Extremal cacti with respect to Sombor index

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Abstract

Recently, a novel topological index, Sombor index, was introduced by Gutman, defined as
\[ SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}, \]
where \(d_u\) denotes the degree of vertex \(u\).

In this paper, we first determine the maximum Sombor index among cacti with \(n\) vertices and \(t\) cycles, then determine the maximum Sombor index among cacti with perfect matchings. We also characterize corresponding maximum cacti.

Keywords: Sombor index; cactus; extremal value.

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1 Introduction

In this paper, all notations and terminologies can refer to Bondy and Murty [2].

The Sombor index and reduced Sombor index are defined as [10]
\[ SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}, \]
\[ SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}. \]

Immediately after, R. Cruz et al. [5] studied the extremal Sombor index among unicyclic graphs and bicyclic graphs. The same author also [4] determined the extremal Sombor index of chemical graphs. At the same time, using different methods, Deng et al. [7] also determined molecular trees with extremal values of Sombor indices. Wang et al. [24] obtain the relations between Sombor and other degree-based indices. Liu et al. [17] ordered

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the chemical graphs by their Sombor index. Redžepović [22] studied chemical applicability of Sombor indices. Other results can be found in [1,3,6,9,11,13,18,19,21,23,25,26].

Cacti is a graph that any two cycles have at most one common vertex. Denote by \( \mathcal{H}(n, t) \), \( \mathcal{C}(2\beta, t) \), the collection of cacti with \( n \) vertices and \( t \) cycles, the collection of cacti with perfect matchings, \( 2\beta \) vertices and \( t \) cycles, respectively. There are a lot of research about topological indices of graphs with perfect matching or given matching numbers, we can refer to [8,15,16,20,25] and references cited therein.

In this paper, we first determine the maximum Sombor index among cacti \( \mathcal{H}(n, t) \), then determine the maximum Sombor index among cacti \( \mathcal{C}(2\beta, t) \). We also characterize corresponding maximum cacti.

2 Preliminaries

In the following, we give a few important lemmas which will be useful in the main results.

![Cacti](image)

Figure 1: Cacti \( \mathcal{H}(n, t) \) and \( \mathcal{H}^*(2\beta, t) \).

**Lemma 2.1** [10] Let \( G \in \mathcal{H}(n, 0) \), then \( SO(G) \leq (n - 1)\sqrt{(n - 1)^2 + 1} \), with equality iff \( G \cong \mathcal{H}(n, 0) \).

**Lemma 2.2** [15] Let \( G \in \mathcal{H}(n, 1) \), then \( SO(G) \leq (n - 3)\sqrt{(n - 1)^2 + 1} + 2\sqrt{(n - 1)^2 + 4 + 2\sqrt{2}} \), with equality iff \( G \cong \mathcal{H}(n, 1) \).

**Lemma 2.3** Let \( f_1(x) = \sqrt{x^2 + d^2} - \sqrt{x^2 + (d - r)^2} \), \( d, r \) are constants, \( 0 < r \leq d \). Then \( f_1(x) \) is a monotonically decreasing function.

**Proof.** \( f_1'(x) = \frac{x}{\sqrt{x^2 + d^2}} - \frac{x}{\sqrt{x^2 + (d - r)^2}} < 0 \). Thus \( f_1(x) \) is a monotonically decreasing function. ■
**Lemma 2.4** Let \( f_2(x) = r\sqrt{x^2 + 1^2} + (x - r)\sqrt{x^2 + 2^2} + (x - r)\sqrt{(x - r)^2 + 2^2} \) (r are constants) and \( x \geq r \), then \( f_2(x) \) is a monotonically increasing function.

**Proof.**

\[
f'_2(x) = \frac{rx}{\sqrt{x^2 + 1^2}} + \sqrt{x^2 + 4} + \frac{x(x-r)}{\sqrt{x^2 + 1^2}} + \sqrt{(x-r)^2 + 4} + \frac{(x-r)^2}{\sqrt{(x-r)^2 + 4}} > 0.
\]

Thus \( f_2(x) \) is a monotonically increasing function. \( \blacksquare \)

**Lemma 2.5** Let \( f_3(x) = x\sqrt{x^2 + 2^2} - (x - 2)\sqrt{(x - 2)^2 + 2^2} \), then \( f_3(x) \) is a monotonically increasing function.

**Proof.**

\[
f'_3(x) = \sqrt{x^2 + 2^2} - \sqrt{(x - 2)^2 + 2^2} + \frac{x^2}{\sqrt{x^2 + 2^2}} - \frac{(x-2)^2}{\sqrt{(x-2)^2 + 2^2}} > 0.
\]

Thus \( f_3(x) \) is a monotonically increasing function. \( \blacksquare \)

**Lemma 2.6** \( \{3, 25\} \) Let \( G \in C(2\beta, 0) \), then \( SO(G) \leq \sqrt{5}(\beta - 1) + \sqrt{\beta^2 + 1} + (\beta - 1)\sqrt{\beta^2 + 4} \), with equality iff \( G \cong H^*(2\beta, 0) \).

**Lemma 2.7** \( \{25\} \) Let \( G \in C(2\beta, 1) \), then \( SO(G) \leq \beta(\beta + 1)^2 + 4 + \sqrt{\beta + 1)^2 + 1 + \sqrt{5}(\beta - 1) + 2\sqrt{2} \), with equality iff \( G \cong H^*(2\beta, 1) \).

**Lemma 2.8** Let \( f(x) = (x - 1)\sqrt{x^2 + 2^2} + \sqrt{x^2 + 1^2} \) and \( g(x) = f(x) - f(x + 1) \), then \( g(x) \) \( (x \geq 1) \) is a monotonically decreasing function.

**Proof.**

\[
f'(x) = \sqrt{x^2 + 2^2} + \frac{x(x-1)}{\sqrt{x^2 + 2^2}} + \frac{x}{\sqrt{x^2 + 1^2}}; \quad f''(x) = \frac{x}{\sqrt{x^2 + 2^2}} + \frac{2x-1}{\sqrt{x^2 + 2^2}} - \frac{x^2(x-1)}{(x^2 + 2^2)^{3/2}} + \frac{1}{\sqrt{x^2 + 1^2}} - \frac{x^2}{(x^2 + 1^2)^{3/2}} + \frac{1}{(x + 1)^{3/2}} > 0 \text{ for } x \geq 1.
\]

Thus \( g(x) \) \( (x \geq 1) \) is a monotonically decreasing function. \( \blacksquare \)

3 Maximum Sombor index among cacti \( H(n, t) \)

**Theorem 3.1** Let \( G \in H(n, t) \) \( (n \geq 5) \), then

\[
SO(G) \leq (n - 2t - 1)\sqrt{(n - 1)^2 + 1} + 2t\sqrt{(n - 1)^2 + 4} + 2\sqrt{2t},
\]

with equality iff \( G \cong H(n, t) \).

**Proof.** For convenience, we denote \( Q(n, t) \triangleq (n - 2t - 1)\sqrt{(n - 1)^2 + 1} + 2t\sqrt{(n - 1)^2 + 4} + 2\sqrt{2t} \). In the following we make inductive assumptions about \( n + t \).

By Lemma 2.1 and 2.2, the conclusion holds if \( t = 1 \) or \( t = 2 \). If \( n = 5 \), the conclusion holds clearly. So we only consider \( n \geq 6 \) and \( t \geq 2 \) in the following. \( PV(G) \) denotes
the set of pendant vertices in $G$. We call the vertices connected with pendant vertices support vertices, denoted by $\text{Supp}(G)$.

**Case 1.** $PV \neq \emptyset$.

Let $v$ be a pendant vertex, $N(v) = w$, $N(w) = \{v, x_1, x_2, \ldots, x_{d-1}\}$. $d_{x_i} = 1$ for $1 \leq i \leq r - 1$, $d_{x_i} \geq 2$ for $r \leq i \leq d - 1$.

Let $G^* = G - v - x_1 - x_2 - \cdots - x_{r-1}$, then $G^* \in \mathcal{H}(n - r, t)$. By Lemma 2.3, 2.4 and 2.5, we have

$$SO(G) = SO(G^*) + r\sqrt{d^2 + 1^2} + \sum_{i=r}^{d-1} (\sqrt{d^2 + d_{x_i}^2} - \sqrt{(d-r)^2 + 1^2})$$

$$\leq Q(n, t) + r\sqrt{d^2 + 1^2} + \sum_{i=r}^{d-1} (\sqrt{d^2 + d_{x_i}^2} - \sqrt{(d-r)^2 + 1^2})$$

$$\leq Q(n, t) + 2t\sqrt{(n-r-1)^2 + 1^2} - 2t\sqrt{(n-1)^2 + 1^2} + (n-r-2t-1)\sqrt{(n-r-1)^2 + 1^2}$$

$$- (n-2t-1)\sqrt{(n-1)^2 + 1^2} + r\sqrt{d^2 + 1^2} + (d-r)(\sqrt{d^2 + 2^2} - \sqrt{(d-r)^2 + 2^2})$$

$$\leq Q(n, t) + 2t\sqrt{(n-r-1)^2 + 1^2} - 2t\sqrt{(n-1)^2 + 1^2} + (n-r-2t-1)\sqrt{(n-r-1)^2 + 1^2}$$

$$- (n-2t-1)\sqrt{(n-1)^2 + 1^2} + r\sqrt{(n-1)^2 + 1^2}$$

$$+ (n-r-1)(\sqrt{(n-1)^2 + 2^2} - \sqrt{(n-r-1)^2 + 2^2})$$

$$= Q(n, t) + (n-2t-r-1)[(\sqrt{(n-1)^2 + 2^2} - \sqrt{(n-r-1)^2 + 2^2})$$

$$- (\sqrt{(n-1)^2 + 1^2} - \sqrt{(n-r-1)^2 + 1^2})]$$

$$\leq Q(n, t),$$

with equality iff $G \cong H(n, t)$.

**Case 2.** $PV = \emptyset$.

Suppose that there exists vertices $v_0, v_1, v_2$ on a cycle of $G$, $v_0v_1, v_1v_2 \in E(G)$, $d(v_1) = d(v_2) = 2$, $d(v_0) \geq d \geq 3$. In the following, we classify the circle lengths.

**Subcase 2.1.** The circle length greater than or equal to 4.
Let $G^* = G - v_1 + v_0v_2$, then $G^* \in \mathcal{H}(n - 1, t)$.

\[
SO(G) = SO(G^*) + \sqrt{d^2 + 2^2} + \sqrt{2^2 + 2^2} - \sqrt{d^2 + 2^2} \\
\leq Q(n - 1, t) + 2\sqrt{2} \\
= Q(n, t) + 2t\sqrt{(n - 2)^2 + 2^2} - 2t\sqrt{(n - 1)^2 + 2^2} + (n - 2t - 2)\sqrt{(n - 2)^2 + 1^2} \\
- (n - 2t - 1)\sqrt{(n - 1)^2 + 1^2} + 2\sqrt{2} \\
= Q(n, t) + 2t[\sqrt{(n - 2)^2 + 2^2} - \sqrt{(n - 1)^2 + 2^2}] + (n - 2t - 2)[\sqrt{(n - 2)^2 + 1^2} \\
- \sqrt{(n - 1)^2 + 1^2}] - \sqrt{(n - 1)^2 + 1^2} + 2\sqrt{2} \\
< Q(n, t).
\]

**Subcase 2.2.** The circle length equals 3.

Let $G^* = G - v_1 - v_2$, then $G^* \in \mathcal{H}(n - 2, t - 1)$. By Lemma 2.3, 2.5 we have

\[
SO(G) = SO(G^*) + 2\sqrt{d^2 + 2^2} + \sqrt{2^2 + 2^2} + \sum_{i=1}^{d-2}(\sqrt{d^2 + d_x^2} - \sqrt{(d - 2)^2 + d_x^2}) \\
\leq Q(n - 2, t - 1) + 2\sqrt{d^2 + 2^2} + \sqrt{2^2 + 2^2} + (d - 2)(\sqrt{d^2 + 2^2} - \sqrt{(d - 2)^2 + 2^2}) \\
= Q(n, t) + (2t - 2)\sqrt{(n - 3)^2 + 2^2} - 2t\sqrt{(n - 1)^2 + 2^2} + (n - 2t - 1)\sqrt{(n - 3)^2 + 1^2} \\
- (n - 2t - 1)\sqrt{(n - 1)^2 + 1^2} + 2\sqrt{d^2 + 2^2} + (d - 2)(\sqrt{d^2 + 2^2} - \sqrt{(d - 2)^2 + 2^2}) \\
\leq Q(n, t) + (2t - 2)\sqrt{(n - 3)^2 + 2^2} - 2t\sqrt{(n - 1)^2 + 2^2} + (n - 2t - 1)\sqrt{(n - 3)^2 + 1^2} \\
- (n - 2t - 1)\sqrt{(n - 1)^2 + 1^2} + (n - 1)\sqrt{(n - 1)^2 + 2^2} - (n - 3)\sqrt{(n - 3)^2 + 2^2} \\
= Q(n, t) + (n - 2t - 1)(\sqrt{(n - 1)^2 + 2^2} - \sqrt{(n - 3)^2 + 2^2}) \\
- (\sqrt{(n - 1)^2 + 1^2} + \sqrt{(n - 3)^2 + 1^2}) \\
\leq Q(n, t),
\]

with equality iff $G \cong H(n, t)$.

This completes the proof.  

Using a similar way, for the reduced Sombor index, we also have similar result. We omit the proof.

**Theorem 3.2** Let $G \in \mathcal{H}(n, t)$ $(n \geq 5)$, then

\[
SO_{red}(G) \leq (n - 2t - 1)(n - 2) + 2t\sqrt{(n - 2)^2 + 1} + \sqrt{2}t,
\]

with equality iff $G \cong H(n, t)$.  

\[\Box\]
4 Maximum Sombor index among cacti $C(2\beta, t)$

For convenience, we denote $\Phi(\beta, t) \triangleq SO(H^*(2\beta, t)) = (\beta + t - 1)\sqrt{(\beta + t)^2 + 4} + \sqrt{(\beta + t)^2 + 1} + \sqrt{5(\beta - t - 1) + 2\sqrt{2t}}$. Note that the definition of function $g(x)$ and $f(x)$ has introduced in Lemma 2.8. Suppose $\mathcal{M}$ is a perfect matching of $G \in C(2\beta, t)$.

In the following Lemma 4.1, Lemma 4.2, and Lemma 4.3, we make inductive assumptions about $\beta + t$. By Lemma 2.6 and 2.7, these conclusions hold if $t = 1$ or $t = 0$. If $\beta = 3, t = 2$, the conclusion holds clearly. So we only consider $\beta \geq 4, t \geq 2$ in the following.

**Lemma 4.1** Let $G \in C(2\beta, t)$ ($\beta \geq 2$), $\delta(G) \geq 2$, then $SO(G) < \Phi(\beta, t)$.

**Proof.** Suppose the cycle $C = v_1v_2 \cdots v_{\lambda}v_1$ where $3 \leq d_{v_i} \triangleq d \leq \beta + t$, $d_{v_i} = 2$ for $i = 2, 3, \cdots, \lambda$. $N(v_1) = \{v_2, v_\lambda, x_1, x_2, \cdots, x_{d-2}\}$. Let $G^* = G - v_1v_2$, then $G^* \in C(2\beta, t - 1)$, and $SO(G^*) \leq \Phi(\beta, t - 1)$. By Lemma 2.3 and 2.8, we have

$$SO(G) = SO(G^*) + \sqrt{d^2 + 2^2} + (\sqrt{2^2 + 2^2 - \sqrt{2^2 + 1^2}}) + \sum_{i=1}^{d-1}(\sqrt{d^2 + d_{v_i}^2} - \sqrt{(d - 1)^2 + d_{v_i}^2})$$

$$\leq \Phi(\beta, t) + (\beta + t - 2)\sqrt{(\beta + t - 1)^2 + 2^2} + \sqrt{(\beta + t - 1)^2 + 1^2}$$

$$- (\beta + t - 1)\sqrt{(\beta + t)^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} + t\sqrt{t^2 + 2^2} - (t - 1)\sqrt{(t - 1)^2 + 2^2}$$

$$= \Phi(\beta, t) + g(\beta + t - 1) - g(d - 1) + [(\sqrt{t^2 + 2^2} - \sqrt{(t - 1)^2 + 2^2})$$

$$- (\sqrt{t^2 + 1^2} - \sqrt{(t - 1)^2 + 1^2})]$$

$$< \Phi(\beta, t),$$

This completes the proof.

The support vertices are the vertices connected with pendant vertices.

**Lemma 4.2** Let $G \in C(2\beta, t)$ ($\beta \geq 2$), $\delta(G) = 1$ and there exists a support vertex $u$ with degree 2 of the corresponding pendant vertex $v$, then $SO(G) \leq \Phi(\beta, t)$, with equality iff $G \cong H^*(2\beta, t)$.

**Proof.** Let $N(u) = \{v, w\}$, $N(w) = \{u, x_1, x_2, \cdots, x_r, x_{r+1}, \cdots, x_{d-1}\}$. $d_{x_i} = 1$ for $1 \leq i \leq r$, $d_{x_i} \geq 2$ for $r + 1 \leq i \leq d - 1$. For convenience, denote $d_w = d$. Let $G^* = G - v - u$, 

then \( G^* \in \mathcal{C}(2\beta - 2, t) \). By Lemma 2.3 and 2.8, we have

\[
SO(G) = SO(G^*) + \sum_{i=r+1}^{d-1} (\sqrt{d^2 + d_i^2} - \sqrt{(d - 1)^2 + d_i^2}) \\
+ r(\sqrt{d^2 + 1^2} - \sqrt{(d - 1)^2 + 1^2}) + \sqrt{d^2 + 2^2} + \sqrt{2^2 + 1^2} \\
\leq \Phi(\beta - 1, t) + (d - r - 1)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) \\
+ r(\sqrt{d^2 + 1^2} - \sqrt{(d - 1)^2 + 1^2}) + \sqrt{d^2 + 2^2} + \sqrt{2^2 + 1^2} \\
= \Phi(\beta, t) + (\beta + t - 2)(\beta + t - 1)^2 + 2^2 + \sqrt{(\beta + t - 1)^2 + 1^2} \\
- (\beta - 1)(\beta + t - 1)^2 + 2^2 - \sqrt{(\beta + t)^2 + 1^2} \\
+ (d - r - 1)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) \\
+ r(\sqrt{d^2 + 1^2} - \sqrt{(d - 1)^2 + 1^2}) + \sqrt{d^2 + 2^2} \\
= \Phi(\beta, t) + g(\beta + t - 1) + r(\sqrt{d^2 + 1^2} - \sqrt{(d - 1)^2 + 1^2}) \\
+ (d - r - 1)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) + \sqrt{d^2 + 2^2}.
\]

Since \( G \in \mathcal{C}(2\beta, t) \), then \( r \leq 1 \). We consider the following two cases.

**Case 1.** \( r = 0 \).

\[
SO(G) \leq \Phi(\beta, t) + g(\beta + t - 1) + (d - 1)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) + \sqrt{d^2 + 2^2} \\
= \Phi(\beta, t) + g(\beta + t - 1) - g(d - 1) + [(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) \\
- (\sqrt{d^2 + 1^2} - \sqrt{(d - 1)^2 + 1^2})] \\
< \Phi(\beta, t).
\]

**Case 2.** \( r = 1 \).

\[
SO(G) \leq \Phi(\beta, t) + g(\beta + t - 1) + (\sqrt{d^2 + 1^2} - \sqrt{(d - 1)^2 + 1^2}) \\
+ (d - 2)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) + \sqrt{d^2 + 2^2} \\
= \Phi(\beta, t) + g(\beta + t - 1) - g(d - 1) \\
\leq \Phi(\beta, t),
\]

with equality iff \( G \cong H^*(2\beta, t) \).

This completes the proof.  

\[\square\]

**Lemma 4.3** Let \( G \in \mathcal{C}(2\beta, t) \) \( (\beta \geq 2) \), \( \delta(G) = 1 \) and the degrees of all support vertices are at least 3, then \( SO(G) \leq \Phi(\beta, t) \), with equality iff \( G \cong H^*(2\beta, t) \).
Proof. Suppose that $\mathcal{C} = v_1v_2 \cdots v_\lambda v_1$ is such a cycle that $v_i(2 \leq i \leq \lambda)$ does not on other cycles of $G$, i.e., $d_{v_i} = 2$ or $3$ for $2 \leq i \leq \lambda$. $3 \leq d_{v_1} \neq d \leq \beta + t$. Without loss of generality, suppose $v_1v_2 \notin \mathcal{M}$. In the following, we classify the circle lengths.

**Case 1.** The circle length equals $3$.

Let $N(v_1) = \{v_2, v_3, x_1, x_2, \cdots, x_r, x_{r+1}, \cdots, x_{d-2}\}$ where $r = 0$ or $1$, $d_{x_i} = 1$ for $1 \leq i \leq r$, $d_{x_i} \geq 2$ for $r + 1 \leq i \leq d - 2$.

**Subcase 1.1.** $d_{v_2} = d_{v_3} = 2$.

Let $G^* = G - v_2 - v_3$, then $G^* \in C(2\beta - 2, t - 1)$, $SO(G^*) \leq \Phi(\beta - 1, t - 1)$.

\[
SO(G) = SO(G^*) + \sum_{i=r+1}^{d-2} \left( \sqrt{d^2 + d_{x_i}^2} - \sqrt{(d - 2)^2 + d_{x_i}^2} \right) + r(\sqrt{d^2 + 1^2} - \sqrt{(d - 2)^2 + 1^2})
+ 2\sqrt{d^2 + 2^2} + \sqrt{2^2 + 2^2}
\leq \Phi(\beta, t) + (\beta + t - 3)\sqrt{(\beta + t - 2)^2 + 2^2} + \sqrt{(\beta + t - 2)^2 + 1^2}
- (\beta + t - 1)\sqrt{(\beta + t)^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} + \sum_{i=r+1}^{d-2} \left( \sqrt{d^2 + d_{x_i}^2} - \sqrt{(d - 2)^2 + d_{x_i}^2} \right)
+ r(\sqrt{d^2 + 1^2} - \sqrt{(d - 2)^2 + 1^2}) + 2\sqrt{d^2 + 2^2}.
\]

**Subcase 1.11.** $r = 0$.

By Lemma 2.3 and 2.8, we have

\[
SO(G) \leq \Phi(\beta, t) + (\beta + t - 3)\sqrt{(\beta + t - 2)^2 + 2^2} + \sqrt{(\beta + t - 2)^2 + 1^2}
- (\beta + t - 1)\sqrt{(\beta + t)^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2}
+ (d - 2)(\sqrt{d^2 + 2^2} - \sqrt{(d - 2)^2 + 2^2}) + 2\sqrt{d^2 + 2^2}
= \Phi(\beta, t) + [f(\beta + t - 2) - f(\beta + t)] - [f(d - 2) - f(d)]
+ [(\sqrt{d^2 + 2^2} - \sqrt{(d - 2)^2 + 2^2}) - (\sqrt{d^2 + 1^2} - \sqrt{(d - 2)^2 + 1^2})]
< \Phi(\beta, t) + [g(\beta + t - 2) + g(\beta + t - 1)] - [g(d - 2) + g(d - 1)]
= \Phi(\beta, t) + [g(\beta + t - 2) - g(d - 2)] + [g(\beta + t - 1) - g(d - 1)]
\leq \Phi(\beta, t).
\]

**Subcase 1.12.** $r = 1$.
By Lemma 2.3 and 2.8, we have

\[
SO(G) \leq \Phi(\beta, t) + (\beta + t - 3)\sqrt{(\beta + t - 2)^2 + 2^2} + \sqrt{(\beta + t - 2)^2 + 1^2} \\
- (\beta + t - 1)\sqrt{(\beta + t)^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} + (\sqrt{d^2 + 1^2} - \sqrt{(d - 2)^2 + 1^2}) \\
+ (d - 3)(\sqrt{d^2 + 2^2} - \sqrt{(d - 2)^2 + 2^2}) + 2\sqrt{d^2 + 2^2} \\
= \Phi(\beta, t) + [f(\beta + t - 2) - f(\beta + t)] - [f(d - 2) - f(d)] \\
= \Phi(\beta, t) + [g(\beta + t - 2) + g(\beta + t - 1)] - [g(d - 2) + g(d - 1)] \\
= \Phi(\beta, t) + [g(\beta + t - 2) - g(d - 2)] + [g(\beta + t - 1) - g(d - 1)] \\
\leq \Phi(\beta, t),
\]

with equality iff \( G \cong H^*(2\beta, t) \).

Subcase 1.2. \( d_{v_2} = d_{v_3} = 3 \).

Let \( N(v_2) = \{v_1, v_3, v'_2\} \) and \( N(v_3) = \{v_1, v_2, v'_3\} \). Let \( G^* = G - v'_2 - v'_3 \), then \( G^* \in C(2\beta - 2, t) \), \( SO(G^*) \leq \Phi(\beta - 1, t) \). Note that \( \beta \geq 4, t \geq 2 \).

\[
SO(G) = SO(G^*) + 2(\sqrt{d^2 + 3^2} - \sqrt{d^2 + 2^2}) + \sqrt{3^2 + 3^2} + 2\sqrt{3^2 + 1^2} - \sqrt{2^2 + 2^2} \\
\leq \Phi(\beta - 1, t) + 2(\sqrt{d^2 + 3^2} - \sqrt{d^2 + 2^2}) + 2\sqrt{10} + \sqrt{2} \\
= \Phi(\beta, t) + g(\beta + t - 1) + 2(\sqrt{d^2 + 3^2} - \sqrt{d^2 + 2^2}) - \sqrt{5} + 2\sqrt{10} + \sqrt{2} \\
\leq \Phi(\beta, t) + g(5) + 2(\sqrt{3^2 + 3^2} - \sqrt{3^2 + 2^2}) - \sqrt{5} + 2\sqrt{10} + \sqrt{2} \\
= \Phi(\beta, t) + 4\sqrt{5^2 + 2^2} + \sqrt{5^2 + 1^2} - 5\sqrt{6^2 + 2^2} - \sqrt{6^2 + 1^2} \\
+ 2(\sqrt{3^2 + 3^2} - \sqrt{3^2 + 2^2}) - \sqrt{5} + 2\sqrt{10} + \sqrt{2} \\
< \Phi(\beta, t).
\]

Subcase 1.3. \( d_{v_2} = 2, d_{v_3} = 3 \).

Let \( N(v_3) = \{v_1, v_2, v'_3\} \) and \( N(v_1) = \{v_2, v_3, x_1, x_2, \cdots, x_{d-2}\} \). Let \( G^* = G - v_3 - v'_3 \),

\[
SO(G) \leq \Phi(\beta, t) + (\beta + t - 3)\sqrt{(\beta + t - 2)^2 + 2^2} + \sqrt{(\beta + t - 2)^2 + 1^2} \\
- (\beta + t - 1)\sqrt{(\beta + t)^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} + (\sqrt{d^2 + 1^2} - \sqrt{(d - 2)^2 + 1^2}) \\
+ (d - 3)(\sqrt{d^2 + 2^2} - \sqrt{(d - 2)^2 + 2^2}) + 2\sqrt{d^2 + 2^2} \\
= \Phi(\beta, t) + [f(\beta + t - 2) - f(\beta + t)] - [f(d - 2) - f(d)] \\
= \Phi(\beta, t) + [g(\beta + t - 2) + g(\beta + t - 1)] - [g(d - 2) + g(d - 1)] \\
= \Phi(\beta, t) + [g(\beta + t - 2) - g(d - 2)] + [g(\beta + t - 1) - g(d - 1)] \\
\leq \Phi(\beta, t),
\]

with equality iff \( G \cong H^*(2\beta, t) \).
then $G^* \in \mathcal{C}(2\beta - 2, t - 1)$, $SO(G^*) \leq \Phi(\beta - 1, t - 1)$.

$$SO(G) = SO(G^*) + \sum_{i=1}^{d-2} (\sqrt{d^2 + d_{x_i}^2} - \sqrt{(d - 1)^2 + d_{x_i}^2}) + \sqrt{d^2 + 3^2} + \sqrt{d^2 + 2^2}$$

$$+ \sqrt{2^2 + 3^2} + \sqrt{1^2 + 3^2} - \sqrt{(d - 1)^2 + 1^2}$$

$$\leq \Phi(\beta - 1, t - 1) + (d - 2)(\sqrt{\beta^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2}) + \sqrt{d^2 + 3^2} + \sqrt{d^2 + 2^2}$$

$$+ \sqrt{2^2 + 3^2} + \sqrt{1^2 + 3^2} - \sqrt{(d - 1)^2 + 1^2}$$

$$\leq \Phi(\beta, t) + (\beta + t - 3)\sqrt{(\beta + t - 2)^2 + 2^2} + \sqrt{(\beta + t - 2)^2 + 1^2}$$

$$- (\beta + t - 1)\sqrt{(\beta + t)^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} + (d - 2)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2})$$

$$+ \sqrt{d^2 + 3^2} + \sqrt{d^2 + 2^2} + \sqrt{1^2 + 10 - 2\sqrt{2}} - \sqrt{(d - 1)^2 + 1^2}$$

$$= \Phi(\beta, t) + [f(\beta + t - 2) - f(\beta + t)] + (d - 2)(\sqrt{d^2 + 2^2} - \sqrt{(d - 1)^2 + 2^2})$$

$$+ \sqrt{d^2 + 3^2} + \sqrt{d^2 + 2^2} + \sqrt{1^2 + 10 - 2\sqrt{2}} - \sqrt{(d - 1)^2 + 1^2}$$

$$= \Phi(\beta, t) + [f(\beta + t - 2) - f(\beta + t)] - [f(d - 1) - f(d)]$$

$$+ \sqrt{d^2 + 3^2} - \sqrt{d^2 + 1^2} + \sqrt{1^2 + 10 - 2\sqrt{2}}$$

$$= \Phi(\beta, t) + [f(\beta + t - 1) - f(\beta + t)] - [f(d - 1) - f(d)] + [f(\beta + t - 2) - f(\beta + t - 1)]$$

$$+ \sqrt{d^2 + 3^2} - \sqrt{d^2 + 1^2} + \sqrt{1^2 + 10 - 2\sqrt{2}}$$

$$= \Phi(\beta, t) + [g(\beta + t - 1) - g(d - 1)] + g(\beta + t - 2)$$

$$+ \sqrt{d^2 + 3^2} - \sqrt{d^2 + 1^2} + \sqrt{1^2 + 10 - 2\sqrt{2}}$$

$$\leq \Phi(\beta, t) + g(\beta + t - 2) + \sqrt{d^2 + 3^2} - \sqrt{d^2 + 1^2} + \sqrt{1^2 + 10 - 2\sqrt{2}}.$$

If $d \geq 3$, then

$$SO(G) \leq \Phi(\beta, t) + g(4) + \sqrt{3^2 + 3^2} - \sqrt{3^2 + 1^2} + \sqrt{1^2 + 10 - 2\sqrt{2}}$$

$$= \Phi(\beta, t) + 3\sqrt{4^2 + 2^2} + \sqrt{4^2 + 2^2} - 4\sqrt{3^2 + 2^2} - \sqrt{5^2 + 1^2}$$

$$+ \sqrt{3^2 + 3^2} - \sqrt{3^2 + 1^2} + \sqrt{1^2 + 10 - 2\sqrt{2}}$$

$$< \Phi(\beta, t).$$

If $d = 2$, then $\beta = 2$ and $t = 1$. Thus $G \cong H^*(4, 1)$.

**Case 2.** The circle length greater than or equal to 4.

**Subcase 2.1.** $d_{v_2} = 3$.

Let $N(v_2) = \{v_1, v_3, v_2\}$, then $d_{v_3} = 2$ or 3.
Let $G^* = G - v_2 - v'_2 + v_1v_3$, then $G^* \in C(2\beta - 2, t)$, $SO(G^*) \leq \Phi(\beta - 1, t)$.

$$SO(G) = SO(G^*) + \sqrt{d^2 + 3^2} + \sqrt{3^2 + 1^2} + \sqrt{3^2 + d^2_{v_3}} - \sqrt{d^2 + d^2_{v_3}}$$

$$\leq \Phi(\beta - 1, t) + \sqrt{d^2 + 3^2} + \sqrt{3^2 + 1^2} + \sqrt{3^2 + d^2_{v_3}} - \sqrt{d^2 + d^2_{v_3}}$$

$$= \Phi(\beta, t) + (\beta - 2)\sqrt{(\beta + t - 1)^2 + 2^2} + \sqrt{(\beta + t - 1)^2 + 1^2}$$

$$- (\beta + t - 1)\sqrt{(\beta + t )^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} - \sqrt{5}$$

$$+ \sqrt{d^2 + 3^2} + \sqrt{3^2 + 1^2} + \sqrt{3^2 + d^2_{v_3}} - \sqrt{d^2 + d^2_{v_3}}.$$

**Subcase 2.11. $d_{v_3} = 2$.**

$$SO(G) \leq \Phi(\beta, t) + (\beta - 2)\sqrt{(\beta + t - 1)^2 + 2^2} + \sqrt{(\beta + t - 1)^2 + 1^2}$$

$$- (\beta + t - 1)\sqrt{(\beta + t )^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} - \sqrt{5}$$

$$+ \sqrt{d^2 + 3^2} - \sqrt{d^2 + 2^2} + \sqrt{10} + \sqrt{13}$$

$$\leq \Phi(\beta, t) + g(\beta + t - 1) + 3\sqrt{2} + \sqrt{10} - \sqrt{5}$$

$$\leq \Phi(\beta, t) + g(5) + 3\sqrt{2} + \sqrt{10} - \sqrt{5}$$

$$= \Phi(\beta, t) + 4\sqrt{29} + \sqrt{26} - 5\sqrt{40} - \sqrt{37} + 3\sqrt{2} + \sqrt{10} - \sqrt{5}$$

$$< \Phi(\beta, t).$$

**Subcase 2.12. $d_{v_3} = 3$.**

$$SO(G) \leq \Phi(\beta, t) + (\beta - 2)\sqrt{(\beta + t - 1)^2 + 2^2} + \sqrt{(\beta + t - 1)^2 + 1^2}$$

$$- (\beta + t - 1)\sqrt{(\beta + t )^2 + 2^2} - \sqrt{(\beta + t)^2 + 1^2} - \sqrt{5} + \sqrt{10} + 3\sqrt{2}$$

$$\leq \Phi(\beta, t) + g(\beta + t - 1) + 3\sqrt{2} + \sqrt{10} - \sqrt{5}$$

$$\leq \Phi(\beta, t) + g(5) + 3\sqrt{2} + \sqrt{10} - \sqrt{5}$$

$$= \Phi(\beta, t) + 4\sqrt{29} + \sqrt{26} - 5\sqrt{40} - \sqrt{37} + 3\sqrt{2} + \sqrt{10} - \sqrt{5}$$

$$< \Phi(\beta, t).$$

**Subcase 2.2. $d_{v_2} = 2$.**

Since $v_1v_2 \notin \mathcal{M}$, then $v_2v_3 \in \mathcal{M}$, so $d_{v_3} = 2$.

Let $G^* = G - v_3v_4 + v_2v_4$, then $G^* \in C(2\beta, t)$.

$$SO(G) = SO(G^*) + \sqrt{d^2 + 2^2} - \sqrt{d^2 + 3^2} + \sqrt{2^2 + 2^2} + \sqrt{d^2_{v_4} + 2^2} - \sqrt{1^2 + 3^2} - \sqrt{d^2_{v_4} + 3^2}$$

$$\leq SO(G^*) + \sqrt{d^2 + 2^2} - \sqrt{d^2 + 3^2} + 4\sqrt{2} - \sqrt{10} - \sqrt{13}$$

$$< SO(G^*) + 4\sqrt{2} - \sqrt{10} - \sqrt{13}$$

$$< SO(G^*).$$
When \( \lambda - 1 = 3 \), by Case 1, we know \( SO(G^*) \leq \Phi(\beta, t) \); When \( \lambda - 1 \geq 4 \), by Case 2.1, we know \( SO(G^*) < \Phi(\beta, t) \). Thus we have \( SO(G) < \Phi(\beta, t) \).

This completes the proof. ■

By Lemma 4.1, 4.2 and 4.3, we can obtain the maximum Sombor index among cacti \( C(2\beta, t) \).

**Theorem 4.4** Let \( G \in C(2\beta, t) \) \((\beta \geq 2)\), then \( SO(G) \leq \Phi(\beta, t) \), with equality iff \( G \cong H^*(2\beta, t) \).

Using a similar way, for the reduced Sombor index, we also have similar result. We omit the proof.

**Theorem 4.5** Let \( G \in C(2\beta, t) \) \((\beta \geq 2)\), then \( SO_{\text{red}}(G) \leq SO_{\text{red}}(H^*(2\beta, t)) \), with equality iff \( G \cong H^*(2\beta, t) \).

**References**

[1] S. Alikhani, N. Ghanbari, Sombor index of polymers, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 715–728.

[2] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, New York, 2008.

[3] H. Chen, W. Li, J. Wang, Extremal values on the Sombor index of trees, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 23–49.

[4] R. Cruz, I. Gutman, J. Rada, Sombor index of chemical graphs, *Appl. Math. Comput.* **399** (2021) #126018.

[5] R. Cruz, J. Rada, Extremal values of the Sombor index in unicyclic and bicyclic graphs, *J. Math. Chem.* **59** (2021) 1098–1116.

[6] K. C. Das, A. S. Cevik, I. N. Cangul, Y. Shang, On Sombor index, *Symmetry* **13** (2021) #140.

[7] H. Deng, Z. Tang, R. Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum. Chem.* **121** (2021) #e26622.
[8] Z. Du, B. Zhou, N. Trinajstić, Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number, J. Math. Chem. 47 (2010) 842–855.

[9] X. Fang, L. You, H. Liu, The expected values of Sombor indices in random hexagonal chains, phenylene chains and Sombor indices of some chemical graphs, Int. J. Quantum. Chem. 121 (2021) #e26740.

[10] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, MATCH Commun. Math. Comput. Chem. 86 (2021) 11–16.

[11] I. Gutman, Some basic properties of Sombor indices, Open J. Discret. Appl. Math. 4 (2021) 1–3.

[12] Y. Huang, H. Liu, Bounds of modified Sombor index, spectral radius and energy, AIMS Mathematics 6 (2021) 11263–11274.

[13] B. Horoldagva, C. Xu, On Sombor index of graphs, MATCH Commun. Math. Comput. Chem. 86 (2021) 703–713.

[14] X. Li, Z. Wang, Trees with extremal spectral radius of weighted adjacency matrices among trees weighted by degree-based indices, Linear Algebra Appl. 620 (2021) 61–75.

[15] H. Liu, H. Deng, Z. Tang, Minimum Szeged index among unicyclic graphs with perfect matchings, J. Comb. Optim. 38 (2019) 443-455.

[16] H. Liu, Z. Tang, The hyper-Zagreb index of cacti with perfect matchings, AKCE Int. J. Graph Combin. 17 (2020) 422-428.

[17] H. Liu, L. You, Y. Huang, Ordering chemical graphs by Sombor indices and its applications, MATCH Commun. Math. Comput. Chem. 87 (2022) 5–22.

[18] H. Liu, L. You, Y. Huang, X. Fang, Spectral properties of p-Sombor matrices and beyond, MATCH Commun. Math. Comput. Chem. 87 (2022) 59–87.

[19] H. Liu, L. You, Z. Tang, J. B. Liu, On the reduced Sombor index and its applications, MATCH Commun. Math. Comput. Chem. 86 (2021) 729–753.

[20] F. Ma, H. Deng, On the sum-connectivity index of cacti, Math. Comput. Model. 54 (2011) 497–507.
[21] I. Milovanović, E. Milovanović, M. Matejić, On some mathematical properties of Sombor indices, *Bull. Int. Math. Virtual Inst.* **11** (2021) 341–353.

[22] I. Redžepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.* **86** (2021) 445–457.

[23] T. Réti, T. Došlić, A. Ali, On the Sombor index of graphs, * Contrib. Math.* **3** (2021) 11–18.

[24] Z. Wang, Y. Mao, Y. Li, B. Furtula, On relations between Sombor and other degree-based indices, *J. Appl. Math. Comput.* (2021) doi:10.1007/s12190-021-01516-x.

[25] T. Zhou, Z. Lin, L. Miao, The Sombor index of trees and unicyclic graphs with given matching number, [arXiv:2103.04645v1](https://arxiv.org/abs/2103.04645).

[26] W. Zhang, L. You, H. Liu, Y. Huang, The expected values and variances for Sombor indices in a general random chain, *Appl. Math. Comput.* **411** (2021) #126521.