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Extremal Graphs for Sombor Index with Given Parameters

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Abstract: In this paper, we present the upper and lower bounds on Sombor index $SO(G)$ among all connected graphs (respectively, connected bipartite graphs). We give some sharp lower and upper bounds on $SO(G)$ among connected graphs in terms of some parameters, including chromatic, girth and matching number. Meanwhile, we characterize the extremal graphs attaining those bounds. In addition, we give upper bounds on $SO(G)$ among connected bipartite graphs with given matching number and/or connectivity and determine the corresponding extremal connected bipartite graphs.

Keywords: chromatic number; girth; connectivity; matching number; Sombor index

MSC: 05C50; 05C12; 15A18

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1. Introduction

In this paper, we only consider finite, undirected and simple connected (respectively, connected bipartite) graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Let S (respectively, F) be a vertex (respectively, an edge) subset of G. Then $G-S$ denotes the graph obtained from G by deleting S and the edges incident with them, and $G-F$ denotes the graph obtained from G by deleting F. If $S=\{v\}$ and $F=\{uv\}$, the subgraphs $G-S$ and $G-F$ will be written as $G-v$ and $G-uv$ for short, respectively. For any two nonadjacent vertices x and y of a graph G, we let $G+xy$ be the graph obtained from G by adding an edge xy. For a positive integer n, we will use the notation $[n]=\{1,2,\ldots,n\}$.

Recently, Gutman [1] devised two new topological indices. For a graph G, its Sombor index $SO(G)$ and reduced Sombor index $SO_{red}(G)$ are defined, respectively, as follows:

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

$$SO_{red}(G)=\sum_{uv\in E(G)}\sqrt{(d_G(u)-1)^2+(d_G(v)-1)^2}.$$

Gutman et al. [1] studied the problem of finding graphs attaining the maximum (respectively, minimum) Sombor index from the class of all trees (respectively, graphs and connected graphs) with given order n. Réti et al. [2] characterized the extremal graphs having the maximum Sombor index in the classes of all connected unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs with order n.

Liu et al. [3] obtained some bounds for the reduced Sombor index of graphs with given several parameters and some special graphs. F. Wang and B. Wu [4] proved a conjecture on the reduced Sombor index proposed by Liu et al. in [3]. They gave an upper bound for the reduced Sombor index of a bipartite graph and determined the extremal graph among all k-chromatic graphs with maximum reduced Sombor index. F. Wang and B. Wu [5] characterized the extremal molecular tree on the reduced Sombor index and exponential reduced Sombor index.

Some authors made a more extensive study to determine the extremal values of the Sombor index of graphs with given some parameters. Sun et al. [6] characterized extremal graphs having extremal values of the Sombor index in terms of the domination number. In [7], Zhou et al. characterized the extremal trees and unicyclic graphs with the extremal Sombor index in terms of the matching number. They also considered the extremal Sombor index in the same graph family with given maximum degree in [8]. Das et al. [9] gave some bounds on the Sombor index of trees in terms of order, independence number, and number of pendent vertices, and characterized the extremal cases. Liu et al. [10] collected the existing bounds and extremal results related to the Sombor index and its variants. Aashtab et al. [11] found an interesting property of the Sombor index. Let G be a connected graph of order n and size m, if for each G' with order n and size m, $SO(G) \leq SO(G')$, then G is an almost regular graph. Using this property, Liu et al. [12] determined the minimum Sombor index of tricyclic and tetracyclic graphs.

If there exists a vertex $v \in V(G)$ such that $G - v$ is a tree (respectively, unicycle), then the graph G is said to be a quasi-tree (respectively, quasi-unicyclic). Das et al. [9] determined the extremal graphs in the set of quasi-trees. Ning et al. [13] gave an upper bound of the Sombor index of the set of quasi-unicyclic graphs with order n, and characterized the corresponding extremal graph. Horoldagva et al. [14] gave some lower or upper bounds on the Sombor index of connected graphs in terms of some parameters, such as the maximum degree. Das et al. [15] gave an upper bound of the Sombor index of connected graphs with a given independence number. Some authors obtained a series of results related to Nordhaus–Gaddum relations for the Sombor index in [14–16].

The extremal values of the Sombor index of chemical graphs are also studied by several authors. A chemical graph is a graph with the degree of each vertex of this graph at most 4. Deng et al. [17] gave an upper bound of the Sombor index in chemical trees with n vertices. Cruz et al. [18] characterized the extremal connected chemical graphs of order n, and determined the extremal graphs in catacondensed hexagonal systems. Liu et al. [19] gave lower and upper bounds of the Sombor index in chemical trees with n vertices and k pendent vertices, and characterized the corresponding extremal chemical trees. Liu et al. [20] determined the first fourteen minimum chemical trees, the first four minimum chemical unicyclic graphs, the first three minimum chemical bicyclic graphs, and the first seven minimum chemical tricyclic graphs.

Some authors considered the relationships between the Sombor index and other indices. Filipovski et al. [21] considered the relations between the Sombor index and some degree-based topological indices. Rata et al. [22] considered the relationship between the Sombor index and the Second Zagreb index.

Recently, Réti et al. [2] introduced a new notion, called k-Sombor index of a graph as follows. For a positive real number k, the k-Sombor index of graph G, denoted by $SO_k(G)$, is defined as

$$SO_k(G) = \sum_{uv \in E(G)} \sqrt[k]{d_G(u)^k + d_G(v)^k}.$$

F. Wang, B. Wu [23] presented the extremal values of the k-Sombor index of trees with some given parameters, such as matching number, the number of pendent vertices, and diameter. Some related results about the Sombor index can be found in [24–26].

In this paper, we present the upper and lower bounds on $SO(G)$ among all connected graphs (respectively, bipartite graphs). In Section 3, we consider some extremal problems on $SO(G)$ with given parameters, such as chromatic number, girth and matching number among connected graphs. In Section 4, we give some sharp upper bounds on the $SO(G)$ in bipartite graphs with given matching number and connectivity. In addition, we characterize the extremal graphs attaining these bounds. In Section 5, we conclude our paper.

2. Preliminaries

For two sets A and B of vertices of G, we write $[A, B]$ for the set of edges $uv \in E(G)$ with $u \in A$ and $v \in B$. An induced subgraph $G[A]$ is the subgraph of G whose vertex set is A and whose edge set consists of all edges of G which have both ends in A. If F is a set of edges, the edge-induced subgraph $G[F]$ is the subgraph of G whose edge set is F and whose vertex set consists of all ends of edges of F. If $V(G_1) \cap V(G_2) = \emptyset$, we denote by $G_1 \cup G_2$ the graph, which consists of two components G_1 and G_2. The join of G_1 and G_2, denoted by $G_1 \vee G_2$, is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{uv|u \in V(G_1), v \in V(G_2)\}$. A matching of G is a subset of mutually independent edges of G. For a graph G, the matching number $\beta(G)$ is the maximum cardinality among the independent sets of edges in G.

A graph G is called k-connected if $G - X$ is connected for every subset $X \subseteq V(G)$ with $|X| < k$. The greatest integer k such that G is k-connected is the connectivity $\kappa(G)$ of G.

Throughout this paper, we use P_n, S_n, C_n, K_n and $\overline{K}_n$ to denote the path graph, star graph, cycle graph, complete graph, and independence set on n vertices, respectively.

In what follows, we give some lemmas which will be used frequently in the proofs of the main results.

Proposition 1. *Let G be a connected graph with at least three vertices.*
(a) If $G \ncong K_n$, then $SO(G+e) > SO(G)$, where $e \in E(\overline{G})$;
(b) If G has an edge e not being a cut edge, then $SO(G-e) < SO(G)$.

Lemma 1 ([1]). *Let P_n be the path of order n. Then for any connected graph G of order n,*

$$SO(P_n) \leq SO(G) \leq SO(K_n).$$

Equality holds if and only if $G \cong P_n$ or $G \cong K_n$. Moreover, $SO(P_2) = \sqrt{2}$, whereas $SO(P_n) = 2\sqrt{5} + 2(n-3)\sqrt{2}$ for $n \geq 3$.

Lemma 2 ([1]). *Let S_n be the star of order n. Then for any tree T of order n.*

$$SO(P_n) \leq SO(T) \leq SO(S_n).$$

Equality holds if and only if $T \cong P_n$ or $T \cong S_n$. Moreover, $SO(S_n) = (n-1)\sqrt{n^2 - 2n + 2}$.

Lemma 3 ([27]). *Every k-chromatic graph has at least k vertices of degree at least $k-1$.*

Lemma 4. *(The Tutte-Berge Formula) For any graph G:*

$$\beta(G) = \frac{1}{2} min\{n - (o(G-S) - |S|) : S \subset V(G)\}$$

Lemma 5. *Suppose that G_0 is a nontrivial connected graph. Let G be a graph obtained from G_0 by connecting a central vertex $v \in S_{s+1}$ to a vertex $u \in V(G_0)$. Let G' be a graph obtained from G by deleting all edges of $G[V(S_{s+1})]$ and connecting each vertex of $V(S_{s+1})$, apart from v, to u, see Figure 1. Then*

$$SO(G') > SO(G).$$

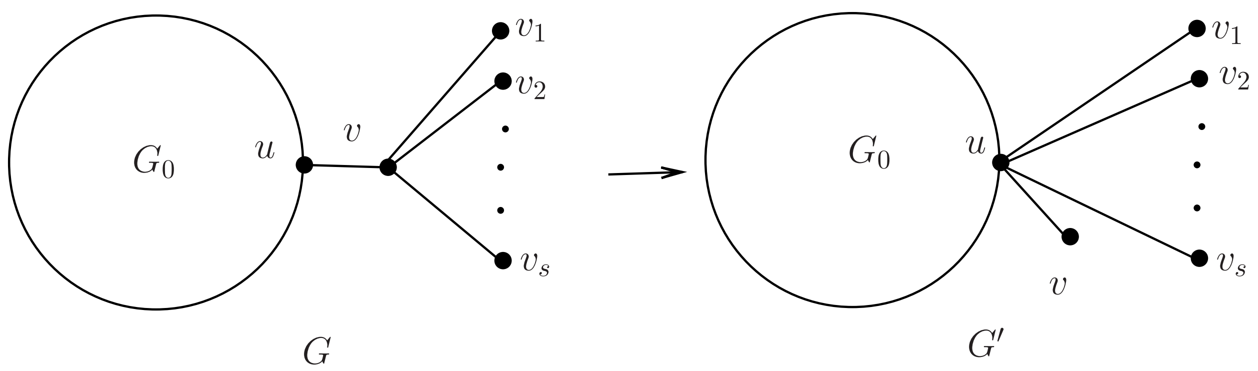

Figure 1. The graphs used in the proof of the Lemma 5.

Proof. Consider the difference between $SO(G')$ and $SO(G)$.

$$
\begin{aligned}
& SO(G') - SO(G) \\
= & \sum_{uv \in V(G')} \sqrt{d^2_{G'}(u) + d^2_{G'}(v)} - \sum_{uv \in V(G)} \sqrt{d^2_G(u) + d^2_G(v)} \\
= & (s+1)\sqrt{(s+1+d_{G_0}(u))^2 + 1} + \sum_{x \in N_{G_0}(u)} \sqrt{d^2_{G_0}(x) + (d_{G_0}(u) + s + 1)^2} \\
& - s\sqrt{(s+1)^2 + 1} - \sqrt{(s+1)^2 + (d_{G_0}(u) + 1)^2} - \sum_{x \in N_{G_0}(u)} \sqrt{d^2_{G_0}(x) + (d_{G_0}(u) + 1)^2} \\
= & \sum_{x \in N_{G_0}(u)} \left(\sqrt{d^2_{G_0}(x) + (d_{G_0}(u) + s + 1)^2} - \sqrt{d^2_{G_0}(x) + (d_{G_0}(u) + 1)^2}\right) \\
& + \left(\sqrt{(s+1+d_{G_0}(u))^2 + 1} - \sqrt{(s+1)^2 + (d_{G_0}(u) + 1)^2}\right) \\
& + s\left(\sqrt{(s+1+d_{G_0}(u))^2 + 1} - \sqrt{(s+1)^2 + 1}\right) \\
> & \ 0.
\end{aligned}
$$

□

3. Connected Graphs with Given Parameters

3.1. Extremal Graphs with Regard to $SO(G)$ in Terms of Order n and Chromatic Number c

Let $\mathcal{X}_n^c$ be the set of connected graphs on n vertices with chromatic number c. A c-partite graph is complete if any two vertices in different parts are adjacent. A simple complete c-partite graph on n vertices whose parts are of equal or almost equal sizes (that is, $\lfloor n/c \rfloor$ or $\lceil n/c \rceil$) is called a *Turán graph* and denoted by $T_n(c)$. We consider the extremal value of $SO(G)$ of graphs G from $\mathcal{X}_n^c$, and determine the corresponding extremal graphs.

In [28], Das et al. gave an upper bound on $SO(G)$ in terms of order n and chromatic number c, and characterized the extremal graphs in the following theorem. The extremal graph is exactly the Turán graph $T_n(c)$.

Theorem 1 ([28])**.** *Let $G \in \mathcal{X}_n^c, q = \lfloor \frac{n}{c} \rfloor$ and $r = n - cq$. Then*

$$SO(G) \leq SO(T_n(c)),$$

the equality holds if and only if $G \cong T_n(c)$.

Moreover, $SO(T_n(c)) = r(c-r)\lfloor \frac{n}{c} \rfloor \lceil \frac{n}{c} \rceil \sqrt{\left(n - \lfloor \frac{n}{c} \rfloor\right)^2 + \left(n - \lceil \frac{n}{c} \rceil\right)^2} + \sqrt{2}\binom{r}{2}\lceil \frac{n}{c} \rceil^2 \left(n - \lceil \frac{n}{c} \rceil\right) + \sqrt{2}\binom{c-r}{2}\lfloor \frac{n}{c} \rfloor^2 \left(n - \lfloor \frac{n}{c} \rfloor\right)$.

In what follows, we give a lower bound on $SO(G)$ in terms of order n and chromatic number c, and characterize the extremal graph in the following theorem. Denote by $KP(n,c)$ a connected graph obtained from K_c by attaching a path P_{n-c+1} to a vertex $v \in K_c$.

Theorem 2. *Let $G \in \mathcal{X}_n^c$ with $2 \leq c \leq n-1$. Then*

$$SO(G) \geq SO(KP(n,c)),$$

the equality holds if and only if $G \cong KP(n,c)$.

Proof. Suppose that $G (\in \mathcal{X}_n^c)$ is a graph having minimum value of $SO(G)$. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$. Since G has chromatic number c, by Lemma 3, there is a vertex subset $S \subseteq V(G)$ with cardinality at least c. Moreover, the degree of each vertex $v \in S$ is at least $c-1$. According to the definition of $SO(G)$ and Proposition 1, it is easy to see that the value of $SO(G)$ decreases when deleting edges in G. It implies that the value $SO(G)$ of G reaches its minimum when the graph G contains as few edges as possible. Based on these facts, we conclude that $G[S]$ is a complete subgraph K_c. Note that the graph G contains as few edges as possible, and each vertex v belongs to S with $d_G(v) \geq c-1$. We have that $G - E(G[S])$ contains as few edges as possible. Thus, $G - E(G[S])$ must be a union of some trees. Thus, $G - E(G[S]) = \bigcup_{i=1}^{t} T_{v_{i_j}}$, where $T_{v_{i_j}}$ is a tree containing v_{i_j} as its root in $G - E(G[S])$ for $1 \leq j \leq t$ and $t \leq c$. Denote by G_1 the graph obtained from $G[S](\cong K_c)$ by attaching a vertex of tree $T_{v_{i_j}}$ to a vertex v_{i_j} of $G[S]$ for $1 \leq j \leq t$.

Without loss of generality, suppose that $G - E(G[S]) = \bigcup_{i=1}^{t} T_{v_i}$, $1 \leq i \leq t$. Let $|V(T_{v_i})| = n_i$ for $1 \leq i \leq t$ and $t \leq c$.

For each subscript $i \in [t]$, by repeating the use of Lemma 5, we obtain a new graph G_2 obtained from $G[S](\cong K_c)$ by attaching a path P_{n_i} to $u_i(\in G[S])$ for $1 \leq i \leq t$. It is not difficult to see that $SO(G_2) < SO(G_1)$.

Replacing the clique $G[S](\cong K_c)$ in G_2 with a copy of K_1, namely v_0, we obtain a new *star-like* tree G_3 with $|G_3| = n - c + 1$. In fact, G_3 is isomorphic to a tree T. By Lemma 2, we can obtain a new tree T' from T such that $T' \cong P_{n-c+1}$ and $SO(T') \leq SO(T)$. In what follows, we consider two cases of whether v_0 is an end vertex of T' or not.

Case 1. $d_{T'}(v_0) = 1$.

In this case, we replace $v_0 \in T'$ (respectively, T) by C_g to obtain a graph G_3 (respectively, G_1). According to the result obtained above, we obtain $SO(G_3) \leq SO(G_1)$ immediately. It is easy to see that $G_3 \cong KP(n,c)$. The result holds.

Case 2. $d_{T'}(v_0) = 2$.

In this case, we replace $v_0 \in T'$ by K_c to obtain a new graph G_4. Let p and q be two positive integers. The graph G_4 can be viewed as a graph obtained from K_c by attaching two paths P_p and P_q to two distinct vertices v_i and v_j of K_c for $1 \leq i < j \leq t$.

Let $P_q = P_{u_0,u_1,\ldots,u_q}$ and $P_p = P_{w_0,w_1,\ldots,w_p}$. Suppose that $1 \leq q \leq p < n - c$. Consider the Sombor index of G_4. Let $G_4 = G(q,p)$ and consider the Sombor index of $G(q,p)$.

$$\begin{aligned}
SO(G_4) &= \sum_{uv \in V(G)} \sqrt{d_G^2(u) + d_G^2(v)} \\
&= 2\sqrt{2}(p+q-4) + 2\sqrt{5} + 2\sqrt{4+c^2} + \sqrt{2}c \\
&\quad + 2(c-2)\sqrt{2c^2-2c+1} + \sqrt{2}\binom{c-2}{2}(c-1) \\
&= 2\sqrt{2}(n-c-4) + 2\sqrt{5} + 2\sqrt{4+c^2} + \sqrt{2}c \\
&\quad + 2(c-2)\sqrt{2c^2-2c+1} + \sqrt{2}\binom{c-2}{2}(c-1).
\end{aligned}$$

The expression of $SO(G_4)$ is independent of p and q. This implies that $SO(G(q,p)) = SO(G(q-1,p+1)) = \cdots = SO(G(1,p+q-1))$. In what follows, compare the difference between $SO(G(1,p+q-1))$ and $SO(G(0,p+q))$:

$$\begin{aligned}
&SO(G(1,p+q-1)) - SO(G(0,p+q)) \\
&= \left[\sqrt{1+c^2} + (c-2)\sqrt{c^2+(c-1)^2} + \sqrt{2c^2} + \sqrt{5}\right] \\
&\quad - \left[(c-2)\sqrt{2(c-1)^2} + \sqrt{(c-1)^2+c^2} + \sqrt{8} + \sqrt{5}\right] \\
&\geq 0.
\end{aligned}$$

Thus, $SO(G(1,p+q-1)) \geq SO(G(0,p+q))$. Since $G(0,p+q) \cong KP(n,c)$, we know that $KP(n,c)$ is exactly the extremal graph with a minimum value of $SO(KP(n,c))$ in this case.

Combining the two cases above, we complete the proof of Theorem 2. $\square$

3.2. Extremal Graphs with Regard to $SO(G)$ in Terms of Order n and Girth g

Let $\mathcal{G}_n^g$ be the set of all connected graphs with given order n and girth g. In this subsection, we characterize the extremal graph having a minimum value of the Sombor index in $\mathcal{G}_n^g$.

Let C_g be a cycle of length g. Denote by $CP(n,g)$ the graph obtained by connecting a pendent vertex of a path P_{n-g} with one vertex $v \in C_g$.

Theorem 3. *Let $G \in \mathcal{G}_n^g$. Then*

$$SO(G) \geq SO(CP(n,g)),$$

and the equality holds if and only if $G \cong CP(n,g)$. Moreover, $SO(CP(n,g)) = 2\sqrt{2}n - 8\sqrt{2} + \sqrt{5} + 2\sqrt{13}$.

Proof. Suppose that $G \in \mathcal{G}_n^g$ is a graph with a minimum value of $SO(G)$. Let C_g be the shortest cycle of G. We first claim that the cycle C_g is the only cycle of G. In fact, suppose, to the contrary, that there exists another cycle C_t different from C_g, where $t \geq g$. By Proposition 1, we know that deleting edges will decrease the value of $SO(G)$. Delete an edge of C_t, and then we obtain a new graph G_1 satisfying $G_1 \in \mathcal{G}_n^g$. It is easy to see that $SO(G_1) < SO(G)$, a contradiction.

By Proposition 1 and the choice of G, it is easy to see that $G - E(C_g)$ contains as few edges as possible. Based on the analysis above, we know that $G - E(C_g)$ must be a forest. Let $V(C_g) = \{u_1, u_2, \ldots, u_g\}$. Denote by $T_{u_{i_j}}$ the tree containing u_{i_j} in $G - E(C_g)$, where $i_j \in [g]$. There exist some trees being single vertices. Without of loss generality, suppose that $T_{u_1}, T_{u_2}, \ldots, T_{u_a}$ are trees of order at least 2, where $a \leq g$.

Replace the cycle C_g in G by a copy of K_1 and denote it by v_0. We obtain a new graph G_2 with $|G_2| = n - g + 1$. In fact, G_2 is isomorphic to a tree T. By Lemma 2, we can obtain a new tree T' from T such that $T' \cong P_n$ and $SO(T') \leq SO(T)$. In what follows, we consider two cases whether v_0 is an end vertex of T' or not.

Case 1. $d_{T'}(v_0) = 1$.

In this case, we replace $v_0 \in T'$ (respectively, T) by C_g to obtain a graph G_3 (respectively, G_1). According to the result obtained above, $SO(T') \leq SO(T)$, we obtain $SO(G_3) \leq SO(G_1)$ immediately. It is easy to see that $G_3 \cong CP(n,g)$. The result follows.

Case 2. $d_{T'}(v_0) = 2$.

Let $b(\geq 1)$ and $d(\geq 1)$ be two integers. We replace v_0 by C_g to obtain a new graph G_4. We see that G_4 can be viewed as two paths P_b and P_d connected to two distinct vertices u_1 and u_2 of cycle C_g, respectively. Note that $b + d + g = n$. Suppose that $b \leq d$. Denote by G_5 a new graph obtained by deleting the edge between u_1 and the path P_b, and attaching P_b to anther end vertex of P_d. We know that G_5 can be viewed as a graph obtained by connecting a path P_{b+d} to any vertex of C_g. Note that $G_5 \cong CP(n,g)$. Next, compare the difference between $SO(G_5)$ and $SO(G_4)$:

$$\begin{aligned} SO(G_5) - SO(G_4) &= \sum_{uv \in V(G')} \sqrt{d_{G'}^2(u) + d_{G'}^2(v)} - \sum_{uv \in V(G)} \sqrt{d_G^2(u) + d_G^2(v)} \\ &= 4\sqrt{4+4} - \left(\sqrt{1+4} + 3\sqrt{4+9}\right) \\ &= 8\sqrt{2} - \sqrt{5} - 3\sqrt{13} \\ &< 0. \end{aligned}$$

Thus, we have $SO(G_5) < SO(G_4)$. In this case, $SO(G_5)(\cong CP(n,g))$ has the minimum value of $SO(CP(n,g))$.

Combing the two cases, we conclude that $CP(n,g)$ has a minimum value of $SO(CP(n,g))$ in $\mathcal{G}_n^g$. This completes the proof of this theorem. $\square$

Let $G \in \mathcal{G}_n^3$. By Proposition 1, adding edges increases the value of the Sombor index. It is easy to see that G contains as many edges as possible. Thus, $SO(G) \le SO(K_n)$. The equality holds if and only if $G \cong K_n$. Moreover, $SO(K_n) = \frac{\sqrt{2}}{2} n(n-1)^2$. If $g \ge 4$, it is difficult to determine the extremal graphs having a maximum value of the Sombor index in $\mathcal{G}_n^g$.

3.3. Extremal Graphs with Regard to $\xi^d(G) - D'(G)$ in Terms of Matching Number

Let $\mathcal{G}_n^\beta$ be the set of connected graphs of order n and matching number β. In what follows, we will determine the extremal graph G in $\mathcal{G}_n^\beta$ with maximum $SO(G)$, and calculate the corresponding value of $SO(G)$.

Firstly, consider some special cases. If $n \ge 3$ and $\beta = 1$, then $SO(G) = SO(S_n) = (n-1)\sqrt{n^2 - 2n + 2}$. If $n = 4$ and $\beta = 2$, then $SO(P_4) \le SO(G) \le SO(K_4)$. Moreover, $SO(P_4) = 2\sqrt{2} + 2\sqrt{5}$ and $SO(K_4) = 18\sqrt{2}$. So, in what follows, we always assume that $\beta \ge 2$ and $n \ge 5$.

If $\beta = \lfloor \frac{n}{2} \rfloor$ and $n \ge 5$, then $SO(P_n) \le SO(G) \le SO(K_n)$. The left equality holds if and only if $G \cong P_n$ and the right equality holds if and only if $G \cong K_n$. Moreover, $SO(P_n) = 2\sqrt{2}(n-3) + 2\sqrt{5}$ and $SO(K_n) = \frac{\sqrt{2}}{2}(n^3 - 2n^2 + n)$.

Theorem 4. *Let $G \in \mathcal{G}_n^\beta$. If $2 \le \beta < \lfloor \frac{n}{2} \rfloor$ and $n \ge 5$, then*

$$SO(G) \le SO(K_\beta \vee \overline{K}_{n-\beta}),$$

the equality holds if and only if $G \cong K_\beta \vee \overline{K}_{n-\beta}$.

Moreover, $SO(K_\beta \vee \overline{K}_{n-\beta}) = \beta(n-\beta)\sqrt{\beta^2+1} + \beta(\beta-1)(n-1)$.

Proof. We characterize the structure of extremal graph $G(\in \mathcal{G}_n^\beta)$ with maximum $SO(G)$. Suppose t and s are two positive integers. Let n_i, $1 \le i \le t$ be all odd positive integers.

We first show that $SO(G) \le SO(K_s \vee (\bigcup_{i=1}^t K_{n_i}))$. Let $\bar{G} = K_s \vee (\bigcup_{i=1}^t K_{n_i})$. Suppose that there exists a graph $G^{**}(\ncong \bar{G})$ having the maximum $SO(G^{**})$. According to Lemma 4, we conclude that there exists a set $S \subseteq V(G^{**})$ with $|S| = s$, such that $G^{**} - S$ contains t odd components $G_1, G_2, \ldots, G_t$ and $\beta(G^{**}) = \frac{1}{2}(n - t + s)$. Note that $\sum_{i=1}^t |V(G_i)| \le n - s$, and then $t \le n - s$. Since $\beta(G^{**}) = \frac{1}{2}(n - t + s)$, we have $n + s - 2\beta(G^{**}) = t \le n - s$. Thus, $\beta(G^{**}) \ge s$.

Suppose that $|V(G_1)| \le |V(G_2)| \le \cdots \le |V(G_t)|$. Let $G_0 = G^{**} - S - (\bigcup_{i=1}^t G_i)$. It is easy to see that G_0 is a union of even components of $G - S$. If $V(G_0) \ne \emptyset$, we add edges to $G^{**}[V(G_0) \cup V(G_t)]$ until there are no edges to add to this induced subgraph. That is, the induced subgraph $G^{**}[V(G_0) \cup V(G_t)]$ is a clique $K_{|G_0|+|G_t|}$. Denote by G' the resulting graph obtained from G^{**} by adding as many edges as possible in $G^{**}[V(G_0) \cup V(G_t)]$. By Lemma 4, we have $\beta(G') \le \frac{1}{2}(n - t + s) = \beta(G^{**})$. According to the fact that adding edges in any graph does not reduce the matching number, we have $\beta(G') \ge \beta(G^{**})$. Then, we have $\beta(G') = \beta(G^{**})$. Thus, $G' \in G_n^\beta$. Since the number of edges in G' are more than the number of edges in G^{**}. By Proposition 1, we have $SO(G') < SO(G^{**})$. This contradicts the choice of G^{**}.

If $V(G_0) = \emptyset$, then $V(G^{**}) = S \bigcup (\bigcup_{i=1}^t V(G_i))$. According to the assumption that $G^{**} \ncong K_s \vee (\bigcup_{i=1}^t K_{n_i})$, we can obtain a new graph G'' from G^{**} by adding edges between each pair vertex sets S and $V(G_i)$, $1 \le i \le t$, and adding edges in $G^{**}[S]$ and $G^{**}[V(G_i)]$. According to Proposition 1, we have $SO(G'') > SO(G^{**})$. This contradicts the maximality of $SO(G^{**})$.

Combining above two cases, we have $SO(G) \le SO(K_s \vee (\bigcup_{i=1}^t K_{n_i}))$.

According to the fact above, we know that $\bar{G}(\cong K_s \vee (\bigcup_{i=1}^t K_{n_i}))$ is the extremal structure in $\mathcal{G}_n^\beta$ with maximum value of $SO(K_s \vee (\bigcup_{i=1}^t K_{n_i}))$.

Next, let us conduct further analysis to determine the specific value of each n_i for $i \in [t]$ and optimize the graph $K_s \vee (\bigcup_{i=1}^{t} K_{n_i})$ such that the value of $SO(K_s \vee (\bigcup_{i=1}^{t} K_{n_i}))$ becomes as large as possible. Consider the value of $SO(K_s \vee (\bigcup_{i=1}^{t} K_{n_i}))$, and we have

$$SO(K_s \vee (\bigcup_{i=1}^{t} K_{n_i})) = \sum_{uv \in E(\bar{G})} \sqrt{d^2_{\bar{G}}(u) + d^2_{\bar{G}}(v)}$$
$$= \binom{s}{2}\sqrt{2(n-1)^2} + \sum_{i=1}^{t} \binom{n_i}{2}\sqrt{2(s+n_i-1)^2} + \sum_{i=1}^{t} sn_i\sqrt{(n-1)^2 + (s+n_i-1)^2}$$
$$= (n-1)\binom{s}{2}\sqrt{2} + \sqrt{2}\sum_{i=1}^{t}\binom{n_i}{2}(s+n_i-1) + s\sum_{i=1}^{t} n_i\sqrt{(n-1)^2+(s+n_i-1)^2}$$

Define a function $f(n_1, n_2, \ldots, n_t)$ with t variables as the following.

$f(n_1, n_2, \ldots, n_t) = \sqrt{2}\sum_{i=1}^{t}\binom{n_i}{2}(s+n_i-1) + s\sum_{i=1}^{t} n_i\sqrt{(n-1)^2+(s+n_i-1)^2}$, where $s(\geq 1)$ is constant. Suppose $1 \leq n_1 \leq n_2 \leq \cdots \leq n_t$, and $2 \leq n_i < n_j$ for $1 \leq i < j \leq t$. Consider the following formula:

$$f(n_1, n_2, \ldots, n_i, \ldots, n_j, \ldots, n_t) - f(n_1, n_2, \ldots, n_i - 1, \ldots, n_j + 1, \ldots, n_t)$$
$$= \left[\sqrt{2}\binom{n_i}{2}(s+n_i-1) + sn_i\sqrt{(n-1)^2+(s+n_i-1)^2} + \sqrt{2}\binom{n_j}{2}(s+n_j-1)\right.$$
$$\left. + sn_j\sqrt{(n-1)^2+(s+n_j-1)^2}\right] - \left[s(n_i-1)\sqrt{(n-1)^2+(s+n_i-2)^2}\right.$$
$$\left. + \sqrt{2}\binom{n_i-1}{2}(s+n_i-2) + \sqrt{2}\binom{n_j+1}{2}(s+n_j) + s(n_j+1)\sqrt{(n-1)^2+(s+n_j)^2}\right]$$

Define two functions as following $h(x) = \sqrt{2}\binom{x}{2}(s+x-1) - \sqrt{2}\binom{x-1}{2}(s+x-2)$. $g(x) = sx\sqrt{(n-1)^2+(s+x-1)^2} - s(x-1)\sqrt{(n-1)^2+(s+x-2)^2}$.

Taking the first derivative, we have $h'(x) = \frac{\sqrt{2}}{2}(2s-3) > 0$. $g'(x) = s\sqrt{(n-1)^2+(s+x-1)^2} + sx\frac{s+x-1}{\sqrt{(n-1)^2+(s+x-1)^2}} - s\sqrt{(n-1)^2+(s+x-2)^2} - s(x-1)\frac{s+x-2}{\sqrt{(n-1)^2+(s+x-2)^2}} > 0$.

Since $2 \leq n_i < n_j$, we have $h(n_i) < h(n_j)$ and $g(n_i) < g(n_j)$. It is easy to see that $f(n_1, n_2, \ldots, n_i, \ldots, n_j, \ldots, n_t) < f(n_1, n_2, \ldots, n_i - 1, \ldots, n_j + 1, \ldots, n_t)$.

From the above, we see that the function $f(n_1, n_2, \ldots, n_i, \ldots, n_j, \ldots, n_t)$ increases when the pair (n_i, n_j) changes by the following chain $(n_i, n_j) \to (n_i - 1, n_j + 1) \to \cdots \to (1, n_j + n_i + 1)$.

For any pair (n_i, n_t), $1 \leq i < t$, if $n_i \geq 2$, we repeat the above process until the graph $\bar{G}$ (i.e., $K_s \vee (\bigcup_{i=1}^{t} K_{n_i})$) becomes a new graph $\hat{G}$ (i.e., $K_s \vee ((t-1)K_1 \bigcup K_{n-s-t+1})$). The graphs $\widetilde{G}$ and $\hat{G}$ are given in Figure 2. By Proposition 1, we obtain $SO(\bar{G}) < SO(\hat{G})$.

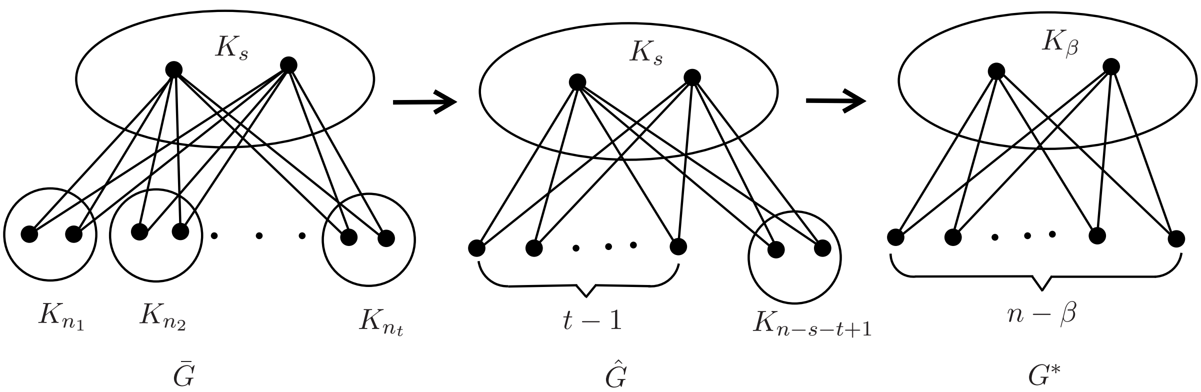

Figure 2. The graphs used in the proof of the Theorem 4.

Next, continue to increase the value of $SO(\hat{G})$. Notice that $\beta(\hat{G}) = \beta = \frac{1}{2}(n+s-t)$. We calculate this value by the following:

$$\begin{aligned}
SO(K_s \vee ((t-1)K_1 \cup K_{n-s-t+1})) &= \sum_{uv \in E(\hat{G})} \sqrt{d_{\hat{G}}^2(u) + d_{\hat{G}}^2(v)} \\
&= s(t-1)\sqrt{(n-1)^2 + s^2} + s(n-s-t+1)\sqrt{(n-1)^2 + (n-t)^2} \\
&\quad + \binom{s}{2}\sqrt{2(n-1)^2} + \binom{n-s-t+1}{2}\sqrt{2(n-t)^2} \\
&= s(t-1)\sqrt{(n-1)^2 + s^2} + s(n-s-t+1)\sqrt{(n-1)^2 + (n-t)^2} \\
&\quad + \sqrt{2}\binom{s}{2}(n-1) + \sqrt{2}\binom{n-s-t+1}{2}(n-t) \\
&= s(n+s-2\beta-1)\sqrt{(n-1)^2 + s^2} + s(2\beta-2s+1)\sqrt{(n-1)^2 + (2\beta-s)^2} \\
&\quad + \sqrt{2}\binom{s}{2}(n-1) + \sqrt{2}\binom{2\beta-2s+1}{2}(2\beta-s)
\end{aligned}$$

Let $g_1(x) = x(n+x-2\beta-1)\sqrt{(n-1)^2+x^2} + x(2\beta-2x+1)\sqrt{(n-1)^2+(2\beta-x)^2} + \sqrt{2}\binom{x}{2}(n-1) + \sqrt{2}\binom{2\beta-2x+1}{2}(2\beta-x)$, with $1 \le x \le \beta < \frac{n-1}{2}$. Taking the first derivative, we have $g_1'(x) = (n+2x-2\beta-1)\sqrt{(n-1)^2+x^2} + \frac{x^3+(n-2\beta-1)x^2}{\sqrt{(n-1)^2+x^2}} + (2\beta-4x+1)\sqrt{(n-1)^2+(2\beta-x)^2} + (2\beta x - 2x^2 + x)\frac{x-2\beta}{\sqrt{(n-1)^2+(2\beta-x)^2}} + \frac{\sqrt{2}}{2}(2x-1)(n-1) - \sqrt{2}\binom{2\beta-2x+1}{2} - \sqrt{2}(2\beta-x)(2\beta-2x) - \sqrt{2}(2\beta-x)(2\beta-2x+1)$.

For $1 \le x \le \beta < \frac{n-1}{2}$, we check that $g_1'(x) > 0$. That is, the function $g_1(x)$ is increasing when $x \in [1, \beta]$. Then, we conclude that $g_1(x)$ reaches its maximum value at $x = \beta$ with $1 \le x \le \beta < \frac{n-1}{2}$. Note that $G^* = K_s \vee ((n+s-2\beta-1)K_1 \cup K_{2\beta-2s+1}) \cong K_\beta \vee \overline{K}_{n-\beta}$ (see Figure 2) for $x = s = \beta$, and then $SO(\hat{G}) < SO(G^*)$.

That is, $SO(K_s \vee ((t-1)K_1 \cup K_{n+s-t+1})) < SO(K_\beta \vee \overline{K}_{n-\beta})$.

This completes the proof. □

4. Bipartite Graphs with Given Parameters

4.1. Extremal Bipartite Graphs with Regard to $SO(G)$ in Terms of Matching Number β

Let $\mathcal{B}_n^\beta$ be the class of all bipartite graphs of order n and matching number β. In this subsection, we give some upper bounds on $SO(G)$ of all connected graph $G \in \mathcal{B}_n^\beta$. Meanwhile, we determine the corresponding extremal graphs.

Theorem 5. *Let $G \in \mathcal{B}_n^\beta$. Then*

$$SO(G) \le SO(K_{\beta,n-\beta}),$$

the equality holds if and only if $G \cong K_{\beta,n-\beta}$. Moreover, $SO(K_{\beta,n-\beta}) = \beta(n-\beta)\sqrt{n^2-2\beta n+2\beta^2}$.

Proof. Suppose that $G \in \mathcal{B}_n^\beta$ is an extremal graph with maximum $SO(G)$. Let A, B be the bipartition of the vertex set of G, $|A| = a$ and $|B| = b$. Let M be a maximal matching of G, and $|M| = \beta$. Suppose $a \ge b \ge \beta$. Let $A_0 = A \bigcap V(G[M])$, and $B_0 = B \bigcap V(G[M])$. It is easy to see that $|A_0| = |B_0| = \beta$. Since $\beta \le \lfloor \frac{n}{2} \rfloor$, we consider two cases depending on the value of β. If $\beta = \lfloor \frac{n}{2} \rfloor$, then $A = \lceil \frac{n}{2} \rceil$ and $B = \lfloor \frac{n}{2} \rfloor$. We claim that $G \cong K_{\beta,n-\beta}$. Suppose, to the contrary, that $G \ncong K_{\beta,n-\beta}$. Construct a new graph G' obtained from G by adding edges between two sets A and B. According to Proposition 1, adding edges will increase the value of the Sombor index, and then we have $SO(G') > SO(G)$. This contradicts the choice of G. Thus, $G \cong K_{\beta,n-\beta}$.

If $\beta < \lfloor \frac{n}{2} \rfloor$ and $b = \beta$, then $G \cong K_{\beta,n-\beta}$. In what follows, we assume that $b > \beta$. We show that $[A \setminus A_0, B \setminus B_0] = \emptyset$. Otherwise, if there exists an edge $e \in [A \setminus A_0, B \setminus B_0]$, then we find a new matching $M' = M \bigcup \{e\}$. Thus, $|M'| = \beta + 1$. This is a contradiction. Construct a new graph G^* from G by adding as many edges as possible between the two sets A_0 and B_0 (respectively, A_0 and $B \setminus B_0$, B_0 and $A \setminus A_0$). We have $SO(G^*) > SO(G)$. Note that $G^*[A_0 \bigcup B_0] = K_{\beta,\beta}$ and $\beta(G^*[A_0 \bigcup B_0]) = \beta$. It is easy to see that $|B \setminus B_0| = b - \beta$, and $|A \setminus A_0| = a - \beta$. Choose M_0 as a proper subset of maximum matching of $G^*[A_0 \bigcup B_0]$. That is, $|M_0| < \beta$. Since $\beta(G^*[A_0 \bigcup B \setminus B_0]) \geq \beta - |M_0|$ and $\beta(G^*[B_0 \bigcup A \setminus A_0]) \geq \beta - |M_0|$, we can find maximal matching with order $|M_0| + 2(\beta - |M_0|) = \beta + (\beta - |M_0|) \geq \beta + 1$ in G^*. Hence, $G^* \notin \mathcal{B}_n^\beta$ and $G^* \neq G$. Next, construct a new graph $\hat{G}$ from G^* by deleting red edges and adding blue edges such that $[A_0, B \setminus B_0] = \emptyset$, and $\hat{G}[B_0 \bigcup (B \setminus B_0)] = K_{b-\beta,\beta}$. The graphs G^* and $\hat{G}$ are given in Figure 3. It is easy to check that $\hat{G} \in \mathcal{B}_n^\beta$ with $\beta(\hat{G}) = \beta$.

In what follows, we claim that $\hat{G} \cong K_{\beta,n-\beta}$. Compare the difference between $SO(\hat{G})$ and G^*:

$$
\begin{aligned}
SO(G^*) - SO(\hat{G}) &= \sum_{uv \in V(G^*)} \sqrt{d_{G^*}^2(u) + d_{G^*}^2(v)} - \sum_{uv \in V(\hat{G})} \sqrt{d_{\hat{G}}^2(u) + d_{\hat{G}}^2(v)} \\
&= (b-\beta)\beta\sqrt{\beta^2 + b^2} + \beta^2\sqrt{a^2 + b^2} + (a-\beta)\beta\sqrt{a^2 + \beta^2} - \beta^2\sqrt{\beta^2 + (a+b-\beta)^2} \\
&\quad - (b-\beta)\beta\sqrt{\beta^2 + (a+b-\beta)^2} - (a-\beta)\beta\sqrt{(a+b-\beta)^2 + \beta^2} \\
&< 0.
\end{aligned}
$$

Thus, $SO(G^*) < SO(\hat{G})$. This implies that $\hat{G} \cong G \cong K_{\beta,n-\beta}$.

We complete the proof of the Theorem 5. □

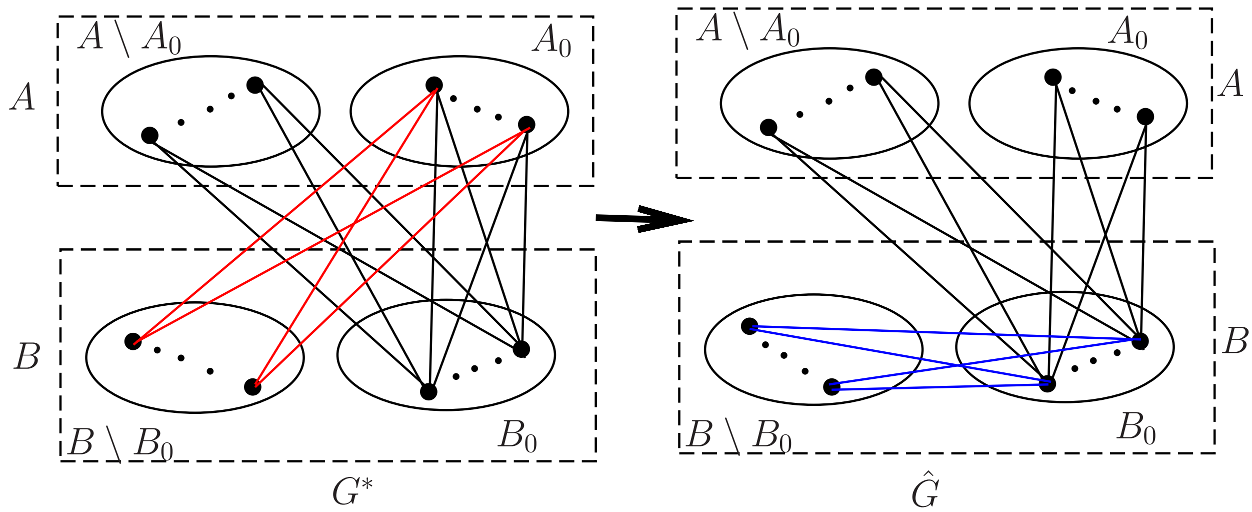

Figure 3. The graphs used in the proof of the Theorem 5.

4.2. Extremal Bipartite Graphs with Regard to $SO(G)$ in Terms of Connectivity k

Let $\mathcal{B}_n^k$ be the class of all bipartite graphs of order n and connectivity k. In what follows, we determine the extremal graphs in $\mathcal{B}_n^k$ with the maximum Sombor index. Denote by $K_{a,b}$ the complete bipartite graph with two partitions A and B. Let $a = |A| \geq |B| = b$. In [29], Li et al. gave two definitions of two operations $\vee_1$ and $\vee_2$. Denote by $\overline{K}_s \vee_1 (K_{n_1,n_2} \bigcup K_{m_1,m_2})$ the graph obtained by connecting each vertex of $\overline{K}_s$ to each vertex of one partition with order n_1 (respectively, m_1) of K_{n_1,n_2} (respectively, K_{m_1,m_2}). Denote by $\overline{K}_s \vee_2 (K_{n_1,n_2} \bigcup K_{m_1,m_2})$ the graph obtained by connecting each vertex of $\overline{K}_s$ to each vertex of one partition with order n_2 (respectively, m_2) of K_{n_1,n_2} (respectively, K_{m_1,m_2}).

Theorem 6. *Let $G \in \mathcal{B}_n^k$ with $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$.*

(I) If $k = \lfloor \frac{n-1}{2} \rfloor$ or $\lfloor \frac{n-3}{2} \rfloor$, then $G \cong K_{s,n-s}$.

Moreover, $SO(K_{s,n-s}) = s(n-s)\sqrt{(n-s)^2 + s^2}$.

(II) If $1 \le k \le \lfloor \frac{n-5}{2} \rfloor$, then $G \cong \overline{K}_s \vee_1 (K_1 \bigcup K_{p,q})$ for some p and q.

Moreover, $SO(\overline{K}_s \vee_1 (K_1 \bigcup K_{p,q})) = s\sqrt{s^2 + (p+1)^2} + sp\sqrt{(s+q)^2 + (p+1)^2} + pq\sqrt{(s+q)^2 + p^2}$.

Proof. Suppose that G is a graph in $\mathcal{B}_n^k$ with maximum $SO(G)$. Let S be a minimal vertex cut set with $|S| = k$, and $G_1, G_2, \ldots, G_t$ be the connected components of $G - S$, where $t \ge 2$. If there exists $i \in [t]$ such that $|G_i| \ge 2$, then $G[G_i]$ must be a complete bipartite subgraph. Otherwise, we can obtain a new graph G' obtained from G by adding edges in $G[G_i]$. By Proposition 1, adding edges increases the value of the Sombor index, we have $SO(G') > SO(G)$. This contradicts the choice of G. If there exists $j \in [t]$ such that $|G_j| = 1$, then $G[G_j, S]$ must be a complete bipartite subgraph $K_{1,s}$. Otherwise, we can find a smaller vertex cut set than S such that the connectivity of G is less than k. This is a contradiction. Moreover, $G[S] = \overline{K}_s$. If there exists an edge $e \in G[S]$, then we can find a triangle in G, a contradiction.

Case 1 $k = \lfloor \frac{n-1}{2} \rfloor$ or $\lfloor \frac{n-3}{2} \rfloor$.

In this case, each component of $G - S$ must be a single vertex K_1. Otherwise, suppose that there exists a component G_i with $|G_i| \ge 2$ for $i \in [t]$. Obviously, $G[G_i]$ is a complete bipartite subgraph. Denote by A the partition of $G[G_i]$ such that A and S are in different partition of G. It is easy to see that A is a vertex cut set with $|A| < s$. This is a contradiction. Thus, $G - S = \overline{K}_{n-s}$. Then, $G \cong K_{s,n-s}$.

Case 2 $1 \le k \le \lfloor \frac{n-5}{2} \rfloor$.

We claim that $G - S$ contains exactly two components G_1 and G_2. Otherwise, suppose that $t \ge 3$. Since each component G_i with order at least 2 is a complete bipartite subgraph, we can obtain a new graph G'' obtain from G by adding edges in $G[\bigcup_{i=2}^t G_i]$ such that $G[\bigcup_{i=2}^t G_i]$ becomes a complete bipartite subgraph. By Proposition 1, we obtain a contradiction that $SO(G'') > SO(G)$.

Without loss of generality, let $|G_1| \ge 2$, and $|G_2| = 1$. Let X, Y be two partitions of G_1 with $|X| = p$, $|Y| = q$ and $p \ge q$. Let $G''' = \overline{K}_s \vee_1 (K_1 \bigcup K_{p,q})$. It is easy to see that $p \ge s$. Otherwise, X is a vertex cut set with $|X| = p < s$. This is a contradiction.

Calculate the Sombor index of $\overline{K}_s \vee_1 (K_1 \bigcup K_{p,q})$.

$$
\begin{aligned}
SO(\overline{K}_s \vee_1 (K_1 \bigcup K_{p,q})) &= \sum_{uv \in E(G''')} \sqrt{d_{G'''}^2(u) + d_{G'''}^2(v)} \\
&= s\sqrt{s^2 + (p+1)^2} + sp\sqrt{(s+q)^2 + (p+1)^2} + pq\sqrt{(s+q)^2 + p^2}.
\end{aligned}
$$

□

5. Concluding Remarks

In this paper, we give some further results on $SO(G)$. We determine the upper and lower bounds on $SO(G)$ among general connected graphs in terms of several graph parameters, i.e., chromatic number, and characterize the extremal graphs. In addition, we consider the extremal value of the Sombor index in bipartite graphs in terms of connectivity and matching number, and determine the corresponding extremal bipartite graphs.

Naturally, it is interesting to consider the extremal connected bipartite graphs in terms of other parameters. We state a few challenging open problems on Sombor index for connected graphs and connected bipartite graphs.

Problem 1. *Determine an upper bound on Sombor index for connected graphs in terms of girth.*

Problem 2. *How can we determine lower and upper bounds on Sombor index for connected bipartite graphs in terms of diameter.*

Problem 3. *Determine lower and upper bounds on Sombor index for connected bipartite graphs in terms of radius.*

Problem 4. *Determine lower and upper bounds on the Sombor index for connected bipartite graphs in terms of domination.*

Our research on the Sombor index among connected graphs and connected bipartite graphs with some given parameters is just the beginning. We will continue to conduct research along this line in the future.

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