired results.

Case 2. G hasn't a pendent vertex v' with its adjacent vertex u' of degree 2 and $(p,q,r) \neq (2,1,2)$. Then G can be obtained from $P(p,q,r)$ by attaching some pendent edges at some vertices of $P(p,q,r)$. Let $P_{p+1} = uu_1u_2\ldots u_{p-1}v$, u_i' be the pendent vertex which is adjacent to $u_i (i = 1,2,\ldots,p-1)$, respectively, and $P = v_0v_1\ldots v_s$ be the longest internal path in G.

Subcase 2.1. $s = 1$. If $d_G(u) = 4$, $G \cong C(P(p,q,r))$. By Lemma 2.2 and *Case 1*, we have the desired results. If $d_G(u) = 3$, then $d_G(v) = 3, q = 1$ and $p \geq 3$.

If $p \geq 4$, let G' be the graph obtained from G by deleting u_2u_3 and adding u_1u_3. By Lemmas 1.1 and 1.2, we have

$$\begin{aligned}
z(G) &= z(G - u_2u_3) + z(G - \{u_2, u_3\}) = z(G - u_2u_3) + z(G - \{u_2, u_2', u_3, u_3'\}) \\
&= z(G - u_2u_3) + z(G - \{u_1', u_2, u_2', u_3, u_3'\}) + z(G - \{u_1, u_1', u_2, u_2', u_3, u_3'\}) \\
z(G') &= z(G' - u_1u_3) + z(G' - \{u_1, u_3\}) = z(G' - u_1u_3) + 2z(G' - \{u_1, u_1', u_2, u_2', u_3, u_3'\}), \\
i(G) &= i(G - u_3) + i(G - N_G[u_3]) = i(G - u_3) + 2i(G - N_G[u_3] \cup \{u_2'\}) \\
&= i(G - u_3) + 2[i(G - N_G[u_3] \cup \{u_1', u_2'\}) + i(G - N_G[u_3] \cup \{u_1, u_1', u_2'\})] \\
&= i(G - u_3) + 2[i(G - N_G[u_3] \cup N_G[u_1] \cup \{u_1', u_2'\}) + 2i(G - N_G[u_3] \cup \{u_1, u_1', u_2'\})] \\
i(G') &= i(G' - u_3) + i(G' - N_{G'}[u_3]) = i(G' - u_3) + 6i(G' - N_{G'}[u_3] \cup \{u_1', u_2, u_2'\}).
\end{aligned}$$

Note that

$$\begin{aligned}
&G - u_2u_3 \cong G' - u_1u_3, G - \{u_1, u_1', u_2, u_2', u_3, u_3'\} \cong G' - \{u_1, u_1', u_2, u_2', u_3, u_3'\}, \\
&G' - \{u_1, u_1', u_2, u_2', u_3, u_3'\} \subset G - \{u_1', u_2, u_2', u_3, u_3'\};
\end{aligned}$$

$$G-u_3 \cong G'-u_3, G-N_G[u_3]\cup\{u_1,u_1',u_2'\}) \cong G'-N_{G'}[u_3]\cup\{u_1',u_2,u_2'\},$$
$$G-N_G[u_3]\cup N_G[u_1]\cup\{u_1',u_2'\} \subset G'-N_{G'}[u_3]\cup\{u_1',u_2,u_2'\}.$$

Then $z(G)>z(G')$ and $i(G)<i(G')$. By *Case 1*, we have the desired results.

If $p=3$, then $r\leq 3$, and $G\in\{W_{11},W_{12}\}$. By (3.5), (3.6), Lemma 3.1 and Theorem 3.2, we have $z(G)>z(B_{2m}), i(G)<i(B_{2m})$.

Subcase 2.2. $s=2$, then at least one of v_0,v_2 must be in $\{u,v\}$. Otherwise, v_1 must be an unmatched vertex, a contradiction. Then there are at most two internal paths of length 2.

Subcase 2.2.1. G has only one internal path of length 2.

When $v_0v_2\notin E(G)$, by Lemma 2.1, we can obtain a connected graph G' such that $G'\cong C(P(p',q',r'))$. By *Subcase 2.1.*, we have the desired results.

When $v_0v_2\in E(G)$, then $B(G)\cong P(p,1,2)$, where $p\geq 3$. Without loss of generality, let v_1v_2 be a matching edge and $u=v_0, v=v_2$, then $d_G(u)=4, d_G(v)=3$. Set u' be the pendent vertex which is adjacent to u. Let G' be the graph obtained from G by deleting u_1u_2 and adding uu_2. Obviously, G' has a pendent vertex which is adjacent to a vertex of degree 2. By Lemmas 1.1 and 1.2, we have

$$\begin{aligned}
z(G) &= z(G-u_1u_2)+z(G-\{u_1,u_2\}) = z(G-u_1u_2)+z(G-\{u_1,u_1',u_2,u_2'\})\\
&= z(G-u_1u_2)+z(G-\{u',u_1,u_1',u_2,u_2'\})+z(G-\{u,u',u_1,u_1',u_2,u_2'\}),\\
z(G') &= z(G'-uu_2)+z(G'-\{u,u_2\}) = z(G'-uu_2)+2z(G'-\{u,u',u_1,u_1',u_2,u_2'\}),\\
i(G) &= i(G-u_2)+i(G-N_G[u_2]) = i(G-u_2)+4i(G-\{u_1,u_1',u_2,u_2',u_3,u_3'\})\\
&= i(G-u_2)+4i(G-\{u',u_1,u_1',u_2,u_2',u_3,u_3'\})+4i(G-\{u,u',u_1,u_1',u_2,u_2',u_3,u_3'\})\\
&= i(G-u_2)+4i(G-\{u',u_1,u_1',u_2,u_2',u_3,u_3'\}\cup N_G[u])\\
&\quad +8i(G-\{u,u',u_1,u_1',u_2,u_2',u_3,u_3'\})\\
i(G') &= i(G'-u_2)+i(G'-N_{G'}[u_2]) = i(G'-u_2)+12i(G'-\{u,u',u_1,u_1',u_2,u_2'\}).
\end{aligned}$$

Note that

$$G-u_1u_2\cong G'-uu_2, G-\{u,u',u_1,u_1',u_2,u_2'\}\cong G'-\{u,u',u_1,u_1',u_2,u_2'\},$$
$$G'-\{u,u',u_1,u_1',u_2,u_2'\}\subset G-\{u',u_1,u_1',u_2,u_2'\};$$
$$G-u_2\cong G'-u_2, G-\{u',u_1,u_1',u_2,u_2',u_3,u_3'\}\cup N_G[u]\subset G'-\{u,u',u_1,u_1',u_2,u_2'\}.$$

Then $z(G)>z(G')$ and $i(G)<i(G')$. By *Case 1*, we have the desired results.

Subcase 2.2.2. G have two internal paths of length 2, let $P=v_0v_1v_2$ and $P'=v_0'v_1'v_2'$ be the two paths. Then at least one of $v_0v_2, v_0'v_2'$ is not an edge of G, by Lemma 2.1, we can obtain a graph G' such that $z(G)>z(G')$ and $i(G)<i(G')$, and G' has one internal path of length 2, by *Subcase 2.2.1.*, we have the desired results.

Subcase 2.3. $s=3$.

If there exists an internal path $P=v_0v_1v_2v_3$ with $v_0v_3\notin E(G)$. By *Transformation A*, Lemma 2.1 and Case 1, we have the desired results. Otherwise, any internal path $P=v_0v_1v_2v_3$ in G, it has $v_0v_3\in E(G)$. Obviously, there are at most two such internal paths.

When there are two such internal paths in G, then $B(G)\cong P(3,1,3)$. Then $G\in\{W_8,W_{10}\}$. By (3.5), (3.6), Lemma 3.1 and Theorem 3.2, we have $z(G)>z(B_{2m}), i(G)<i(B_{2m})$.

When there is only one such internal path in G, then $B(G) \cong P(3,1,q)$. Let G' be the graph obtained from G by deleting v_1v_2 and adding uv_2. By Lemmas 1.1 and 1.2, we have

$$\begin{aligned} z(G) &= z(G - v_1v_2) + z(G - \{v_1, v_2\}), \\ z(G') &= z(G' - uv_2) + z(G' - \{u, v_2\}) = z(G' - uv_2) + z(G' - \{u, v_1, v_2\}), \\ i(G) &= i(G - v_2) + i(G - N_G[v_2]) = i(G - v_2) + i(G - \{v, v_1, v_2\}) \\ &= i(G - v_2) + i(G - \{u, v, v_1, v_2\}) + i(G - \{v, v_1, v_2\} \cup N_G[u]), \\ i(G') &= i(G' - v_2) + i(G' - N_{G'}[v_2]) = i(G' - v_2) + 2i(G' - \{u, v, v_1, v_2\}). \end{aligned}$$

Note that

$$\begin{aligned} &G - v_1v_2 \cong G' - uv_2, G' - \{u, v_1, v_2\} \subset G - \{v_1, v_2\}; \\ &G - v_2 \cong G' - v_2, G - \{u, v, v_1, v_2\} \cong G' - \{u, v, v_1, v_2\}, \\ &G - \{v, v_1, v_2\} \cup N_G[u] \subset G' - \{u, v, v_1, v_2\}. \end{aligned}$$

Then $z(G) > z(G')$ and $i(G) < i(G')$. Hence $s = 2$ in G', by *Subcase 2.2.*, we have the desired results.

Subcase 2.4. $s \geq 4$. By *Translation A*, Lemma 2.1 and *Case 1*, we have the desired results.

Case 3. G hasn't a pendent vertex v' with its adjacent vertex u' of degree 2 and $(p, q, r) = (2, 1, 2)$. Then $G \in \{W_1, W_2, C(P(2, 1, 2))\}$. Note that $z(C(P(2, 1, 2))) = 38, i(C(P(2, 1, 2))) = 52$. By (3.5), (3.6), Lemma 3.1 and Theorem 3.2, we have $z(G) > z(B_{2m}), i(G) < i(B_{2m})$.

This completes the proof. ∎

By Lemma 3.1, Theorem 3.2 and 3.3, we obtain our main results.

Theorem 3.3. *Let G be a graph in* $\mathscr{B}(2m, m), m \geq 2$.

(i) *If* $m = 2$, $G \cong P(2, 1, 2), z(G) = 8, i(G) = 6$;
(ii) *If* $m \geq 3$, $z(G) \geq 4 \cdot 2^{m-1} + (m-3) \cdot 2^{m-2}$ *and* $i(G) \leq 2 \cdot 3^{m-1} + 2^{m-3}$, *the equalities hold if and only if* $G \cong B_{2m}$.

References

[1] B. Bollobás, *Modern Graph Theory*, Graduate Texts in Mathematics, 184, Springer, New York, 1998.
[2] A. Chang, F. Tian and A. Yu, On the index of bicyclic graphs with perfect matchings, *Discrete Math.* **283** (2004), no. 1–3, 51–59.
[3] H. Deng and S. Chen, The extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* **59** (2008), no. 1, 171–190.
[4] H. Deng, The largest Hosoya index of $(n, n+1)$-graphs, *Comput. Math. Appl.* **56** (2008), no. 10, 2499–2506.
[5] H. Deng, The smallest Hosoya index in $(n, n+1)$-graphs, *J. Math. Chem.* **43** (2008), no. 1, 119–133.
[6] H. Deng, The smallest Merrifield-Simmons index of $(n, n+1)$-graphs, *Math. Comput. Modelling* **49** (2009), no. 1-2, 320–326.
[7] H. Deng, S. Chen and J. Zhang, The Merrifield-Simmons index in $(n, n+1)$-graphs, *J. Math. Chem.* **43** (2008), no. 1, 75–91.
[8] R. E. Merrifield and H. E. Simmons, *Topological Methods in Chemistry*, Wiley, New York, 1989.
[9] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
[10] H. Hua, Hosoya index of unicyclic graphs with prescribed pendent vertices, *J. Math. Chem.* **43** (2008), no. 2, 831–844.
[11] H. Hua, Minimizing a class of unicyclic graphs by means of Hosoya index, *Math. Comput. Modelling* **48** (2008), no. 5-6, 940–948.
[12] Y. Hou, On acyclic systems with minimal Hosoya index, *Discrete Appl. Math.* **119** (2002), no. 3, 251–257.

[13] A. J. Hoffman and J. H. Smith, On the spectral radii of topologically equivalent graphs, in *Recent Advances in Graph Theory (Proc. Second Czechoslovak Sympos., Prague, 1974)*, 273–281, Academia, Prague.
[14] S. Li and Z. Zhu, The number of independent sets in unicyclic graphs with a given diameter, *Discrete Appl. Math.* **157** (2009), 1387–1395.
[15] H. Prodinger and R. F. Tichy, Fibonacci numbers of graphs, *Fibonacci Quart.* **20** (1982), no. 1, 16–21.
[16] J. Ou, On extremal unicyclic molecular graphs with maximal Hosoya index, *Discrete Appl. Math.* **157** (2009), no. 2, 391–397.
[17] H. Liu, X. Yan and Z. Yan, On the Merrifield-Simmons indices and Hosoya indices of trees with a prescribed diameter, *MATCH Commun. Math. Comput. Chem.* **57** (2007), no. 2, 371–384.
[18] H. Liu and M. Lu, A unified approach to extremal cacti for different indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007), no. 1, 183–194.
[19] A. S. Pedersen and P. D. Vestergaard, The number of independent sets in unicyclic graphs, *Discrete Appl. Math.* **152** (2005), no. 1–3, 246–256.
[20] L. Turker, Contemplation on the Hosoya indices, *Journal of Molecular structure (Theochem)*, **623** (2003), 75–77.
[21] L. Tan and Z. Zhu, The extremal θ-graphs with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* **63** (2010), no. 3, 789–798.
[22] H. Wang and H. Hua, Unicycle graphs with extremal Merrifield-Simmons index, *J. Math. Chem.* **43** (2008), no. 1, 202–209.
[23] S. Wagner, Extremal trees with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* **57** (2007), no. 1, 221–233.
[24] S. Wagner and I. Gutman, Maxima and minima of the Hosoya index and the Merrifield-Simmons index: A survey of results and techniques, *Acta Appl. Math.* **112** (2010), no. 3, 323–346.
[25] K. Xu and I. Gutman, The greatest Hosoya index of bicyclic graphs with given maximum degree, *MATCH Commun. Math. Comput. Chem.* **66** (2011), no. 3, 795–824.
[26] K. Xu, On the Hosoya index and the Merrifield-Simmons index of graphs with a given clique number, *Appl. Math. Lett.* **23** (2010), no. 4, 395–398.
[27] K. Xu and B. Xu, Some extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index, *MATCH Commun. Math. Comput. Chem.* **62** (2009), no. 3, 629–648.
[28] A. Yu and F. Tian, A kind of graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices, *MATCH Commun. Math. Comput. Chem.* **55** (2006), no. 1, 103–118.
[29] C. Ye and Z. Hu, On the ordering of trees by two indices, *Bull. Malays. Math. Sci. Soc. (2)* **35** (2012), no. 4, 969–974.
[30] Y. Wu and Q. Yu, A characterization of graphs with equal domination number and vertex cover number, *Bull. Malays. Math. Sci. Soc. (2)* **35** (2012), no. 3, 803–806.