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Extremal Sombor Index of Graphs with Cut Edges and Clique Number

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Abstract: The Sombor index is defined as $SO(G) = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}$, where $d(u)$ and $d(v)$ represent the number of edges in the graph G connected to the vertices u and v, respectively. In this paper, we characterize the largest and second largest Sombor indexes with a given number of cut edges. Moreover, we determine the upper and lower sharp bounds of the Sombor index with a given number of clique numbers, and we characterize the extremal graphs.

Keywords: Sombor index; cut edge; clique number

MSC: 05C35

1. Introduction

In graph theory, studying extremal graphs and indices for a class of graphs with given parameters is an interesting problem. Recently, Gutman introduced a novel topological index, named the Sombor index in [1] and defined as $SO(G) = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}$, where $d(u)$ and $d(v)$ represent the number of edges connected to vertices u and v in G, respectively, and further established some mathematical properties for the index. Chen et al. in [2] considered the extremal values of the Sombor index of trees with some given parameters such as matching number, pendent vertices, diameter, segment number, and branching number. In the meantime, the corresponding extremal trees are characterized. Li et al. showed the extremal graphs with respect to the Sombor index among all the n-order trees with a given diameter [3]. In [4], Redžpović studied the chemical applicability of the Sombor index. In addition, Cruz et al. in [5] determined the extremal chemical graphs and hexagonal systems for the Sombor index. In [6], Zhou et al. studied the Sombor index of trees and unicyclic graphs with a given maximum degree. In [7], they found the maximum Sombor index of unicyclic graphs with a fixed girth. In [8], they showed applications of the Sombor index. For more studies in this direction, one may refer to [9–24].

Let $G = (V(G), E(G))$ be a finite, simple, and connected graph with $V(G) = \bigcup_{i=1}^{n} V_i$ and $E(G) = \bigcup_{i=1}^{m} E_i$. For any vertex $v \in V(G)$, we denote $N_G(v) = \{u | uv \in E(G)\}$ and $N_G[v] = \{u | uv \in E(G)\} \cup \{v\}$. The degree $d(v)$ of the vertex v is the number of edges connected to the vertex v. The vertex v is called pendent vertex if $d(v) = 1$. The stem is the vertex adjacent to at least one pendent vertex, and the pendent edge is the edge incident with the pendent vertex and the stem. If $u, v \in G$, then the distance $d(u, v)$ is the length of the shortest path connecting the two vertices u and v. We use P_n, C_n, and $K_{1,n-1}$ to represent the path, cycle, and star graph with n vertices, respectively.

A *clique* is a subset $V' \in V(G)$ that makes $G[V']$ to a complete graph. The order of the largest complete subgraph in graph G is called the clique number $\psi(G)$ of G. The chromatic number $\chi(G)$ of the graph G is the minimum number of colors needed to stain each vertex

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on a graph so that the two adjacent vertices are different colors. See reference [25] for some notations and terms that we have not mentioned here.

Let $\mathcal{C}_{n,k}$ be a class of graphs having n vertices and k cut edges. Denote $E' = \{e_1, e_2, \cdots, e_k\}$. It can be divided into two classes, namely, pendent edges with size k', and non-pendent edges with size $k - k'$. We know the resulting graph $G - E'$ are either 2-edge-connected graphs or isolated vertices. The maximum number of cut edges in a connected graph with n vertices and at least one cycle is limited to $n - 3$; therefore, we assume that the graph G with cut edges and k ($k \geq 1$) is less than or equal to $n - 3$.

In this paper, we determine the Sombor index of the graph with a given number of cut edges and determine the types of the graphs with the largest and second largest Sombor indexes. At the same time, we use clique number to determine the upper and lower sharp bounds for the Sombor index in $\mathcal{C}_{n,k}$. We will introduce some graph transformations.

2. The Extremal Graph of the Sombor Index with Cut Edges

If any graphs G_1 and G_2 with $V(G_1) \cap V(G_2) = \{v\}$, then label the graph as $G_1 v G_2$. If the graphs $G_1, G_2, \cdots, G_t$ ($t \geq 2$) share a common vertex v, then the graph is labeled as $G_1 v G_2 v \cdots v G_t$. In the same way, if there is a cut edge uv between any graphs G_1 and G_2 with $u \in V(G_1)$ and $v \in V(G_2)$, in the same way, we label this graph as $G_1 uv G_2$. According to the definition and direct computation, we can obtain the following results.

Lemma 1. *Let $G = (V, E)$ be a graph and $u, v \in V(G)$. If uv is not an edge in $E(G)$, we have $SO(G) < SO(G + uv)$. If uv is an edge in $E(G)$, then we have $SO(G) > SO(G - uv)$.*

Proof. Since the increase (or decrease) in a new edge in the graph increases (or decreases) by some vertex degree, the lemma obviously holds. □

Here, we explain the graph transformation I on graph $G \in \mathcal{C}_{n,k}$. Denote that $G = G_1 uv G_2$ is a graph that does not contain cut edge uv, where G_1 and G_2 are both 2-edge-connected graphs (Figure 1a). Let $G^* = G - \{uv\} + \{u(v)w\}$ (Figure 1b). Then, the resulting graph G^* is obtained from G via the graph transformation I. Since the graph G^* posses k cut edges, the number of pendent vertices increases by 1.

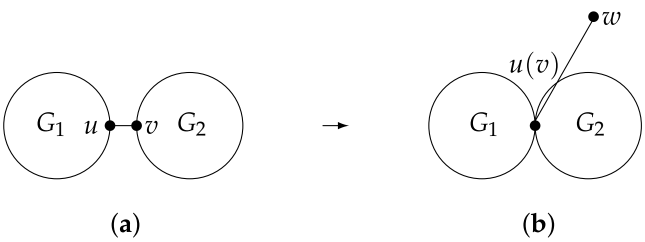

Figure 1. The graph transformation I: $G \to G^*$. (**a**) G. (**b**) G^*.

Lemma 2. *Suppose that G^* is the graph derived by $G \in \mathcal{C}_{n,k}$ using the graph transformation I, as described in Figure 1. Then, $SO(G^*) > SO(G)$.*

Proof. Set $N_G(u) - \{v\} = \{u_1, u_2, \cdots, u_r\}$ and $N_G(v) - \{u\} = \{v_1, v_2, \cdots, v_s\}$ with $r, s \geq 2$. Then, $d_G(u) = r + 1$, $d_G(v) = s + 1$, and $d_{G^*}(u(v)) = r + s + 1$. It is clear that the vertices $u_1, u_2, \cdots, u_r$ are in $V(G_1)$; and $v_1, v_2, \cdots, v_s$ are in $V(G_2)$ by assumption. Further,

$$SO(G^*) - SO(G) = \sqrt{\sum_{x \in N_{G^*}(u)} d^2_{G^*}(x) + d^2_{G^*}(u)} - \sqrt{\sum_{x \in N_G(u) \setminus v} d^2_G(x) + d^2_G(u)}$$
$$- \sqrt{\sum_{x \in N_G(v) \setminus u} d^2_G(x) + d^2_G(v)} = \sqrt{1 + (r + s + 1)^2}$$

$$+\sqrt{\sum_{x\in N_G(u)\setminus v} d_G^2(x)+(r+s+1)^2}+\sqrt{\sum_{x\in N_G(v)\setminus u} d_G^2(x)+(r+s+1)^2}$$
$$-\sqrt{\sum_{x\in N_G(u)\setminus v} d_G^2(x)+(r+1)^2}-\sqrt{\sum_{x\in N_G(v)\setminus u} d_G^2(x)+(s+1)^2}$$
$$-\sqrt{(r+1)^2+(s+1)^2}=\sqrt{1+(r+s+1)^2}$$
$$+\sqrt{\sum_{i=1}^{r} d_G^2(u_i)+(r+s+1)^2}+\sqrt{\sum_{j=1}^{s} d_G^2(v_j)+(r+s+1)^2}$$
$$-\sqrt{\sum_{i=1}^{r} d_G^2(u_i)+(r+1)^2}-\sqrt{\sum_{j=1}^{s} d_G^2(v_j)+(s+1)^2}-\sqrt{(r+1)^2+(s+1)^2}$$
$$=\left(\sqrt{1+(r+s+1)^2}-\sqrt{(r+1)^2+(s+1)^2}\right)$$
$$+\left(\sqrt{\sum_{i=1}^{r} d_G^2(u_i)+(r+s+1)^2}-\sqrt{\sum_{i=1}^{r} d_G^2(u_i)+(r+1)^2}\right)$$
$$+\left(\sqrt{\sum_{j=1}^{s} d_G^2(v_j)+(r+s+1)^2}-\sqrt{\sum_{j=1}^{s} d_G^2(v_j)+(s+1)^2}\right).$$

Note that

$$\sqrt{1+(r+s+1)^2}-\sqrt{(r+1)^2+(s+1)^2}>0.$$
$$\sqrt{\sum_{i=1}^{r} d_G^2(u_i)+(r+s+1)^2}-\sqrt{\sum_{i=1}^{r} d_G^2(u_i)+(r+1)^2}>0.$$
$$\sqrt{\sum_{j=1}^{s} d_G^2(v_j)+(r+s+1)^2}-\sqrt{\sum_{j=1}^{s} d_G^2(v_j)+(s+1)^2}>0.$$

where $d_G(u_i), d_G(v_j)\geq 1$ and $SO(G^*)-SO(G)>0$. We have finished. □

Here, we explain the graph transformation II on a graph $G\in\mathcal{C}_{n,k}$. Set uv as not a pendent cut edge in $G=G_1uvK_{1,r}$, Figure 2a. Let $G^{**}=G_1uK_{1,r+1}$ (Figure 2b). In this way, the graph G^{**} is attained at G by applying graph transformation II.

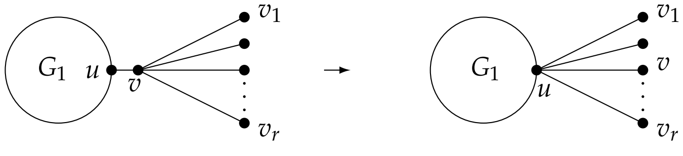

Figure 2. The graph transformation II: $G\to G^{**}$. (**a**) G. (**b**) G^{**}.

Based on the graph transformation II, we obtain:

Lemma 3. *Let G_1 be a 2-edge-connected graph and uv be a non-pendent cut edge of $G=G_1uvK_{1,r}$; G^{**} will be the resulting graph from G by applying the graph transformation II (Figure 2). Then, we have $SO(G^{**})>SO(G)$.*

Either a cut edge or a non-pendent edge can be transformed into a pendent edge via graph transformations I and II, as shown in Figure 3.

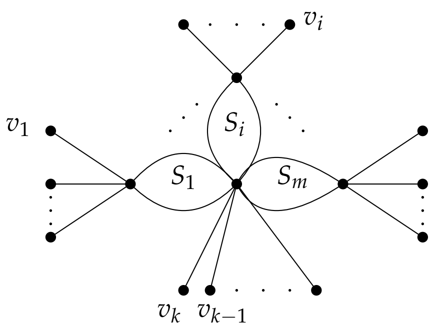

Figure 3. The graph $G^*_{k''}$.

Here, we explain the graph transformation III on graph $G \in \mathcal{C}_{n,k}$. Assume that $u, v \in V(G)$ and the vertices $u_1, u_2, \cdots, u_s$ are pendent vertices adjacent to vertex u; the vertices $v_1, v_2, \cdots, v_t$ are pendent vertices adjacent to vertex v, as shown in Figure 4a. Let $G' = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$, as shown in Figure 4b. Then, G' is the resulting graph from G through graph transformation III.

Lemma 4. *Let G' be a graph obtained from G by applying the graph transformation III (Figure 3). Then, $SO(G') > SO(G)$.*

By repeating this transformation in the graph, all pendent edges are connected to the same vertex.

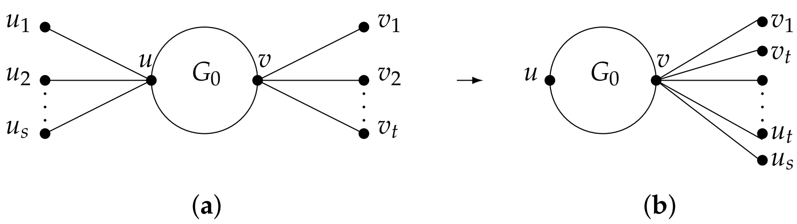

Figure 4. The graph transformation III: $G \to G'$. (**a**) G. (**b**) G'.

We will discuss the graph of $\mathcal{C}_{n,k}$ with the largest Sombor index in the following. Let K_n be a complete graph with n vertices, and Q_n^k be a graph obtained by connecting k independent vertices to one of the vertices of K_{n-k}.

Theorem 1. *In all connected graphs in $\mathcal{C}_{n,k}$, the Sombor index takes the maximum value on Q_n^k, i.e., the graph obtained by connecting k independent vertices to one of the vertex of the graph K_{n-k}.*

Proof. According to above lemmas, we provide the Sombor index for graphs in $\mathcal{C}_{n,k}$ that achieve the upper bound.

Claim 1. If a graph $G \in \mathcal{C}_{n,k}$, then $SO(G) \leq SO(G^*)$.

Let $G \in \mathcal{C}_{n,k}$ and $G \ncong G^*$, then based on the above lemmas, we know $SO(G) < SO(G^*)$. Obviously, the equality holds when $G \cong G^*$.

Claim 2. For two graphs G^* and H in Figure 4, $SO(G^*) \leq SO(H)$, the equality holds when $G^* \cong H$.

Assume $G \in \mathcal{C}_{n,k}$ is a graph with cut edges $\{e_1, e_2, \cdots e_k\}$. Then, via Lemma 1, we have $SO(G + e) > SO(G)$, where $e \notin E(G)$. Recall that by adding some edges to 2-edge-connected graphs S_i for $i \in \{1, 2, \cdots, m\}$, it is converted to the complete subgraphs $K_{n_i+1} for (i \in \{1, 2, \cdots, m\}$; therefore, the graph G^* is converted to the graph H, which has k cut edges, so that $H \subset G \in \mathcal{C}_{n,k}$. According to Lemma 1, if $G^* \subset H$, then we have $SO(G^*) < SO(H)$ and the equality holds when $G^* \cong H$.

Claim 3. For two graphs H and Q_n^k in Figure 5, we have $SO(H) \leq SO(Q_n^k)$, and the equality holds when $H \cong Q_n^k$, i.e., $m = 1$.

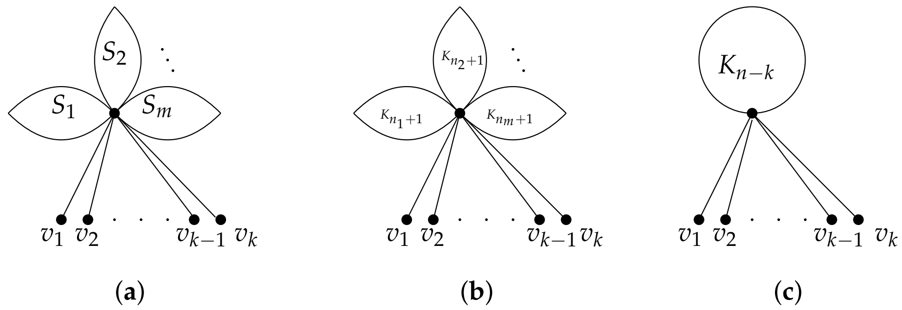

Figure 5. Simple graphs G^*, H and Q_n^k with k cut edges. (**a**) G^*. (**b**) H. (**c**) Q_n^k.

The graph H becomes the graph Q_n^k if we connect every pair of vertices in the complete subgraphs $K_{n_i+1} (i \in \{1, 2, \cdots, m\})$ of H and it has k cut edges. Obviously, $Q_n^k \in \mathcal{C}_{n,k}$ and $H \subset Q_n^k$. Therefore, using Lemma 1, we obtain $SO(H) < SO(Q_n^k)$, and the equality holds when $H \cong Q_n^k$, i.e., $m = 1$.

With the above three claims, the theorem holds. □

In the following, we characterize the graph with the second largest Sombor index in $\mathcal{C}_{n,k}$.

Theorem 2. *In all graphs $G \in \mathcal{C}_{n,k}$ and $G \ncong Q_n^k$, it holds that $SO(G) \leq SO(G_2)$; the equality holds when $G \cong G_2$.*

Proof of Theorem 2. For all graphs $G \in \mathcal{C}_{n,k}$, if G achieves the maximum $SO(G)$, then it must be one of the graphs shown in Figure 6, namely G_1, G_2, or G_3.

Recall that either a cut edge or a non-pendent cut edge can eventually be transformed into a pendent edge by repeating the graph transformation I or II. We denote the resulting graph as $G^*_{k''}$ in Figure 3, where S_i for $1 \leq i \leq m$ represents the 2-edge-connected graphs. Then, we have $SO(G^*_{k''}) \geq SO(G)$. In Figure 3, k'' represents the number of non-pendent vertices attached to cut edges. In the following, we will discuss two cases according to parameters m and k''.

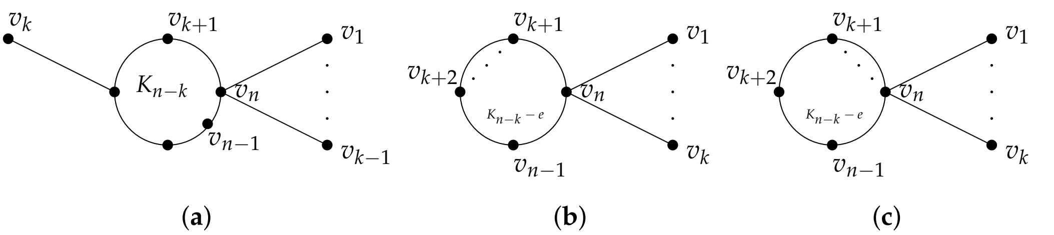

Figure 6. Simple graphs G_1, G_2, and G_3 with cut edges. (**a**) G_1. (**b**) G_2. (**c**) G_3.

Case 1. If $m = 1$.

If $k'' = 1$, additional edges are added to the vertices of the subgraph S_1 which is 2-edge-connected; via transformation, S_1 turns into G_2 or G_3 (see Figure 7). By adding an additional edge to either G_2 or G_3, then it becomes the graph Q_n^k. Therefore, based on the Lemma 1, it holds that

$$SO(G) \leq SO(G^*_{k''}) \leq SO(G_2) \leq SO(Q_n^k) \text{ or } SO(G) \leq SO(G^*_{k''}) \leq SO(G_3) \leq SO(Q_n^k).$$

If $k'' \geq 2$, edges are initially added to the vertices of the S_1 which is a 2-edge-connected subgraph, and it is converted to K_{n-k}, denoting the graph as H_1 (See Figure 8). By applying

Lemma 1, we obtain $SO(H) \geq SO(G^*_{k''})$. Next, repeating the graph transformation III on graph H, at last we obtain G_1. If we move only one edge from G_1, it becomes Q_n^k. By repeating this transformation in the graph, each pendent edge is attached to the same vertex. Via Lemma 4, we have $SO(G) \leq SO(H_1) \leq SO(G_1) \leq SO(Q_n^k)$.

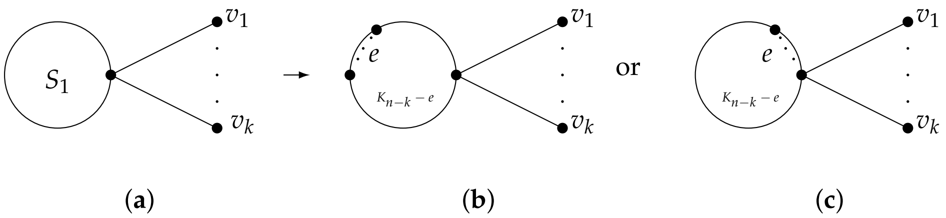

Figure 7. The graphs with $m = 1, k'' = 1$. (**a**) $G^*_{k''}$. (**b**) G_2. (**c**) G_3.

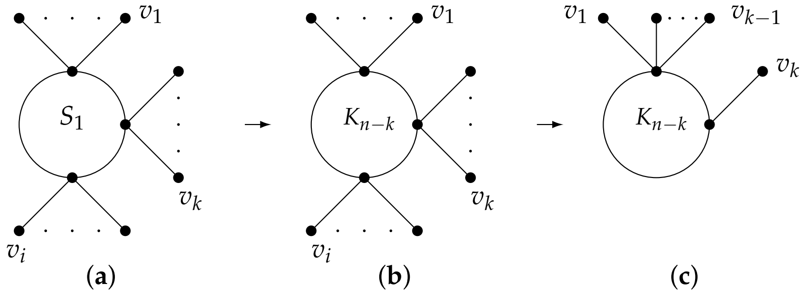

Figure 8. The graph transformation with $m = 1, k'' \geq 2$. (**a**) $G^*_{k''}$. (**b**) H_1. (**c**) G_1.

Case 2. If $m \geq 2$, we consider the same way in Case 1.

If $k'' = 1$, the complete graphs $K_{i+1}(i = 1, 2, \cdots, m)$ are constructed by adding edges to the 2-edge-connected subgraphs $S_i(i = 1, 2, \cdots, m)$ in $G^*_{k''}$, forming the graph H_2 (Figure 9). Then, we have $SO(H_2) \geq SO(G^*_{k''})$ via Lemma 1. Add some edges between $K_{n_i+1}(i = 1, 2, \cdots, m)$, composing the graph G_2 (Figure 9). If adding another edge to G_2, it becomes Q_n^k. Via Lemma 1, it holds that $SO(G^*_{k''}) \leq SO(H_2) \leq SO(G_2) \leq SO(Q_n^k)$.

If $k'' \geq 2$, add some edges to $S_i(i = 1, 2, \cdots, m)$ of $G^*_{k''}$ to obtain the complete graph $K_{n_i+1}(i = 1, 2, \cdots, m)$; by adding edges among $K_{n_i+1}(i = 1, 2, \cdots, m)$, we can obtain the graph H_3. Finally, we can obtain the graph G_1 by applying the graph transformation III on H_3, and we can obtain the graph Q_n^k by adding an edge to G_1 (Figure 10). Then, according to the above lemmas, it holds that $SO(G^*_{k''}) \leq SO(H_3) \leq SO(G_1) \leq SO(Q_n^k)$.

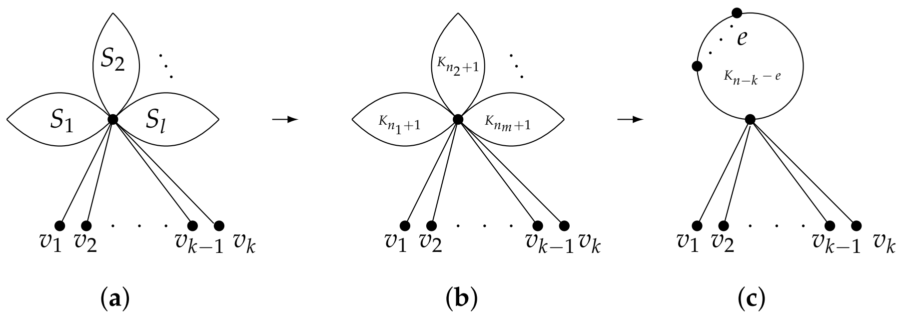

Figure 9. The graph transformation with $m \geq 2, k'' = 1$. (**a**) $G^*_{k''}$. (**b**) H_2. (**c**) G_2.

From the above cases, we know that the second largest value of the Sombor index is taken by one of the graphs G_1, G_2, and G_3. In our next work, we only need to compare the Sombor index of G_1, G_2, and G_3. Therefore,

$$SO(G_1) = (k-1)\sqrt{(n-2)^2+1} + \sqrt{(n-2)^2+(n-k)^2} + \sqrt{(n-k)^2+1}$$
$$+ \sqrt{(n-2)^2+(n-k-1)^2}(n-k-2) + \sqrt{(n-k)^2+(n-k-1)^2}$$
$$+ \sqrt{2(n-k-1)^2}(n-k-3).$$
$$SO(G_2) = k\sqrt{(n-1)^2+1} + \sqrt{(n-1)^2+(n-k-2)^2} + \sqrt{(n-1)^2+(n-k-1)^2}(n-k)$$
$$+ \sqrt{2(n-k-1)^2}(n-k-4) + \sqrt{(n-k-2)^2+(n-k-1)^2}(2n-2k-5).$$
$$SO(G_3) = k\sqrt{(n-2)^2+1} + (n-k-2)\Big(\sqrt{(n-k-2)^2+(n-k-1)^2}$$
$$+ \sqrt{(n-2)^2+(n-k-1)^2}\Big) + \sqrt{2(n-k-1)^2}(n-k-3).$$

Therefore, we compare the graph G_2 with the graph G_1, where $n \geq k+3$ and $k \geq 1$, then, through direct calculation, we have $SO(G_2) - SO(G_1) > 0$.

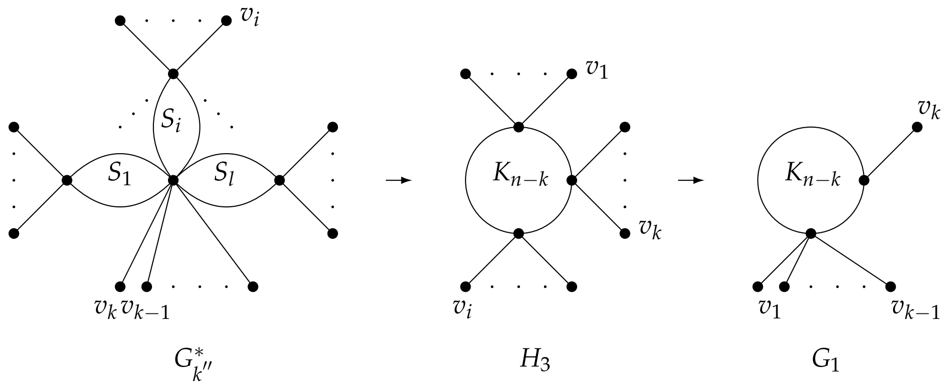

Figure 10. The graph transformation with $m \geq 2, k'' \geq 2$.

Next, we compare the graph G_2 with the graph G_1 using easy calculation, where $n \geq k+3$ and $k \geq 1$, then $SO(G_2) - SO(G_3) > 0$. Therefore, the Sombor index attained the maximum value on G_2. The theorem is proven. □

3. Extremal Sombor Index of Graphs with a Clique Number

Let $\chi_{n,k}$ and $\psi_{n,k}$ be a class of graphs with n vertices, and chromatic number k and clique number k, respectively.

Let $Q_n(k)$ be a complete k-partite graph with a partition set differing in size by no more than 1. Let $T_k((n-k)^1)$ be the graph in which a vertex of a a complete graph K_k is connected to a path graph P_{n-k+1} (see Figure 11). Next, we will prove that the graph $Q_n(k)$ and the tadpole graph $T_k((n-k)^1)$ has a maximal and minimal Sombor index in $\psi_{n,k}$, respectively.

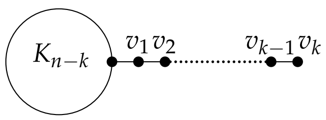

Figure 11. The tadpole graph $T_k((n-k)^1)$.

In order to obtain our main result, we first provide some necessary lemmas. From the definition of the Sombor index of the graph, these lemmas are obvious and fundamental.

Assume that $\sum_{i=1}^{k} n_i = n$. Set $Q_{n_1,n_2,\cdots,n_k}$ as the complete k-partite graph with n vertices, and the number of the partition set as $n_1, n_2, \cdots, n_k$, respectively.

Lemma 5. $SO(Q_{n_1,n_2,\cdots,n_k}) = \sum_{s=1}^{k}\sum_{t=s+1}^{k} n_s n_t \sqrt{(n-n_s)^2+(n-n_t)^2}$.

Proof. In a partition set of size n_j of $Q_{n_1,n_2,\cdots,n_k}$ for $j \in \{1,2,\cdots,k\}$, the degree of each vertex is $n-n_j$ between two partition sets of sizes n_i, n_j , where $1 \le i < j \le k$, respectively. In $Q_{n_1,n_2,\cdots,n_k}$, there are $n_i n_j$ edges connected to two sets. In addition, the degrees of the two vertices incident with each of these edges are $n-n_i$ and $n-n_j$, respectively. Then, we have $SO(Q_{n_1,n_2,\cdots,n_k}) = \sum_{s=1}^{k}\sum_{t=s+1}^{k} n_s n_t \sqrt{(n-n_s)^2+(n-n_t)^2}$, and we complete the proof of the lemma. □

In the next, we consider the maximal Sombor index of graphs from $\chi_{n,k}$. The set $\chi_{n,k}$ contains connected graph K_1 when $k=1$, and the only graph in $\chi_{n,k}$ is the complete graph K_n when $k=n$.

Lemma 6. *Let $G \in \chi_{n,k}$ be the graph with a maximal Sombor index. Then, $G \cong Q_{n_1,n_2,\cdots,n_k}$.*

Proof. The lemma holds immediately based on Lemma 1, and by the definition of the set $\chi_{n,k}$. □

Further, we will introduce some notations. If $u,v \in V(G)$ are not the same vertices in graph G for $p,q>0$, we denote by $G_{u,v}(p,q)$ the graph from G by attaching a path of length p and q at the vertex u and v of G, respectively. For $v \in V(G)$, let $G_v(l)$ be the graph attaining at v a path of length l. Let $1 \le k \le n-2$, and through the graph transformations, we get the following Lemma:

Lemma 7. *Let G be a connected graph with $G \ncong K_1$; v is a vertex in G. $G_v(k,n-1-k)$ is the graph resulting from attaching at v two paths of lengths k and $n-1-k$, respectively. Then, $SO(G_v(k,n-1-k)) > SO(G_v(n-1))$.*

By repeating the above lemma, it is easy to obtain the following result.

Remark 1 ([6]). *When the tree T with t vertices on the graph G is replaced by the path P_{t+1}, then $SO(G)$ of the graph decreases.*

Remark 2 ([6]). *Assume $s,t>0$, and two vertices $u,v \in V(G)$ so that $d(u) \ge d(v) > 1$. Then, $SO(G_{u,v}(s,t)) > SO(G_v(s+t))$.*

Now, we first consider the maximal Sombor index for a graph from $\chi_{n,k}$. In the discussion in this part, we assume that the graph G has k chromatic numbers for $1<k<n$ and $n = kq+r$, $(0 \le r < k)$, where $q = \lfloor \frac{n}{k} \rfloor$.

Lemma 8. *Let $G \in \chi_{n,k}$, then*

$$\begin{aligned} SO(G) &\le SO(Q_n(k)) \\ &= \binom{k-r}{2}\left\lfloor\frac{n}{k}\right\rfloor^2\sqrt{2(n-\lfloor\frac{n}{k}\rfloor)^2} \\ &+ r(k-r)\left\lfloor\frac{n}{k}\right\rfloor\left\lceil\frac{n}{k}\right\rceil\sqrt{(n-\lfloor\frac{n}{k}\rfloor)^2+(n-\lceil\frac{n}{k}\rceil)^2} \\ &+ \binom{r}{2}\left\lceil\frac{n}{k}\right\rceil^2\sqrt{2(n-\lceil\frac{n}{k}\rceil^2)}, \end{aligned}$$

where the first equality holds when $G \cong Q_n(k)$.

Proof. For any graph $G \in \chi_{n,k}$, there are k color classes, and each color class is an independent set. If the order of k classes is $n_1, n_2, \cdots, n_k$, according to Lemma 6 and by $\chi_{n,k}$, it takes the maximal Sombor index, which is the complete k-partite graph $Q_{n_1,n_2,\cdots,n_k}$. Suppose that a graph $G \in \chi_{n,k}$ takes the maximal Sombor index. We claim that G is $Q_n(k)$. On the contrary, suppose that n_p and n_q represent the size of vertices of two classes, $1 \le p < q \le k$, such that $n_q - n_p \ge 2$. Let $\sum\limits_{i}^{j} n_i = 0$ if $j < i$ for convenience. Thus, using Lemma 5, we obtain:

$$
\begin{aligned}
SO(Q_{n_1,n_2,\cdots,n_p,\cdots,n_q,\cdots,n_k}) &= \sum_{i=1}^{p-1}\sum_{j=i+1}^{k} n_i n_j \sqrt{(n-n_i)^2+(n-n_j)^2} \\
&+ \sum_{i=p+1}^{q-1}\sum_{\substack{j=i+1\\ j\neq q}}^{k} n_i n_j \sqrt{(n-n_i)^2+(n-n_j)^2} \\
&+ \sum_{i=q+1}^{k}\sum_{j=i+1}^{k} n_i n_j \sqrt{(n-n_i)^2+(n-n_j)^2} \\
&+ n_p(n-n_p)\Big(\sum_{i=1}^{p-1} \sqrt{(n-n_i)^2+(n-n_j)^2} \\
&+ \sum_{j=p+1}^{k} \sqrt{(n_j)^2+(n-n_j)^2}\Big) \\
&+ n_q(n-n_q)\Big(\sum_{i=1}^{p-1} \sqrt{n_i^2+(n-n_j)^2} \\
&+ \sum_{j=p+1}^{q-1} \sqrt{n_j^2+(n-n_j)^2} + \sum_{j=q+1}^{k} \sqrt{n_j^2+(n-n_j)^2}\Big).
\end{aligned}
$$

Let

$$
A_1 = \sum_{i=1}^{p-1}\sum_{j=i+1}^{k} n_i n_j \sqrt{(n-n_i)^2+(n-n_j)^2}, A_2 = \sum_{i=p+1}^{q-1}\sum_{\substack{j=i+1\\ j\neq q}}^{k} n_i n_j \sqrt{(n-n_i)^2+(n-n_j)^2},
$$

$$
A_3 = \sum_{i=q+1}^{k}\sum_{j=i+1}^{k} n_i n_j \sqrt{(n-n_i)^2+(n-n_j)^2}, and
$$

$$
B = \sum_{i=1}^{p-1} \sqrt{n_i^2+(n-n_i)^2} + \sum_{i=q+1}^{q-1} \sqrt{n_i^2+(n-n_i)^2} + \sum_{j=q+1}^{k} \sqrt{n_i^2+(n-n_i)^2}.
$$

Then, we have

$$
\begin{aligned}
SO(Q_{n_1,n_2,\cdots,n_p,\cdots,n_q,\cdots,n_k}) &= A_1 + A_2 + A_3 + \Big(n(n_p+n_q) - (n_p^2+n_q^2)\Big) \sum_{i=1}^{p-1} \sqrt{n_i^2+(n-n_i)^2} \\
&+ \Big(nn_p(1-p) + n_q(n-n_q)\Big) \sum_{i=p+1}^{q-1} \sqrt{n_i^2+(n-n_i)^2} \\
&+ \Big(n_p(n-n_p) + n_q(n-n_q)\Big) \sum_{j=q+1}^{k} \sqrt{n_i^2+(n-n_i)^2} \\
&+ n_p n_q (n-n_p)(n-n_q) = A_1 + A_2 + A_3 \\
&+ \Big(n(n_p+n_q) - (n_p^2+n_q^2)\Big) B + nn_p n_q (1-p)(n-n_q),
\end{aligned}
$$

$$
\begin{aligned}
SO(Q_{n_1,n_2,\cdots,n_{p+1},\cdots,n_{q-1},\cdots,n_k}) &= A_1 + A_2 + A_3 \\
&+ \Big((n_p+1)(n-n_p-1) + (n_q-1)(n-n_q+1)\Big)B \\
&+ (n_p+1)(n_q-1)(n-n_p-1)(n-n_q+1).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
SO(Q_{n_1,n_2,\cdots,n_{p+1},\cdots,n_{q-1},\cdots,n_k}) - SO(Q_{n_1,n_2,\cdots,n_p,\cdots,n_q,\cdots,n_k}) &= 2(n_q-n_p-1)B \\
&+ (n_pn_q + n_q - n_p - 1)(n-n_p-1)(n-n_q+1) \\
&- n_pn_q(n-n_p)(n-n_q) \\
&\geq n_pn_q\Big((n-n_p) - (n-n_q) - 1\Big) \\
&> n_q - n_p - 1 > 0.
\end{aligned}
$$

This contradicts the maximality of the Sombor index of G. We know that $n = r + k\lfloor \frac{n}{k} \rfloor = r\lceil \frac{n}{k} \rceil + (k-r)\lfloor \frac{n}{k} \rfloor$. Combining with Lemma 5, the values of Sombor index $SO(Q_n(k))$ can be obtained immediately. □

Lemma 9 ([26]). *Assume that $G_1 = (V, E_1)$ is the graph, $\psi(G) \leq k$. Then, there is a k-partite graph $G_2 = (V, E_2)$, and it holds that $d_{G_1}(v) \leq d_{G_2}(v)$ for $v \in V$.*

According to the above lemmas, we obtain:

Theorem 3. *Let $G \in \psi_{n,k}$. Then,*

$$
\begin{aligned}
SO(G) \leq & \binom{k-r}{2} \left\lfloor \frac{n}{k} \right\rfloor^2 \sqrt{2(n - \lfloor \frac{n}{k} \rfloor)^2} \\
& + r(k-r) \left\lfloor \frac{n}{k} \right\rfloor \left\lceil \frac{n}{k} \right\rceil \sqrt{(n - \lfloor \frac{n}{k} \rfloor)^2 + (n - \lceil \frac{n}{k} \rceil)^2} \\
& + \binom{r}{2} \left\lceil \frac{n}{k} \right\rceil^2 \sqrt{2(n - \lceil \frac{n}{k} \rceil^2)},
\end{aligned}
$$

the equality holds when $G \cong Q_n(k)$.

Proof. It is trivial that when $k = n$, then we assume that $k < n$. Assume that G from $\psi_{n,k}$ has the maximum Sombor index. Let $G \in \chi_{n,k}$. If not, from the case $\psi(G) = k$ of Lemma 9, we obtain the k-partite graph G_2 with the same set of vertices as G makes $v \in V(G) = V(G_2)$, $d_G(v) \leq d_{G_2}(v)$. Clearly, $G_2 \in \psi_{n,k}$. According to the definition, we obtain $SO(G_2) \geq SO(G)$. According to Lemma 8, this theorem holds immediately due to the uniqueness of extremal graphs in $\chi_{n,k}$. □

Theorem 4. *Let $G \in \psi_{n,k}$, then $SO(G) \geq \left(\binom{k}{2} - (k-1)\right)\sqrt{2(k-1)^2} + (k-1)$ $\sqrt{k^2+(k-1)^2} + \sqrt{k^2+4} + 2\sqrt{2}(n-k-2) + \sqrt{5}$, where equality holds when $G \cong T_k$ $((n-k)^1)$.*

Proof. Assume that the graph $G_1 \in \psi_{n,k}$ has the smallest Sombor index. Using the definition of $\psi_{n,k}$, G_1 has a subgraph Q_k, which is a complete graph. Let $V(Q_k) = \{v_1, v_2, \cdots, v_k\}$. Via Lemma 1, G_1 is a graph obtained via Q_k by connecting some trees rooted in some vertices of Q_k. From G_1, let $V_0 = \{v_i | i \in \{1, 2, \cdots, k\}, d_{G_1}(v_i) > k-1$ (i.e., there is a tree connected to v_i for any vertex $v_i \in V_0$, and vertices in V_0 are labeled as $v_1, v_2, \cdots, v_t$, with $k \geq t$.

From Lemma 9, all trees connected to some vertices of Q_k must be paths in G_1, i.e., all vertices of V_0 of G_1 have degree k. Suppose that $|V_0| = 1$. Contrary to assumption, we can find two vertices at least, such that $v_i, v_j \in V_0$. The graph $G_{v_i,v_j}(p_i, p_j)$ is denoted by G_1. However, from the graph transformation, $G_1 \cong G_{v_i,v_j}(p_i, p_j)$ is converted into $G_{v_i}(p_i + p_j)$ or $G_{v_j}(p_i + p_j)$ with a smaller Sombor index. In this way, it contradicts the choice of G_1. Hence, $G_1 \cong T_k((n-k)^1)$, and through simple calculation, we have $SO\big(T_k((n-k)^1)\big) = \left(\binom{k}{2} - (k-1)\right)\sqrt{2(k-1)^2} + (k-1)\sqrt{k^2 + (k-1)^2} + \sqrt{k^2+4} + 2\sqrt{2}(n-k-2) + \sqrt{5}$.

This theorem is proven. □

4. Conclusions

In this paper, firstly, we determine the Sombor index of the graph with a given number of cut edges and we determine the types of graphs with the largest and second largest Sombor indexes through the graph transformations I, II, and III. Secondly, we use the clique number to characterize the extremal graphs for the Sombor index, and we provide the upper and lower bounds for the index. As a result, we provide the following results in Table 1.

Table 1. Main results.

Class of Graph	Extremal Graph	Maximum or Minimum
$\mathcal{C}_{n,k}$	Q_n^k	maximum
$\chi_{n,k}$	$Q_n(k)$	maximum
$\psi_{n,k}$	$T_k((n-k)^1)$	minimum

5. Notations

We provide some symbols in Table 2 in the following.

Table 2. Notations.

Symbol	Definition
$\mathcal{C}_{n,k}$	The set of graphs having n vertices and k cut edges
Q_n^k	The graph obtained by connecting k independent vertices to one of the vertices of K_{n-k}
$\chi_{n,k}$	The set of chromatic number k of connected graphs with n vertices
$\psi_{n,k}$	The set of clique number k of connected graphs with n vertices
$Q_n(k)$	The complete k-partite graph and its partition sets differ in size by no more than 1
$T_k((n-k)^1)$	The graph in which a vertex on a complete graph K_k is connected to a pendent vertex on a path graph P_{n-k+1}
$Q_{n_1,n_2,\cdots,n_k}$	The complete k-partite graph with n vertices; the number of the partition set is $n_1, n_2, \cdots, n_k$, respectively
$G_{u,v}(p,q)$	The graph attained from G by attaching at u a path of length p and at v a path of length q
$G_v(l)$	The graph attained at v a path of length l

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