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ON SOMBOR INDEX OF BICYCLIC GRAPHS WITH GIVEN MATCHING NUMBER†

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Abstract. Nowadays, it is an important task to find extremal values on any molecular descriptor with respect to different graph parameters. The Sombor index is a novel topological molecular descriptor introduced by Gutman in 2021. The research on determining extremal values for the Sombor index of a graph is very popular recently. In this paper, we present the maximum Sombor index of bicyclic graphs with given matching number. Furthermore, we identify the corresponding extremal bicyclic graphs.

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1. Introduction

As a numerical parameter of molecular structure, topological molecular descriptors (or topological indices) play an important role in chemistry, pharmacology and materials science, etc. (see [10], [11], [26]). In 2021, Gutman [8] put forward a novel topological molecular descriptor named Sombor index. And for a (molecular) graph G, it is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2},$$

where $d_G(u)$ denotes the degree of vertex u in G. Sombor index has attracted a significant attention from researchers within a very short time. Redžepović [23] found that Sombor index can be successfully used to simulate the thermodynamic properties of compounds since it possesses satisfactory prediction potential in modeling entropy and enthalpy of vaporization of alkanes. For mathematical

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investigations of Sombor index, the readers can refer to [1-4], [6-9], [12-17], [19], [20], [24], [25], [27], [29], [30].

We only deal with connected graphs without multiple edges and loops. We use $G = (V(G), E(G))$ to denote the graph with vertex set $V(G)$ and edge set $E(G)$. Let $N_G(x)$ be the set of all neighbours of $x \in V(G)$ in G, and $d_G(x) = |N_G(x)|$. If $d_G(x) = 1$, we call x is a pendant vertex, and denoted by $PV(G)$ the set of all pendant vertices in G. We denote the distance between vertices u and v of G by $d_G(u, v)$. Let $G - xy$ and $G - x$ be the graph obtained from G by deleting the edge $xy \in E(G)$ and the vertex $x \in V(G)$, respectively. Similarly, $G + uv$ is the graph obtained from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$. Unicyclic graphs U and bicyclic graphs B are connected graphs satisfying $|E(U)| = |V(U)|$ and $|E(B)| = |V(B)| + 1$, respectively. As usual, let's denote the path, the cycle and the star on n vertices by P_n, C_n and S_n, respectively.

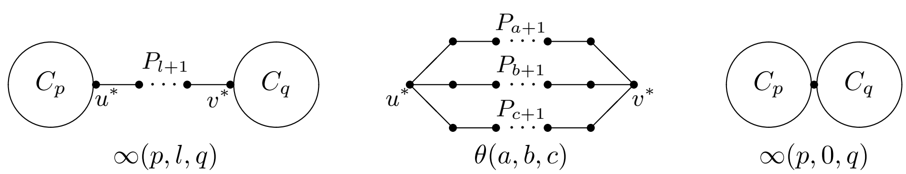

Figure 1. The graphs $\infty(p, l, q)$, $\theta(a, b, c)$ and $\infty(p, 0, q)$.

There are two categories of bases of bicyclic graphs, as described here. Denoted by $\infty(p, l, q)$ the graph obtained from two vertex-disjoint cycles C_p and C_q by connecting one vertex u^* of C_p and one vertex v^* of C_q with a path $P_{l+1} = u^* \cdots v^*$ of length l (if $l = 0$, identifying u^* with v^*), as depicted in Figure 1. Denoted by $\theta(a, b, c)$ the union of three internally disjoint paths P_{a+1}, P_{b+1}, P_{c+1} of length a, b, c ($a, b, c \geq 1$ and at most one of them is 1) respectively with common end vertices u^* and v^*, as depicted in Figure 1. Notice that any bicyclic graph is obtained from a $\theta(a, b, c)$ or an $\infty(p, l, q)$ by attaching trees to some of its vertices. The bicyclic graphs containing $\infty(p, l, q)$ and $\theta(r, s, t)$ as its base are called ∞-graph and θ-graph, respectively.

A subset $M \subseteq E(G)$ is called a matching of G if no pair of edges in M share a common vertex. The matching number of a graph G is the maximum cardinality of a matching in G. If vertex $x \in V(G)$ is incident with some edge of M, where M is a matching of G, then x is said to be M-saturated. M is called a perfect matching if each vertex of G is M-saturated. We can refer to [5] for other terminologies and notations.

At present, studying the behavior of topological indices is an essential subject. There are many papers on topological indices of bicyclic graphs. Recent results can be referred to [3], [18], [21], [28], et al. In this paper, by using the properties of Sombor index and exploring the structures of bicyclic graphs with given matching number, we present the maximum Sombor index of bicyclic graphs with given matching number, and identify the corresponding extremal graphs.

2. Some lemmas

Let $S(x,y)=\sqrt{x^2+y^2}$, where $x,y\geq 1$. One can easily get the Lemmas 2.1 and 2.2. They also can be found in [25].

Lemma 2.1. *Let $h_c(x)=S(x,c+1)-S(x,c)=\sqrt{x^2+(c+1)^2}-\sqrt{x^2+c^2}$, where $x\geq 1$ and c is a positive integer. Then $h_c(x)$ is decreasing for x.*

Lemma 2.2. *Let $\varphi_c(x)=S(x,c)-S(x-1,c)=\sqrt{x^2+c^2}-\sqrt{(x-1)^2+c^2}$, where $x\geq 2$ and c is a positive integer. Then $\varphi_c(x)$ is increasing for x.*

Lemma 2.3. *Let $\psi(m)=(m+1)\sqrt{(m+2)^2+4}+\sqrt{5}(m-3)+\sqrt{(m+2)^2+1}+4\sqrt{2}-(4\sqrt{2}m+8\sqrt{5}-6\sqrt{2})$. Then $\psi(m)>0$ for $m\geq 3$.*

Proof. Notice that for $m\geq 3$,

$$\psi'(m)>\sqrt{(m+2)^2+4}+\sqrt{5}-4\sqrt{2}\geq\sqrt{29}+\sqrt{5}-4\sqrt{2}\approx 1.964>0.$$

So $\psi(m)\geq\psi(3)=4\sqrt{29}+\sqrt{26}-2\sqrt{2}-8\sqrt{5}\approx 5.923>0$. $\square$

Lemma 2.4. *Let $l(t,r)=\sqrt{t^2+1}+(r-1)\big(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\big)+(t-r)\big(\sqrt{t^2+4}-\sqrt{(t-1)^2+4}\big)$, where $r\geq 2$, $t\geq 3$ and $r<t$. Then $l(t,r)$ is increasing for t and r, respectively.*

Proof. Note that $l(t,r)=r\big[\big(\sqrt{(t-1)^2+4}-\sqrt{(t-1)^2+1}\big)-\big(\sqrt{t^2+4}-\sqrt{t^2+1}\big)\big]+t\big(\sqrt{t^2+4}-\sqrt{(t-1)^2+4}\big)+\sqrt{(t-1)^2+1}$. By Lemma 2.1, we have $\big(\sqrt{(t-1)^2+4}-\sqrt{(t-1)^2+1}\big)-\big(\sqrt{t^2+4}-\sqrt{t^2+1}\big)=h_1(t-1)-h_1(t)>0$. So $l(t,r)$ is increasing for r. Furthermore,

$$\begin{aligned}\frac{\partial l(t,r)}{\partial t}=&r\Big[\Big(\frac{t-1}{\sqrt{(t-1)^2+4}}-\frac{t-1}{\sqrt{(t-1)^2+1}}\Big)-\Big(\frac{t}{\sqrt{t^2+4}}-\frac{t}{\sqrt{t^2+1}}\Big)\Big]\\&+\Big(\sqrt{t^2+4}-\sqrt{(t-1)^2+4}\Big)+t\Big(\frac{t}{\sqrt{t^2+4}}-\frac{t-1}{\sqrt{(t-1)^2+4}}\Big)+\frac{t-1}{\sqrt{(t-1)^2+1}}.\end{aligned}$$

Let $g_1(x)=\frac{x}{\sqrt{x^2+4}}-\frac{x}{\sqrt{x^2+1}}$. Then for $x\geq 2$, $g_1'(x)=\frac{4}{\sqrt{(x^2+4)^3}}-\frac{1}{\sqrt{(x^2+1)^3}}=\frac{\sqrt{2(2x^2+2)^3}-\sqrt{(x^2+4)^3}}{\sqrt{(x^2+4)^3(x^2+1)^3}}>0$. Then $\Big(\frac{t-1}{\sqrt{(t-1)^2+4}}-\frac{t-1}{\sqrt{(t-1)^2+1}}\Big)-\Big(\frac{t}{\sqrt{t^2+4}}-\frac{t}{\sqrt{t^2+1}}\Big)=g_1(t-1)-g_1(t)<0$. Since $r<t$, we have

$$\begin{aligned}\frac{\partial l(t,r)}{\partial t}>&t\Big[\Big(\frac{t-1}{\sqrt{(t-1)^2+4}}-\frac{t-1}{\sqrt{(t-1)^2+1}}\Big)-\Big(\frac{t}{\sqrt{t^2+4}}-\frac{t}{\sqrt{t^2+1}}\Big)\Big]\\&+\Big(\sqrt{t^2+4}-\sqrt{(t-1)^2+4}\Big)+t\Big(\frac{t}{\sqrt{t^2+4}}-\frac{t-1}{\sqrt{(t-1)^2+4}}\Big)+\frac{t-1}{\sqrt{(t-1)^2+1}}\\=&\sqrt{t^2+4}-\sqrt{(t-1)^2+4}+\frac{t^2}{\sqrt{t^2+1}}-\frac{(t-1)^2}{\sqrt{(t-1)^2+1}}.\end{aligned}$$

Let $g_2(x)=\frac{x^2}{\sqrt{x^2+1}}$. Then for $x\ge 2$, $g_2'(x)=\frac{x^3+2x}{\sqrt{(x^2+1)^3}}>0$. So $\frac{t^2}{\sqrt{t^2+1}}-\frac{(t-1)^2}{\sqrt{(t-1)^2+1}}=g_2(t)-g_2(t-1)>0$. Therefore, $\frac{\partial l(t,r)}{\partial t}>0$, and $l(t,r)$ is increasing for t. □

Lemma 2.5. ([3])*Let B be an n-vertex ($n\ge 4$) bicyclic graph. Then*

$$SO(B)\ge 2\sqrt{2}n-5\sqrt{2}+4\sqrt{13}.$$

Equality holds only if $B\in\theta(a,b,c)$ (one of a,b,c is equal to 1 and $a+b+c-1=n$) or $B\in\infty(p,1,q)$ ($p+q=n$).

Lemma 2.6. ([29]) *Let U be an $2m$-vertex ($m\ge 2$) unicyclic graph with a perfect matching. Then*

$$SO(U)\le m\sqrt{(m+1)^2+4}+\sqrt{5}(m-2)+\sqrt{(m+1)^2+1}+\sqrt{8}.$$

3. Main results

For integers $m\ge 3$, denoted by $\mathscr{B}_{n,m}$ the set of n-vertex bicyclic graphs with matching number m.

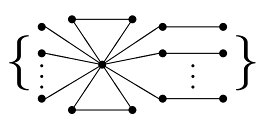

Figure 2. The graph $\boldsymbol{B}^*_{n,m}$.

Let $\boldsymbol{B}^*_{n,m}$ be the bicyclic graphs on n vertices arisen from $\infty(3,0,3)$ by attaching $n-2m+1$ pendant edges and $m-3$ paths of length 2 to the vertex of degree 4 in $\infty(3,0,3)$, as depicted in Figure 2. Let $SO(\boldsymbol{B}^*_{n,m})=f(n,m)$, where

$$\begin{aligned}f(n,m)=&(m+1)\sqrt{(n-m+2)^2+4}+\sqrt{5}(m-3)\\&+(n-2m+1)\sqrt{(n-m+2)^2+1}+4\sqrt{2}.\end{aligned}$$

Lemma 3.1. ([31]) *Let $B\in\mathscr{B}_{2m,m}$ and T be a tree in B attached to a root r, where $m\ge 3$. If $y\in V(T)$ is a vertex furthest from the root r with $d_B(y,r)\ge 2$, then y is a pendant vertex and adjacent to a vertex x of degree 2.*

Lemma 3.2. ([22]) *Let $B\in\mathscr{B}_{2m,m}$. If $PV(B)\ne\emptyset$, then for any vertex $x\in V(B)$, $\mid N_B(x)\cap PV(B)\mid\le 1$.*

Lemma 3.3. ([31]) *Let $B\in\mathscr{B}_{n,m}$ ($n>2m$) and B has at least one pendant vertex. Then there is an m-matching M and a pendant vertex y such that M does not saturate y.*

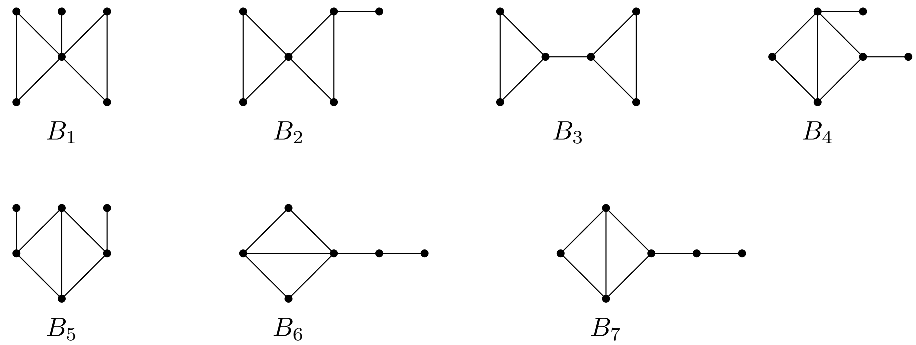

Figure 3. The graphs $B_1, B_2, \cdots, B_6$ and B_7.

By Lemma 2.5, Theorem 3.4 is immediate.

Theorem 3.4. *Let $B \in \mathscr{B}_{2m,m}$, where $m \geq 3$. Then*

$$SO(B) \geq 4\sqrt{2}m - 5\sqrt{2} + 4\sqrt{13}.$$

Equality holds only if $B \in \theta(a,b,c)$ (one of a,b,c is equal to 1 and $a+b+c-1 = 2m$) or $B \in \infty(p,1,q)$ ($p+q = 2m$).

Theorem 3.5. *Let $B \in \mathscr{B}_{2m,m}$, where $m \geq 3$. Then*

$$SO(B) \leq f(2m,m),$$

where $f(2m,m) = (m+1)\sqrt{(m+2)^2+4} + \sqrt{5}(m-3) + \sqrt{(m+2)^2+1} + 4\sqrt{2}$, with equality if and only if $B \cong \boldsymbol{B}^*_{2m,m}$.

Proof. If $PV(B) = \emptyset$, B belongs to the type of $\infty(p,l,q)$ or $\theta(a,b,c)$ (see Figure 1), where $p+l+q = 2m+1$ or $a+b+c = 2m+1$. By Lemma 2.3, for $m \geq 3$, we have $SO(\infty(p,0,q)) = 4\sqrt{2}m + 8\sqrt{5} - 6\sqrt{2} < f(2m,m)$. And for $m \geq 3$, $SO(\infty(p,l,q)) = SO(\theta(a,b,c)) = 4\sqrt{2}m + 6\sqrt{13} - 10\sqrt{2} < 4\sqrt{2}m + 8\sqrt{5} - 6\sqrt{2} = SO(\infty(p,0,q)) < f(2m,m)$ $(l > 1)$ when $u^*v^* \notin B$, $SO(\infty(p,l,q)) = SO(\theta(a,b,c)) = 4\sqrt{2}m + 4\sqrt{13} - 5\sqrt{2} < 4\sqrt{2}m + 8\sqrt{5} - 6\sqrt{2} < f(2m,m)$ $(l = 1)$ when $u^*v^* \in B$. So we suppose that $PV(B) \neq \emptyset$ in the following proof.

By induction on m. If $m = 3$, then $B \in \{B_1, B_2, \cdots, B_7\}$, where $B_1, B_2, \cdots, B_7$ are depicted in Figure 3. By direct calculation, $SO(B_i) < SO(B_1) = SO(\boldsymbol{B}^*_{6,3}) = f(6,3)$, where $i = 2, \cdots, 7$. Thus for $m = 3$, the theorem is true.

We assume that $m \geq 4$ and the result holds for all bicyclic graphs on fewer than $2m$ vertices with a perfect matching. Suppose M is a perfect matching of B. For $y \in PV(B)$, there exists a tree T_r attached on a root $r \in V(\theta(a,b,c))$ or $r \in V(\infty(p,l,q)$ in B such that $y \in V(T_r)$, where T_r is a pendant tree in B. Let $d_{T_r}(r,z) = \max\{d_{T_r}(r,y) | y \in V(T_r)\}$ and $\mathscr{T}_B$ be the set of all pendant trees in B. We discuss in three cases.

Case 1. $\max\{d_{T_r}(r,z) | T_r \in \mathscr{T}_B\} = 1$.

Now, B is a graph arisen from $\infty(p,l,q)$ or $\theta(a,b,c)$ by attaching some pendant edges to its some vertices. In view of Lemma 3.2, it follows that every vertex of $\infty(p,l,q)$ or $\theta(a,b,c)$ is attached by at most one pendant edge.

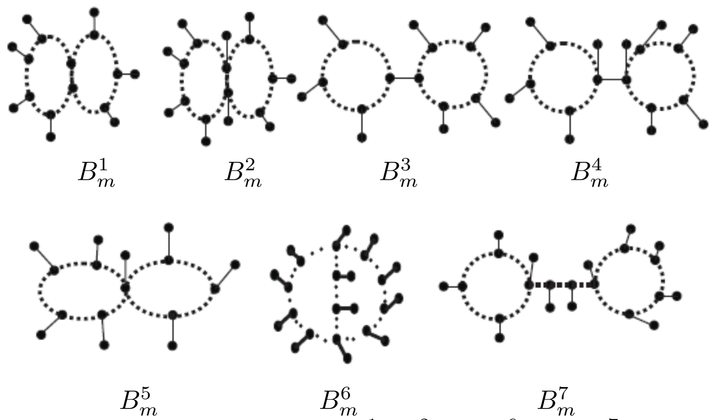

Figure 4. The graphs $B_m^1, B_m^2, \cdots B_m^6$ and B_m^7.

Subcase 1.1. For any $w \in V(B)$, $d_B(w) \neq 2$.

Since B has a perfect matching, then $B \in \{B_m^i | i = 1, 2, \cdots, 7\}$, where B_m^i $(i = 1, 2, \cdots, 7)$ are depicted in Figure 4. It is not difficult to get that $SO(B_m^1) = (3\sqrt{2}+\sqrt{10})m + 6\sqrt{2} - \sqrt{10}$ $(m \geq 3)$, $SO(B_m^2) = (3\sqrt{2}+\sqrt{10})m + 20 + 2\sqrt{17} - 2\sqrt{10} - 8\sqrt{2}$ $(m \geq 4)$, $SO(B_m^3) = (3\sqrt{2}+\sqrt{10})m + 6\sqrt{2} - \sqrt{10}$ $(m \geq 5)$, $SO(B_m^4) = (3\sqrt{2}+\sqrt{10})m + 20 + 2\sqrt{17} - 2\sqrt{10} - 8\sqrt{2}$ $(m \geq 6)$, $SO(B_m^5) = (3\sqrt{2}+\sqrt{10})m + 4\sqrt{34} + \sqrt{26} - \sqrt{10} - 9\sqrt{2}$ $(m \geq 5)$, $SO(B_m^6) = (3\sqrt{2}+\sqrt{10})m + 30 + 2\sqrt{17} - 2\sqrt{10} - 15\sqrt{2}$ $(m \geq 5)$ and $SO(B_m^7) = (3\sqrt{2}+\sqrt{10})m + 30 + 2\sqrt{17} - 2\sqrt{10} - 15\sqrt{2}$ $(m \geq 7)$. By a similar way as the case of $PV(B) = \emptyset$, one can easily check that $SO(\boldsymbol{B}^*_{2m,m}) = f(2m, m) > SO(B_m^5) > SO(B_m^i)$, where $i = 1, 2, 3, 4, 6, 7$.

Subcase 1.2. B contains one vertex w with $d_B(w) = 2$.

Subsubcase 1.2.1. w belongs to the vertices in one of the cycles of B.

Denote $N_B(w) = \{w_1, w_2\}$. Since $B \in \mathscr{B}_{2m,m}$, then $ww_1 \notin M$ or $ww_2 \notin M$. Suppose without loss of generality that $ww_1 \notin M$. Let $d_B(w_1) = t$, $N_B(w_1) \setminus \{w\} = \{u_1, u_2, \cdots, u_{t-1}\}$. Since $B \in \mathscr{B}_{2m,m}$, then $2 \leq t \leq 5$, $2 \leq d_B(w_2) \leq 5$ and $d_B(u_i) \geq 1$, where $i = 1, 2, \cdots, t-1$. In view of Lemma 3.2, there exists at most one vertex of $\{u_1, u_2, \cdots, u_{t-1}\}$ with degree 1. Let $U' = B - ww_1$. Obviously, U' is an $2m$-vertex $(m \geq 4)$ unicyclic graph with a perfect matching. By Lemmas 2.1, 2.2 and 2.6, for $2 \leq t \leq 5$ and $m \geq 4$, it follows that

$$\begin{aligned}SO(B) =& SO(U') + S(2, d_B(w_2)) - S(1, d_B(w_2)) + S(2, t) \\ &+ \sum_{i=1}^{t-1} \Big[S(t, d_B(u_i)) - S(t-1, d_B(u_i)) \Big] \\ \leq& SO(U') + S(2,2) - S(1,2) + S(2,t) + S(t,1) - S(t-1,1)\end{aligned}$$

$$\begin{aligned}
&+(t-2)[S(2,t)-S(2,t-1)]\\
\leq&SO(U')+\sqrt{8}-\sqrt{5}+\sqrt{t^2+1}-\sqrt{(t-1)^2+1}+\sqrt{t^2+4}\\
&+(t-2)\big(\sqrt{t^2+4}-\sqrt{(t-1)^2+4}\big)\\
\leq&m\sqrt{(m+1)^2+4}+\sqrt{5}(m-2)+\sqrt{(m+1)^2+1}\\
&+\sqrt{8}+\sqrt{8}-\sqrt{5}+\sqrt{26}-\sqrt{17}+4\sqrt{29}-3\sqrt{20}\\
<&f(2m,m)
\end{aligned}$$

since

$$\begin{aligned}
&f(2m,m)-m\sqrt{(m+1)^2+4}-\sqrt{5}(m-2)-\sqrt{(m+1)^2+1}-2\sqrt{8}+\sqrt{5}\\
&-\sqrt{26}+\sqrt{17}-4\sqrt{29}+3\sqrt{20}\\
=&m\big(\sqrt{(m+2)^2+4}-\sqrt{(m+1)^2+4}\big)+\sqrt{(m+2)^2+1}-\sqrt{(m+1)^2+1}\\
&+\sqrt{(m+2)^2+4}-\sqrt{26}+\sqrt{17}-4\sqrt{29}+3\sqrt{20}\\
\geq&4(\sqrt{40}-\sqrt{29})+\sqrt{37}-\sqrt{26}+\sqrt{40}-\sqrt{26}+\sqrt{17}-4\sqrt{29}+3\sqrt{20}\\
\approx&1.9657>0.
\end{aligned}$$

Subsubcase 1.2.2. w lie in the path of a ∞-graph.

Now B contains an edge uv which belongs to a cycle such that $d_B(u)=d_B(v)=3$. Denote $N_B(u)=\{v,u_1,u_2\}$ and $N_B(v)=\{u,v_1,v_2\}$. Assume without loss of generality that $d_B(u_1)=d_B(v_1)=1$ and $3\leq d_B(u_2),d_B(v_2)\leq 4$. Let $U''=B-uv$. Then U'' is an $2m$-vertex ($m\geq 4$) unicyclic graph with a perfect matching. By Lemmas 2.1 and 2.6, it follows that

$$\begin{aligned}
SO(B)=&SO(U'')+S(3,3)+2\big(S(3,1)-S(2,1)\big)+S(3,d_B(u_2))-S(2,d_B(u_2))\\
&+S(3,d_B(v_2))-S(2,d_B(v_2))\\
\leq&SO(U'')+S(3,3)+2\big(S(3,1)-S(2,1)\big)+2\big(S(3,3)-S(2,3)\big)\\
\leq&m\sqrt{(m+1)^2+4}+\sqrt{5}(m-2)+\sqrt{(m+1)^2+1}+\sqrt{8}+\sqrt{18}\\
&+2(\sqrt{10}-\sqrt{5})+2(\sqrt{18}-\sqrt{13})\\
<&f(2m,m).
\end{aligned}$$

since

$$\begin{aligned}
&f(2m,m)-m\sqrt{(m+1)^2+4}-\sqrt{5}(m-2)-\sqrt{(m+1)^2+1}-\sqrt{8}-\sqrt{18}\\
&-2(\sqrt{10}-\sqrt{5})-2(\sqrt{18}-\sqrt{13})\\
=&m\big(\sqrt{(m+2)^2+4}-\sqrt{(m+1)^2+4}\big)+\sqrt{(m+2)^2+1}-\sqrt{(m+1)^2+1}\\
&+\sqrt{(m+2)^2+4}+2\sqrt{2}-\sqrt{5}-\sqrt{18}-2(\sqrt{10}-\sqrt{5})-2(\sqrt{18}-\sqrt{13})\\
\geq&4(\sqrt{40}-\sqrt{29})+\sqrt{37}-\sqrt{26}+\sqrt{40}+2\sqrt{2}-\sqrt{5}-\sqrt{18}\\
&-2(\sqrt{10}-\sqrt{5})-2(\sqrt{18}-\sqrt{13})
\end{aligned}$$

$\approx 4.289 > 0.$

Case 2. There is a pendant tree $T_r \in \mathscr{T}_B$ such that $d_{T_r}(r,z) = 2$.

Since $z \in PV(B)$, let $N_B(z) = \{u\}$, by Lemma 3.1, we have $d_B(u) = 2$. Let $N_B(u) = \{r, z\}$, $N_B(r) = \{u, x_1, x_2, \cdots, x_s, v_1, v_2, \cdots, v_t\}$, where x_i belongs to the vertices of the cycles in B and $d_B(x_i) \geq 2$ ($i = 1, 2, \cdots, s$ and $s = 2, 3$ or 4).

Subcase 2.1. $PV(B) \cap N_B(r) \neq \emptyset$.

Suppose without loss of generality that $v_1 \in PV(B)$, then $v_1 r \in M$. By Lemma 3.2, $(N_B(r) \setminus \{v_1\}) \cap PV(B) = \emptyset$. Then $d_B(v_j) \geq 2$ for $2 \leq j \leq t$. Since $d_{T_r}(r,z) = \max\{d_{T_r}(r,y) | y \in V(T_r)\} = 2$, combining with Lemma 3.1, we have $d_B(v_j) = 2$ and $(N_B(v_j) \setminus \{r\}) = \{z_j\} \in PV(B)$, where $2 \leq j \leq t$. Let $B' = B - z - u$, then $B' \in \mathscr{B}_{2m-2,m-1}$. By Lemmas 2.1, 2.2 and induction hypothesis, it follows that

$$\begin{aligned}
SO(B) =& SO(B') + S(t+s+1,1) - S(t+s,1) + S(t+s+1,2) + S(1,2) \\
&+ \sum_{i=1}^{s} \Big[S(t+s+1, d_B(x_i)) - S(t+s, d_B(x_i)) \Big] \\
&+ \sum_{j=2}^{t} \Big[S(t+s+1,2) - S(t+s,2) \Big] \\
\leq& SO(B') + S(t+s+1,1) - S(t+s,1) + S(t+s+1,2) + S(1,2) \\
&+ (t+s-1)[S(t+s+1,2) - S(t+s,2)] \\
\leq& f(2m-2, m-1) + (t+3)[S(t+5,2) - S(t+4,2)] \\
&+ S(t+5,1) - S(t+4,1) + S(t+5,2) + S(1,2) \\
=& f(2m-2, m-1) + m\big(\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\big) \\
&+ \sqrt{(m+2)^2+1} - \sqrt{(m+1)^2+1} + \sqrt{(m+2)^2+4} + \sqrt{5} \\
=& f(2m, m)
\end{aligned}$$

since $t \leq m-3$ and $S(t+s+1,k) - S(t+s,k)$ $(k = 1,2)$, $S(t+s+1,2)$ is increasing for s. With the equalities only if $V(B) = \{x_1, \cdots, x_4, r, v_1, u, z\} \cup \{v_2, \cdots, v_t, z_2, \cdots, z_t\}$, $s = 4$, $d_B(x_1) = \cdots = d_B(x_4) = 2$ and $SO(B') = f(2m-2, m-1)$, which implies that $B' \cong \boldsymbol{B}^*_{2m-2,m-1}$ and $B \cong \boldsymbol{B}^*_{2m,m}$.

Subcase 2.2. $PV(B) \cap N_B(r) = \emptyset$.

Now we can see that $d_B(v_j) \geq 2$, $(N_B(v_j) \setminus \{r\}) = \{z_j\} \in PV(B)$, where $1 \leq j \leq t$ and $v_j z_j \in M$. Since $B \in \mathscr{B}_{2m,m}$, then B contains one vertex $x_j \in N_B(r)$ and x_j also belongs to the vertices of the cycles in B such that $r x_j \in M$. Let $B' = B - z - u$, then $B' \in \mathscr{B}_{2m-2,m-1}$. By Lemmas 2.1, 2.2 and induction hypothesis, it follows that

$$\begin{aligned}
SO(B) =& SO(B') + S(t+s+1,2) + S(1,2) \\
&+ \sum_{i=1}^{s} \Big[S(t+s+1, d_B(x_i)) - S(t+s, d_B(x_i)) \Big]
\end{aligned}$$

$$\begin{aligned}
&+\sum_{j=1}^{t}\Big[S(t+s+1,2)-S(t+s,2)\Big]\\
\le&SO(B')+S(t+s+1,2)+S(1,2)\\
&+(t+s)[S(t+s+1,2)-S(t+s,2)]\\
\le&f(2m-2,m-1)+S(t+5,2)+S(1,2)\\
&+(t+4)[S(t+5,2)-S(t+4,2)]\\
=&f(2m-2,m-1)+\sqrt{(t+5)^2+4}+\sqrt{5}\\
&+(t+4)\big(\sqrt{(t+5)^2+4}-\sqrt{(t+4)^2+4}\big)\\
<&f(2m-2,m-1)+\sqrt{(m+2)^2+4}+\sqrt{5}\\
&+(m+1)\big(\sqrt{(m+2)^2+4}-\sqrt{(m+1)^2+4}\big)\\
=&f(2m,m)+\big(\sqrt{(m+2)^2+4}-\sqrt{(m+2)^2+1}\big)\\
&-\big(\sqrt{(m+1)^2+4}-\sqrt{(m+1)^2+1}\big)\\
=&f(2m,m)+\big(h_1(m+2)-h_1(m+1)\big)\\
<&f(2m,m)
\end{aligned}$$

since $t<m-3$.

Case 3. For all $T_r\in\mathscr{T}_B$, $d_{T_r}(r,z)\neq 2$ and $\max\{d_{T_r}(r,z)|T_r\in\mathscr{T}_B\}\ge 3$.

Similar to Case 2, as $z\in PV(B)$, denote $N_B(z)=\{u\}$, by Lemma 3.1, $d_B(u)=2$. Denote $N_B(u)=\{v,z\}$ and $N_B(v)=\{u,w,v_1,v_2,\cdots,v_t\}$ (maybe $w=r$), then $d_B(w)\ge 2$.

Subcase 3.1. $N_B(v)\cap PV(B)\neq\emptyset$.

Assume without loss of generality that $v_1\in PV(U)$, then $v_1v\in M$. Similar to Subcase 2.1, we have $d_B(v_i)=2$ and $N_B(v_i)\setminus\{v\}=\{z_i\}\in PV(B)$, where $i=2,3,\cdots,t$. Let $B'=B-z-u$. Then $B'\in\mathscr{B}_{2m-2,m-1}$. By Lemmas 2.1, 2.2 and induction hypothesis, it follows that

$$\begin{aligned}
SO(B)=&SO(B')+S(t+2,d_B(w))-S(t+1,d_B(w))+[S(t+2,1)-S(t+1,1)]\\
&+S(t+2,2)+S(2,1)+\sum_{i=2}^{t}\Big[S(t+2,d_B(v_i))-S(t+1,d_B(v_i))\Big]\\
\le&SO(B')+t[S(t+2,2)-S(t+1,2)]+[S(t+2,1)-S(t+1,1)]\\
&+S(t+2,2)+S(2,1)\\
\le&f(2m-2,m-1)+\sqrt{(t+2)^2+4}+\sqrt{5}\\
&+t\big(\sqrt{(t+2)^2+4}-\sqrt{(t+1)^2+4}\big)\\
&+\sqrt{(t+2)^2+1}-\sqrt{(t+1)^2+1}\\
<&f(2m-2,m-1)+\sqrt{(m-1)^2+4}+\sqrt{5}\\
&+\sqrt{(m-1)^2+1}-\sqrt{(m-2)^2+1}
\end{aligned}$$

$$
\begin{aligned}
&+ (m-3)\big(\sqrt{(m-1)^2+4} - \sqrt{(m-2)^2+4}\big)\\
<&f(2m,m)
\end{aligned}
$$

since $t < m-3$ and

$$
\begin{aligned}
&f(2m,m) - f(2m-2,m-1) - \sqrt{(m-1)^2+4} - \sqrt{5} - \sqrt{(m-1)^2+1}\\
&+ \sqrt{(m-2)^2+1} - (m-3)\big(\sqrt{(m-1)^2+4} - \sqrt{(m-2)^2+4}\big)\\
=&(m-3)\Big[\big(\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\big) - \big(\sqrt{(m-1)^2+4} - \sqrt{(m-2)^2+4}\big)\Big]\\
&+ \Big[\big(\sqrt{(m+2)^2+1} - \sqrt{(m+1)^2+1}\big) - \big(\sqrt{(m-1)^2+1} - \sqrt{(m-2)^2+1}\big)\Big]\\
&+ 3\big(\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\big) + \sqrt{(m+2)^2+4} - \sqrt{(m-1)^2+4}\\
=&(m-3)\big(\varphi_2(m+2) - \varphi_2(m-1)\big) + \big(\varphi_1(m+2) - \varphi_1(m-1)\big)\\
&+ 3\big(\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\big) + \sqrt{(m+2)^2+4} - \sqrt{(m-1)^2+4}\\
>&0.
\end{aligned}
$$

Subcase 3.2. $N_B(v) \cap PV(B) = \emptyset$.

Similar to Subcase 2.2, we have $d_B(v_i) = 2$, $N_B(v_i) \setminus \{v\} = \{z_i\} \in PV(B)$, where $v_i z_i \in M$, $i = 1, 2, \cdots, t$. Since $B \in \mathscr{B}_{2m,m}$, then $vw \in M$. Let $B' = B - z - u$. Then $B' \in \mathscr{B}_{2(m-1),m-1}$. By induction hypothesis and Lemmas 2.1, 2.2, we have

$$
\begin{aligned}
SO(B) =&SO(B') + S(t+2,2) + S(2,1) + S(t+2,d_B(w)) + S(t+1,d_B(w))\\
&+ \sum_{i=1}^{t}\Big[S(t+2,d_B(v_i)) - S(t+1,d_B(v_i))\Big]\\
\leq&SO(B') + S(t+2,2) + S(2,1) + (t+1)[S(t+2,2) - S(t+1,2)]\\
\leq&f(2m-2,m-1) + \sqrt{(t+2)^2+4} + \sqrt{5}\\
&+ (t+1)\big(\sqrt{(t+2)^2+4} - \sqrt{(t+1)^2+4}\big)\\
<&f(2m-2,m-1) + \sqrt{(m-1)^2+4} + \sqrt{5}\\
&+ (m-2)\big(\sqrt{(m-1)^2+4} - \sqrt{(m-2)^2+4}\big)\\
<&f(2m,m)
\end{aligned}
$$

since $t < m-3$ and

$$
\begin{aligned}
&f(2m,m) - f(2m-2,m-1) - \sqrt{(m-1)^2+4} - \sqrt{5}\\
&- (m-2)\big(\sqrt{(m-1)^2+4} - \sqrt{(m-2)^2+4}\big)\\
=&(m-2)\Big[\big(\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\big) - \big(\sqrt{(m-1)^2+4} - \sqrt{(m-2)^2+4}\big)\Big]\\
&+ 2\big(\sqrt{(m+2)^2+4} - \sqrt{(m+1)^2+4}\big) + \sqrt{(m+2)^2+1} - \sqrt{(m+1)^2+1}\\
&+ \sqrt{(m+2)^2+4} - \sqrt{(m-1)^2+4}
\end{aligned}
$$

$$
\begin{aligned}
=&(m-2)\big(\varphi_2(m+2)-\varphi_2(m-1)\big)+2\big(\sqrt{(m+2)^2+4}-\sqrt{(m+1)^2+4}\big)\\
&+\sqrt{(m+2)^2+1}-\sqrt{(m+1)^2+1}+\sqrt{(m+2)^2+4}-\sqrt{(m-1)^2+4}\\
>&0.
\end{aligned}
$$

The proof is completed. □

Theorem 3.6. *Let $B \in \mathscr{B}_{n,m}$, where $m \geq 3$. Then*

$$SO(B) \leq f(n,m)$$

with equality if and only if $B \cong \boldsymbol{B}^*_{n,m}$.

Proof. By induction on n. If $n = 2m$, by Theorem 3.5, the result holds. Now suppose that $n > 2m$. If $PV(B) = \emptyset$, B belongs to the type of $\infty(p,l,q)$ or $\theta(a,b,c)$ and $n = 2m+1$, then $p+l+q-1 = n = 2m+1$ and $a+b+c-1 = n = 2m+1$. For $p+l+q-1, a+b+c-1 = 2m+1$, one can easily check that $\max\{SO(\infty(p,l,q))(l \neq 0), SO(\theta(a,b,c)), SO(\infty(p,0,q))\} = SO(\infty(p,0,q))$ and $SO(\infty(p,0,q)) = 4\sqrt{2}m + 8\sqrt{5} - 4\sqrt{2} < SO(\boldsymbol{B}^*_{2m+1,m}) = f(2m+1,m) = (m+1)\sqrt{(m+3)^2+4} + \sqrt{5}(m-3) + 2\sqrt{(m+3)^2+1} + 4\sqrt{2}$ for $m \geq 3$. The theorem holds. Thus we suppose that $PV(B) \neq \emptyset$ in the following proof. In view of Lemma 3.3, it follows that there is a pendant vertex y and an m-matching M such that y is not M-saturated. Let $xy \in E(B)$ and $d_B(x) = t$. Let $N_B(x) \cap PV(B) = \{y_1, y_2, \cdots, y_{r-1}, y_r = y\}$ and $N_B(x) \setminus PV(B) = \{u_1, u_2, \cdots, u_{t-r}\}$. Then $d_B(u_i) \geq 2$ for each $i \in \{1, 2, \cdots, t-r\}$. Furthermore, since B is a bicyclic graph and there exist at least $m-3$ M-saturated vertices in $V(B) \setminus \{x, y_1, y_2, \cdots, y_{r-1}, y_r, u_1, u_2, \cdots, u_{t-r}\}$, then $n = |V(B)| \geq t+1+m-3$, that is $t \leq n-m+2$. Let $B' = B - y$. Then $B' \in \mathscr{B}_{n-1,m}$. We discuss in two cases.

Case 1. $r = 1$.

Now, $y = y_1$. By the induction hypothesis and Lemmas 2.1, 2.2, for $n > 2m$, it follows that

$$
\begin{aligned}
SO(B) =&SO(B') + S(1,t) + \sum_{i=1}^{t-1}\Big[S(d_U(x), d_U(u_i)) - S(d_U(x)-1, d_U(u_i))\Big]\\
\leq&SO(B') + S(1,t) + \sum_{i=1}^{t-1}\Big[S(t,2) - S(t-1,2)\Big]\\
\leq&f(n-1,m) + \sqrt{t^2+1} + (t-1)\big(\sqrt{t^2+4} - \sqrt{(t-1)^2+4}\big)\\
\leq&f(n-1,m) + \sqrt{(n-m+2)^2+1}\\
&+(n-m+1)\big(\sqrt{(n-m+2)^2+4} - \sqrt{(n-m+1)^2+4}\big)\\
<&f(n,m)
\end{aligned}
$$

since

$$
\begin{aligned}
&f(n,m) - f(n-1,m) - \sqrt{(n-m+2)^2+1}\\
&-(n-m+1)\big(\sqrt{(n-m+2)^2+4} - \sqrt{(n-m+1)^2+4}\big)
\end{aligned}
$$

$$
\begin{aligned}
&=(n-2m)\Big[\big(\sqrt{(n-m+1)^2+4}-\sqrt{(n-m+1)^2+1}\big)\\
&\quad-\big(\sqrt{(n-m+2)^2+4}-\sqrt{(n-m+2)^2+1}\big)\Big]\\
&=(n-2m)(h_1(n-m+1)-h_1(n-m+2))\\
&>0.
\end{aligned}
$$

Case 2. $r \geq 2$.

Notice that there exist at least $r-1$ vertices which are not M-saturated, then $n-(r-1) \geq 2m$, that is $r \leq n-2m+1$. By the induction hypothesis and Lemmas 2.1, 2.2, 2.4, it follows that

$$
\begin{aligned}
SO(B) =&SO(B') + S(1,t) + \sum_{i=1}^{r-1}\Big[S(d_U(x), d_U(y_i)) - S(d_U(x)-1, d_U(y_i))\Big]\\
&+\sum_{j=1}^{t-r}\Big[S(d_U(x), d_U(u_j)) - S(d_U(x)-1, d_U(u_j))\Big]\\
\leq& SO(B') + S(1,t) + (r-1)[S(t,1) - S(t-1,1)]\\
&+(t-r)[S(t,2)-S(t-1,2)]\\
\leq& f(n-1,m) + \sqrt{t^2+1} + (r-1)\big(\sqrt{t^2+1}-\sqrt{(t-1)^2+1}\big)\\
&+(t-r)\big(\sqrt{t^2+4}-\sqrt{(t-1)^2+4}\big)\\
\leq&(m+1)\sqrt{(n-m+1)^2+4}+(n-2m)\sqrt{(n-m+1)^2+1}+\sqrt{5}(m-3)+4\sqrt{2}\\
&+\sqrt{(n-m+2)^2+1}+(n-2m)\big(\sqrt{(n-m+2)^2+1}-\sqrt{(n-m+1)^2+1}\big)\\
&+(m+1)\big(\sqrt{(n-m+2)^2+4}-\sqrt{(n-m+1)^2+4}\big)\\
=&(m+1)\sqrt{(n-m+2)^2+4}+\sqrt{5}(m-3)+4\sqrt{2}\\
&+(n-2m+1)\sqrt{(n-m+2)^2+1}\\
=&f(n,m).
\end{aligned}
$$

With the equalities hold only if $SO(B') = f(n-1,m)$, $r = n-2m+1$, $t = n-m+2$ and $d_U(u_j) = 2$ for $j = 1, 2, \cdots, t-r$, which implies that $B' \cong \boldsymbol{B}^*_{n-1,m}$, and $B \cong \boldsymbol{B}^*_{n,m}$. □

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