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On the Steiner (Revised) Szeged Index

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Abstract

The kth Steiner (revised) Szeged index is defined from Steiner distance, in order to generalize the (revised) Szeged index. In this paper, we obtain some upper and lower bounds on the kth Steiner (revised) Szeged index of graphs. Then we give Nordhaus-Gaddum-type results of the kth Steiner (revised) Szeged index of graphs. Moreover, we determine a formula on $rSz_k(G)$ for trees in general, and present a lower bound on the third Steiner Szeged index for trees of order n and characterize the graphs which attained the bound. Finally, we prove that the path P_n gives the maximum value of the third Steiner Szeged index among the star-like trees of order $n \geq 10$.

1 Introduction

All graphs considered in this paper are simple, finite and undirected. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The *degree* of a vertex v in G, denoted by $d_G(v)$, is equal to $|N_G(v)|$, where $N_G(v) = \{u : uv \in E(G)\}$. For $u, v \in V(G)$, $d(u, v)$ denotes the distance between vertices u and v. The *Wiener index* of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V} d(u, v).$$

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This topological index has been extensively studied in the mathematical literature [9,10]. Let $e = uv$ be an edge of G, and define three sets as follows:

$$N_u(e) = \Big\{w \in V(G) : d(u,w) < d(v,w)\Big\},$$
$$N_v(e) = \Big\{w \in V(G) : d(v,w) < d(u,w)\Big\},$$
$$N_0(e) = \Big\{w \in V(G) : d(u,w) = d(v,w)\Big\}.$$

Thus, $\Big\{N_u(e), N_v(e), N_0(e)\Big\}$ is a partition of the vertices of G with respect to e. The number of vertices in $N_u(e), N_v(e)$ and $N_0(e)$ are denoted by $n_u(e), n_v(e)$ and $n_0(e)$, respectively. A long time known property of the Wiener index is the formula [21]:

$$W(G) = \sum_{e=uv} n_u(e)n_v(e),$$

which is applicable for trees. Using the above formula, Gutman [8] introduced a graph invariant named the *Szeged index* as an extention of the Wiener index and defined it by

$$Sz(G) = \sum_{e=uv} n_u(e)n_v(e).$$

Randić [19] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named the *revised Szeged index*. The *revised Szeged index* of a connected graph G is defined as

$$rSz(G) = \sum_{e=uv} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right).$$

Some properties and applications of the Szeged index and the revised Szeged index have been reported in [2,6,11,17,18,20,22].

The *Steiner distance* $d_G(S)$ of a set S of vertices in a connected graph G is the minimum size among all connected subgraphs of G containing S. That is, $d_G(S) = \min\Big\{|E(T)|,\ S \subseteq V(T)\Big\}$, where T is a subtree of G. In [12], Li et al. proposed a generalization of the concept of Wiener index, using Steiner distance. The *kth Steiner Wiener index* $SW_k(G)$ of a connected graph G is defined by

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S| = k}} d_G(S).$$

Let $e = uv$ be an edge of graph G. For an integer $k\,(2 \le k \le |V(G)| - 1)$, we can similarly construct three distinct kinds of $(k-1)$-subsets of $V(G)$ as follows:

$$N_u(e;k) = \Big\{S \subseteq V(G), |S| = k-1 : d_G(S \cup \{u\}) < d_G(S \cup \{v\}), u, v \notin S\Big\},$$

$$N_v(e;k) = \Big\{S \subseteq V(G), |S| = k-1 : d_G(S \cup \{v\}) < d_G(S \cup \{u\}), u, v \notin S\Big\},$$

$$N_0(e;k) = \Big\{S \subseteq V(G), |S| = k-1 : d_G(S \cup \{u\}) = d_G(S \cup \{v\}), u, v \notin S\Big\}.$$

The cardinality of $N_u(e;k), N_v(e;k)$ and $N_0(e;k)$ are denoted by $n_u(e;k), n_v(e;k)$ and $n_0(e;k)$, respectively. Evidently, if n is the number of vertices of the graph G, then

$$n_u(e;k) + n_v(e;k) + n_0(e;k) = \binom{n-2}{k-1}.$$

As a natural counterpart of the generalized (revised) Szeged index, Ghorbani et al. introduced the concept of the Steiner (revised) Szeged index in [7]. Then the *kth Steiner Szeged index $Sz_k(G)$* and the *kth Steiner revised Szeged index $rSz_k(G)$* of a graph G are defined as

$$Sz_k(G) = \sum_{e=uv} \Big(n_u(e;k) + 1\Big)\Big(n_v(e;k) + 1\Big)$$

and

$$rSz_k(G) = \sum_{e=uv} \left(n_u(e;k) + \frac{n_0(e;k)}{2} + 1\right)\left(n_v(e;k) + \frac{n_0(e;k)}{2} + 1\right),$$

respectively. If $k = 2$, then $Sz_2(G) = Sz(G)$ and $rSz_2(G) = rSz(G)$.

The results on the Steiner Wiener index, Steiner degree distance, Steiner Gutman index and the kth Steiner (revised) Szeged index are very limited, some basic results can be found in [1, 5, 7, 12–16]. We denote by S_n and P_n, the star and path on n vertices, respectively, throughout this paper. By $S(n_1, n_2, \ldots, n_q)$ we denote the starlike tree which has a vertex v_1 of degree $q \geq 3$ and which has the property

$$S(n_1, n_2, \ldots, n_q) - v_1 = P_{n_1} \cup P_{n_2} \cup \ldots \cup P_{n_q}.$$

This tree has $n_1 + n_2 + \cdots + n_q + 1 = n$ vertices. Clearly, the parameters $n_1, n_2, \ldots, n_q$ determine the starlike tree up to isomorphism. In what follows, it will be assumed that $n_1 \geq n_2 \geq \cdots \geq n_q \geq 1$. We say that the starlike tree $S(n_1, n_2, \ldots, n_q)$ has q branches, the lengths of which are $n_1, n_2, \ldots, n_q$ respectively. In particular, $S(\underbrace{1, 1, \ldots, 1}_{n-1}) \cong S_n$ and $S(\underbrace{n - n_2 - 1, n_2, 0, \ldots, 0}_{q}) \cong P_n$. Other undefined notations and terminology on the graph theory can be found in [3].

The rest of this paper is organized as follows. We give some upper and lower bounds on $Sz_k(G)$ and $rSz_k(G)$ in Section 2. In Section 3, we obtain Nordhaus-Gaddum-type results on $rSz_k(G) + rSz_k(\overline{G})$. In Section 4, we determine a formula on $rSz_k(G)$ for trees in general and give a lower bound on $Sz_3(T)$ in terms of n for any tree T and characterize the graphs which attained the bound. Finally, we prove that the path P_n gives the maximum value of Sz_3 among the star-like trees of order $n \geq 10$. In Section 5, we add concluding remarks and future work.

2 Upper and lower bounds on the Steiner (revised) Szeged index

In this section we give some upper and lower bounds on the Steiner (revised) Szeged index of graphs. We begin this section with a definition that is used in our later proofs. Let $e = uv$ be an edge of G, we define

$$D(u|e) = \sum_{\substack{S \subseteq V(G) \\ |S| = k-1 \\ u,v \notin S}} d_G(S \cup \{u\}).$$

Lemma 1. *Let G be a connected graph and $e = uv$ be an edge of G. Then $n_u(e;k) = n_v(e;k)$ if and only if $D(u|e) = D(v|e)$.*

Proof. Consider all the $(k-1)$-subsets of $V(G)\backslash\{u,v\}$. Let

$$N_u(e;k) = \{S_1, S_2, \ldots, S_p\}, N_v(e;k) = \{T_1, T_2, \ldots, T_q\}, N_0(e;k) = \{R_1, R_2, \ldots, R_r\}.$$

Now,

$$\begin{aligned}
D(u|e) =& \sum_{\substack{S \subseteq V(G) \\ |S| = k-1 \\ u,v \notin S}} d_G(S \cup \{u\}) \\
=& \sum_{i=1}^{p} d_G(S_i \cup \{u\}) + \sum_{i=1}^{q} d_G(T_i \cup \{u\}) + \sum_{i=1}^{r} d_G(R_i \cup \{u\}) \\
=& \sum_{i=1}^{p} d_G(S_i \cup \{u\}) + \sum_{i=1}^{q} \Big[d_G(T_i \cup \{v\}) + 1\Big] + \sum_{i=1}^{r} d_G(R_i \cup \{u\}) \\
=& q + \sum_{i=1}^{p} d_G(S_i \cup \{u\}) + \sum_{i=1}^{q} d_G(T_i \cup \{v\}) + \sum_{i=1}^{r} d_G(R_i \cup \{u\}).
\end{aligned}$$

Similarly, we obtain

$$D(v|e) = p + \sum_{i=1}^{p} d_G(S_i \cup \{u\}) + \sum_{i=1}^{q} d_G(T_i \cup \{v\}) + \sum_{i=1}^{r} d_G(R_i \cup \{v\}).$$

Since $d_G(R_i \cup \{u\}) = d_G(R_i \cup \{v\})$ $(i = 1, \ldots, r)$, from the above results, we obtain

$$D(u|e) - D(v|e) = q - p = n_v(e;k) - n_u(e;k)$$

and the result follows. ∎

Now, we give an upper bound of $rSz_k(G)$ and $Sz_k(G)$ in terms of n and m.

Theorem 1. *Let G be a connected graph of order n and size m. Then*

$$rSz_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1}+2\right]^2$$

with equality holding if and only if $D(u|e) = D(v|e)$ for every edge $e = uv$ in G.

Proof. Since $n_0(e;k) = \binom{n-2}{k-1} - n_u(e;k) - n_v(e;k)$, we have

$$\begin{aligned}
rSz_k(G) &= \sum_{e=uv}\left(n_u(e;k)+\frac{n_0(e;k)}{2}+1\right)\left(n_v(e;k)+\frac{n_0(e;k)}{2}+1\right)\\
&= \sum_{e=uv}\left(\frac{\binom{n-2}{k-1}+n_u(e;k)-n_v(e;k)+2}{2}\right)\left(\frac{\binom{n-2}{k-1}-n_u(e;k)+n_v(e;k)+2}{2}\right)\\
&= \frac{1}{4}\sum_{e=uv}\left[\left(\binom{n-2}{k-1}+2\right)^2-\left(n_u(e;k)-n_v(e;k)\right)^2\right]\\
&= \frac{m}{4}\left[\binom{n-2}{k-1}+2\right]^2-\frac{1}{4}\sum_{e=uv}\left(n_u(e;k)-n_v(e;k)\right)^2 \leq \frac{m}{4}\left[\binom{n-2}{k-1}+2\right]^2.
\end{aligned}$$

Moreover, the equality holds if and only if $n_u(e;k) = n_v(e;k)$ for every edge $e = uv$ in G. By Lemma 1, the result follows. ■

Corollary 2. *If G is $(n-k+1)$-connected graph of order n and size m, then*

$$rSz_k(G) = \frac{m}{4}\left[\binom{n-2}{k-1}+2\right]^2.$$

Proof. Let $e = uv$ be an edge of graph G. Since G is $(n-k+1)$-connected, it follows that for any $S \subseteq V(G)$, $|S| = k-1$ and $u, v \notin S$, $d_G(S\cup\{u\}) = d_G(S\cup\{v\}) = k-1$, and hence $n_u(e;k) = n_v(e;k) = 0$. By Theorem 1, we get the required result. ■

Corollary 3. *Let G be a connected graph of order n and size m. Then*

$$Sz_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1}+2\right]^2$$

with equality holding if and only if $D(u|e) = D(v|e)$ and $n_0(e;k) = 0$ for every edge $e = uv$ in G.

Proof. From the definition, we have $Sz_k(G) \leq rSz_k(G)$. The result follows from Theorem 1. ■

Lemma 4. *Let T be a tree of order n. Then T is a star graph if and only if* $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ *or* $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ *for any edge* $e = uv \in E(T)$.

Proof. If T is a star graph, then every edge in $E(T)$ is a pendant edge. Obviously, we have $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$. Conversely, let $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ for any edge $e = uv \in E(T)$. We have to prove that T is a star graph. By contradiction, we prove this result. For this we assume that there exists a non-pendant edge $e = uv$ satisfying $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$. By the definitions of $n_u(e;k)$, $n_v(e;k)$ and $n_0(e;k)$, for every $S \subseteq V(T)$, $|S| = k-1$, $u, v \notin S$, we have $d_T(S \cup \{v\}) < d_T(S \cup \{u\})$, that is, $d_T(S \cup \{v\}) + 1 = d_T(S \cup \{u\})$. Since e is a non-pendant edge, then there exist two vertices w and x in T such that $wu \in E(T)$ and $vx \in E(T)$. For $|S| = k-1 \geq 2$, suppose that $w, x \in S$. Then $d_T(S \cup \{v\}) = d_T(S \cup \{u\}) = d_T(S \cup \{v\}) + 1$, a contradiction. Otherwise, $|S| = 1$. Suppose that $w \in S$. Then $d_T(S \cup \{v\}) = 2 > 1 = d_T(S \cup \{u\}) = d_T(S \cup \{v\}) + 1$, a contradiction. This completes the proof of the result. ■

We now give a lower bound on $rSz_k(G)$ and $Sz_k(G)$ of graph G.

Theorem 2. *Let G be a connected graph of order n and size m. Then*

$$rSz_k(G) \geq m\left[\binom{n-2}{k-1} + 1\right]$$

with equality holding if and only if $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ *or* $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ *for every edge $e = uv$ in G.*

Proof. By the proof of Theorem 1, we obtain

$$\begin{aligned} rSz_k(G) &= \frac{1}{4}\sum_{e=uv}\left[\left(\binom{n-2}{k-1} + 2\right)^2 - (n_u(e;k) - n_v(e;k))^2\right] \\ &\geq \frac{1}{4}\sum_{e=uv}\left[\left(\binom{n-2}{k-1} + 2\right)^2 - \binom{n-2}{k-1}^2\right] = m\left[\binom{n-2}{k-1} + 1\right]. \end{aligned}$$

The equality holds if and only if $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ for every edge $e = uv$ in G. ■

Corollary 5. *Let G be a connected graph of order n. Then*

$$rSz_k(G) \geq (n-1)\left[\binom{n-2}{k-1} + 1\right], \tag{1}$$

with equality if and only if $G \cong S_n$.

Proof. Since G is connected, we have $m \geq n-1$. Using this with Theorem 2, we get the result in (1). Moreover, the equality holds in (1) if and only if $m = n-1$ and $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$, or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ for every edge $e = uv$ in G, that is, if and only if $G \cong S_n$, by Lemma 4 and Theorem 2. ■

Theorem 3. *Let G be a connected graph of order n with m edges and p pendant vertices. Then*

$$Sz_k(G) \geq m + p\binom{n-2}{k-1}.$$

Proof. Let $e = uv$ be an edge of graph G. If e is a pendant edge, then $n_v(e;k) = \binom{n-2}{k-1}$, $n_u(e;k) = 0$ or $n_u(e;k) = \binom{n-2}{k-1}$, $n_v(e;k) = 0$. So, we obtain

$$\begin{aligned} Sz_k(G) &= \sum_{e=uv} \Big(n_u(e;k)+1\Big)\Big(n_v(e;k)+1\Big) \\ &= \sum_{\substack{e\,=\,uv \\ d_G(u)\,=\,1 \\ \text{or } d_G(v)\,=\,1}} \left[\binom{n-2}{k-1}+1\right] + \sum_{\substack{e\,=\,uv \\ d_G(u)\,\neq\,1\,\neq\,d_G(v)}} \Big(n_u(e;k)+1\Big)\Big(n_v(e;k)+1\Big) \\ &\geq p\left[\binom{n-2}{k-1}+1\right] + m - p = m + p\binom{n-2}{k-1}. \end{aligned}$$

■

We now consider the difference between $rSz_k(G)$ and $Sz_k(G)$.

Theorem 4. *Let G be a connected graph of order n and size m. Then*

$$rSz_k(G) - Sz_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1}+4\right]\binom{n-2}{k-1}$$

with equality holding if and only if $n_u(e;k) = n_v(e;k) = 0$ for every edge $e = uv$ in G.

Proof. By the definitions of $rSz_k(G)$ and $Sz_k(G)$, we obtain

$$\begin{aligned} & rSz_k(G) \\ &= \sum_{e=uv}\left(n_u(e;k) + \frac{n_0(e;k)}{2}+1\right)\left(n_v(e;k)+\frac{n_0(e;k)}{2}+1\right) \\ &= \sum_{e=uv}\Big(n_u(e;k)+1\Big)\Big(n_v(e;k)+1\Big) + \sum_{e=uv}\frac{n_0(e;k)}{2}\Big(n_u(e;k)+n_v(e;k)+2\Big) \\ &+ \sum_{e=uv}\frac{n_0(e;k)^2}{4} = Sz_k(G) + \frac{1}{2}\sum_{e=uv} n_0(e;k)\ \left(\binom{n-2}{k-1}+2-n_0(e;k)\right) \\ &+ \frac{1}{4}\sum_{e=uv} n_0(e;k)^2 = Sz_k(G) + \frac{1}{2}\sum_{e=uv}\left[n_0(e;k)\ \left(\binom{n-2}{k-1}+2\right) - \frac{n_0(e;k)^2}{2}\right]. \end{aligned}$$

Since $0 \leq n_0(e;k) \leq \binom{n-2}{k-1}$ and $f(x) = x\left(\binom{n-2}{k-1} + 2 - \frac{x}{2}\right)$ is an increasing function on $0 \leq x \leq \binom{n-2}{k-1}$, we obtain

$$\begin{aligned} rSz_k(G) - Sz_k(G) \leq & \sum_{e=uv}\left[\frac{1}{2}\binom{n-2}{k-1}\left(\binom{n-2}{k-1}+2\right) - \frac{1}{4}\binom{n-2}{k-1}^2\right] \\ = & \frac{m}{4}\left[\binom{n-2}{k-1}^2 + 4\binom{n-2}{k-1}\right]. \end{aligned}$$

Moreover, the equality holding if and only if $n_0(e;k) = \binom{n-2}{k-1}$ for every edge $e = uv$ in G, that is, if and only if $n_u(e;k) = n_v(e;k) = 0$ for every edge $e = uv$ in G. ■

3 Nordhaus-Gaddum-type results on $rSz_k(G) + rSz_k(\overline{G})$

In this section we give Nordhaus-Gaddum-type results on the *kth Steiner Szeged index* $Sz_k(G)$ and the *kth Steiner revised Szeged index* $rSz_k(G)$ of graph G.

Theorem 5. *Let G be a connected graph of order n with connected complement $\overline{G}$. Then*
(i)

$$\frac{n(n-1)}{2}\left[\binom{n-2}{k-1}+1\right] \leq rSz_k(G) + rSz_k(\overline{G}) \leq \frac{n(n-1)}{8}\left[\binom{n-2}{k-1}+2\right]^2,$$

(ii)

$$\frac{(n-1)^2(n-2)}{2}\left[\binom{n-2}{k-1}+1\right]^2 < rSz_k(G)\, rSz_k(\overline{G}) \leq \frac{n^2(n-1)^2}{256}\left[\binom{n-2}{k-1}+2\right]^4. \tag{2}$$

Proof. Let m and $\overline{m}$ be the number of edges of G and $\overline{G}$, respectively. Then $m + \overline{m} = \frac{n(n-1)}{2}$. Since both G and $\overline{G}$ are connected, we have $m \geq n-1$ and $\overline{m} \geq n-1$. One can easily obtain that

$$\frac{(n-1)^2(n-2)}{2} \leq m\,\overline{m} = m\left[\frac{n(n-1)}{2} - m\right] \leq \frac{n^2(n-1)^2}{16} \tag{3}$$

with left (or right) equality holds if and only if $m = n-1$ or $m = \frac{(n-1)(n-2)}{2}$ (or $m = \frac{n(n-1)}{4}$).

By Theorems 1 and 2, we obtain

$$\begin{aligned} rSz_k(G) + rSz_k(\overline{G}) \;\; & \leq \;\; \frac{1}{4}m\left[\binom{n-2}{k-1}+2\right]^2 + \frac{1}{4}\overline{m}\left[\binom{n-2}{k-1}+2\right]^2 \\ & = \;\; \frac{m+\overline{m}}{4}\left[\binom{n-2}{k-1}+2\right]^2 = \frac{n(n-1)}{8}\left[\binom{n-2}{k-1}+2\right]^2 \end{aligned}$$

and

$$\begin{aligned} rSz_k(G) + rSz_k(\overline{G}) &\geq m\left[\binom{n-2}{k-1}+1\right] + \overline{m}\left[\binom{n-2}{k-1}+1\right] \\ &= \frac{n(n-1)}{2}\left[\binom{n-2}{k-1}+1\right]. \end{aligned}$$

Thus we get the result in (i). Similarly, by Theorems 1 and 2 with (3), we get the required result in (ii).

By Lemma 4 and Theorem 2 with equality in (3), one can easily see that the left equality holds in (2) if and only if $G \cong S_n$ or $\overline{G} \cong S_n$. Since both G and $\overline{G}$ are connected, the left inequality in (2) is strict. This completes the proof of the theorem. ■

Theorem 6. *Let G be a connected graph of order n with p pendant vertices. Then*

$$\frac{n(n-1)}{2} + p\binom{n-2}{k-1} \leq Sz_k(G) + Sz_k(\overline{G}) \leq \frac{n(n-1)}{8}\left[\binom{n-2}{k-1}+2\right]^2.$$

Proof. From $Sz_k(G) \leq rSz_k(G)$ with Theorem 5, the upper bound is obvious. Let $\overline{p}$ be the number of pendant vertices in $\overline{G}$. Since $m + \overline{m} = \frac{n(n-1)}{2}$ ($\overline{m}$ is the number of edges in $\overline{G}$), by Theorem 3, we obtain

$$\begin{aligned} Sz_k(G) + Sz_k(\overline{G}) &\geq m + p\binom{n-2}{k-1} + \overline{m} + \overline{p}\binom{n-2}{k-1} \\ &= \frac{n(n-1)}{2} + (p+\overline{p})\binom{n-2}{k-1} \geq \frac{n(n-1)}{2} + p\binom{n-2}{k-1}. \end{aligned}$$

■

Corollary 6. *Let G be a connected graph of order n. Then*

$$Sz_k(G) + Sz_k(\overline{G}) \geq \frac{n(n-1)}{2}.$$

4 Results for trees

In [7], the authors give a formula of $Sz_k(T)$ for trees.

Lemma 7. [7] *For a tree T,*

$$Sz_k(T) = \sum_{e=uv\in E(T)} \left(\binom{n_u(e)-1}{k-1}+1\right)\left(\binom{n_v(e)-1}{k-1}+1\right)$$

where $2 \leq k \leq |V(T)| - 1$.

Similarly, we give a formula of $rSz_k(T)$ for trees.

Theorem 7. *Let T be a tree of order n. Then*

$$rSz_k(T) = \frac{n-1}{4}\left[\binom{n-2}{k-1}+2\right]^2 - \frac{1}{4}\sum_{e=uv\in E(T)}\left[\binom{n_u(e)-1}{k-1}-\binom{n_v(e)-1}{k-1}\right]^2.$$

Proof. Let $e = uv$ be an edge of T. It is easy to check that $n_u(e;k) = \binom{n_u(e)-1}{k-1}$ and $n_v(e;k) = \binom{n_v(e)-1}{k-1}$. By the proof of Theorem 1, we obtain

$$\begin{aligned} rSz_k(T) &= \frac{m}{4}\left[\binom{n-2}{k-1}+2\right]^2 - \frac{1}{4}\sum_{e=uv}\Big(n_u(e;k)-n_v(e;k)\Big)^2 \\ &= \frac{n-1}{4}\left[\binom{n-2}{k-1}+2\right]^2 - \frac{1}{4}\sum_{e=uv}\left[\binom{n_u(e)-1}{k-1}-\binom{n_v(e)-1}{k-1}\right]^2. \end{aligned}$$

■

A double star $DS(p,q)$ is a tree obtained from two disjoint stars S_{p+1} and S_{q+1} by join their center with an edge. If n is the number of vertices of $DS(p,q)$, then $n = p+q+2$.

Corollary 8. *Let $DS(p,q)$ be a double star. Then*

$$rSz_k(DS(p,q)) = (p+q+1)\left[\binom{p+q}{k-1}+1\right] + \frac{1}{4}\binom{p+q}{k-1}^2 - \frac{1}{4}\left[\binom{p}{k-1}-\binom{q}{k-1}\right]^2.$$

Proof. By Theorem 7 and the proof of Theorem 1, we obtain

$$\begin{aligned} & rSz_k(DS(p,q)) \\ = \;& \frac{(n-1)}{4}\left[\binom{n-2}{k-1}+2\right]^2 - \frac{1}{4}\sum_{e=uv}\Big(n_u(e;k)-n_v(e;k)\Big)^2 \\ = \;& \frac{(n-1)}{4}\left[\binom{n-2}{k-1}+2\right]^2 - \frac{(n-2)}{4}\binom{n-2}{k-1}^2 - \frac{1}{4}\left[\binom{p}{k-1}-\binom{q}{k-1}\right]^2 \\ = \;& (p+q+1)\left[\binom{p+q}{k-1}+1\right] + \frac{1}{4}\binom{p+q}{k-1}^2 - \frac{1}{4}\left[\binom{p}{k-1}-\binom{q}{k-1}\right]^2. \end{aligned}$$

■

We now give a lower bound on $Sz_3(T)$ of any tree of order n and characterize extremal trees. For this we need the following results.

Lemma 9. *For positive integers n and p, $3 \le p \le \lfloor \frac{n}{2} \rfloor$,*

$$\left(\binom{n-p}{2}+1\right)\left(\binom{p-2}{2}+1\right) \le \left(\binom{n-p-1}{2}+1\right)\left(\binom{p-1}{2}+1\right),$$

with equality if and only if $n = 6, p = 3$.

Proof. Now,

$$\begin{aligned}
&\left(\binom{n-p-1}{2}+1\right)\left(\binom{p-1}{2}+1\right)-\left(\binom{n-p}{2}+1\right)\left(\binom{p-2}{2}+1\right)\\
=\;&\left(\frac{(n-p-1)(n-p-2)}{2}+1\right)\left(\frac{(p-1)(p-2)}{2}+1\right)-\left(\frac{(n-p)(n-p-1)}{2}+1\right)\\
&\qquad\times\left(\frac{(p-2)(p-3)}{2}+1\right)\\
=\;&\frac{(n-p-1)(n-p-2)(p-1)(p-2)-(n-p)(n-p-1)(p-2)(p-3)}{4}\\
&-\frac{(p-2)(p-3)+(n-p)(n-p-1)-(p-1)(p-2)-(n-p-1)(n-p-2)}{2}\\
=\;&\frac{(n-p-1)(p-2)(n-2p+1)}{2}-(n-2p+1)\\
=\;&\frac{(n-2p+1)}{2}\Big[(n-p-1)(p-2)-2\Big]\geq 0
\end{aligned}$$

as $3 \leq p \leq \lfloor \frac{n}{2} \rfloor$. This proves the result. ∎

Corollary 10. *For any positive integer $n \geq 7$,*

$$\begin{aligned}
&\binom{n-3}{2}+1<2\left(\binom{n-4}{2}+1\right)<4\left(\binom{n-5}{2}+1\right)<\cdots\\
&\quad<\left(\binom{\lceil\frac{n}{2}\rceil}{2}+1\right)\left(\binom{\lfloor\frac{n}{2}\rfloor-2}{2}+1\right)<\left(\binom{\lceil\frac{n}{2}\rceil-1}{2}+1\right)\left(\binom{\lfloor\frac{n}{2}\rfloor-1}{2}+1\right).
\end{aligned}$$

Proof. Putting $p = 3, 4, \ldots, \lfloor \frac{n}{2} \rfloor$ in Lemma 9, we get the required result. ∎

Lemma 11. *For positive integer $n \geq 9$,*

$$\binom{n-3}{2}+1<\binom{n-2}{2}+1\leq 2\left(\binom{n-4}{2}+1\right)$$

with right equality holding if and only if $n = 9$.

Let S'_n be a tree of order n with center vertex v such that $T\backslash\{v\} = \lfloor \frac{n}{2} \rfloor K_2$ (n is odd) or $T\backslash\{v\} = \lfloor \frac{n-1}{2} \rfloor K_2 \cup K_1$ (n is even). For $n \leq 7$, one can easily check that

$$Sz_3(T)\geq\sum_{i=1}^{n-1}\left(\binom{i-1}{2}+1\right)\left(\binom{n-i-1}{2}+1\right)$$

with equality if and only if $T \cong P_n$. For $n = 8$, we have $Sz_3(T) \geq 97$ with equality if and only if $T \cong S(2, 2, 2, 1)$. We are now ready to give a lower bound on $Sz_3(T)$ in terms of n when $n \geq 9$.

Theorem 8. *Let T be a tree of order $n \geq 9$. Then*

$$Sz_3(T) \geq \left\lceil \frac{n-1}{2} \right\rceil \left(\binom{n-2}{2} + 1 \right) + \left\lfloor \frac{n-1}{2} \right\rfloor \left(\binom{n-3}{2} + 1 \right)$$

with equality holding if and only if $T \cong S'_n$.

Proof. Let p be the number of pendant edges in T. Let q be the number of edges $e = uv$ such that $n_u(e) = 2$, $n_v(e) = n-2$ or $n_u(e) = n-2$, $n_v(e) = 2$. Since T is a tree, we have $q \leq p$, that is, $q \leq \lfloor \frac{n-1}{2} \rfloor$. First we assume that $p + q = n-1$. In this case we must have $p \geq \lceil \frac{n-1}{2} \rceil$ and $q \leq \lfloor \frac{n-1}{2} \rfloor$. By Lemmas 7 and 11, we obtain

$$\begin{aligned} Sz_3(T) &= p \left(\binom{n-2}{2} + 1 \right) + q \left(\binom{n-3}{2} + 1 \right) \\ &\geq \left\lceil \frac{n-1}{2} \right\rceil \left(\binom{n-2}{2} + 1 \right) + \left\lfloor \frac{n-1}{2} \right\rfloor \left(\binom{n-3}{2} + 1 \right) = Sz_3(S'_n) \end{aligned}$$

with equality holding if and only if $p - \left\lceil \frac{n-1}{2} \right\rceil = \left\lfloor \frac{n-1}{2} \right\rfloor - q = 0$, that is, if and only if $T \cong S'_n$.

Next we assume that $p + q < n-1$. By Lemmas 7 and 11 and Corollary 10, we obtain

$$\begin{aligned} Sz_3(T) &\geq p \left(\binom{n-2}{2} + 1 \right) + q \left(\binom{n-3}{2} + 1 \right) + 2(n-1-p-q) \left(\binom{n-4}{2} + 1 \right) \\ &> p \left(\binom{n-2}{2} + 1 \right) + q \left(\binom{n-3}{2} + 1 \right) + \left(\left\lceil \frac{n-1}{2} \right\rceil - p \right) \left(\binom{n-2}{2} + 1 \right) \\ &\qquad + \left(\left\lfloor \frac{n-1}{2} \right\rfloor - q \right) \left(\binom{n-3}{2} + 1 \right) \\ &= \left\lceil \frac{n-1}{2} \right\rceil \left(\binom{n-2}{2} + 1 \right) + \left\lfloor \frac{n-1}{2} \right\rfloor \left(\binom{n-3}{2} + 1 \right) = Sz_3(S'_n). \end{aligned}$$

This completes the proof of the theorem. ∎

Let $v_{\ell+1}$ be a vertex in a tree T with at least two vertices and suppose that two new paths $P : v_{\ell+1}v_\ell v_{\ell-1} \ldots v_2 v_1$ and $Q : v_{\ell+1}v_{\ell+2}v_{\ell+3} \ldots v_{k+\ell}v_{k+\ell+1}$ of lengths ℓ, k ($k \geq \ell \geq 1$), respectively, are attached to T at $v_{\ell+1}$, to form a new tree $T_{k,\ell}$, where $v_1 v_2 \ldots v_\ell$ and $v_{\ell+2}v_{\ell+3} \ldots v_{k+\ell+1}$ are distinct new vertices. Let $T_{k+1,\ell-1} = T_{k,\ell} - v_1v_2 + v_{k+\ell+1}v_1$. Thus we have

Transformation A: $\qquad T_{k,\ell} \longrightarrow T_{k+1,\ell-1}$.

Let $|V(T)| = n - k - \ell$. Then we have $|V(T_{k+1,\ell-1})| = |V(T_{k,\ell})| = n$.

Lemma 12. *Let T be a tree with at least two vertices and $n \geq 10$. Also let $T_{k,\ell}$ and $T_{k+1,\ell-1}$ be the trees defined as above. If $k \geq 2$, then*

$$Sz_3(T_{k,\ell}) < Sz_3(T_{k+1,\ell-1}).$$

Proof. Now,

$$\begin{aligned} & Sz_3(T_{k+1,\ell-1}) - Sz_3(T_{k,\ell}) \\ &= \sum_{e=uv\in E(T_{k+1,\ell-1})} \left(\binom{n_u(e)-1}{2}+1\right)\left(\binom{n_v(e)-1}{2}+1\right) \\ &\qquad - \sum_{e=uv\in E(T_{k,\ell})} \left(\binom{n_u(e)-1}{2}+1\right)\left(\binom{n_v(e)-1}{2}+1\right) \\ &= \left(\binom{k}{2}+1\right)\left(\binom{n-k-2}{2}+1\right) - \left(\binom{\ell-1}{2}+1\right)\left(\binom{n-\ell-1}{2}+1\right). \end{aligned} \tag{4}$$

Since $n \geq 10$, by Corollary 10 and Lemma 11, we obtain

$$\begin{aligned} & \binom{n-3}{2}+1 < \binom{n-2}{2}+1 < 2\left(\binom{n-4}{2}+1\right) < 4\left(\binom{n-5}{2}+1\right) < \cdots \\ & \qquad < \left(\binom{\lceil\frac{n}{2}\rceil}{2}+1\right)\left(\binom{\lfloor\frac{n}{2}\rfloor-2}{2}+1\right) < \left(\binom{\lceil\frac{n}{2}\rceil-1}{2}+1\right)\left(\binom{\lfloor\frac{n}{2}\rfloor-1}{2}+1\right). \end{aligned}$$

Again since $k \geq 2$, $k \geq \ell \geq 1$ and $k+\ell \leq n-2$, using the above result, we get

$$\left(\binom{k}{2}+1\right)\left(\binom{n-k-2}{2}+1\right) > \left(\binom{\ell-1}{2}+1\right)\left(\binom{n-\ell-1}{2}+1\right).$$

Using this in (4), we obtain $Sz_3(T_{k+1,\ell-1}) > Sz_3(T_{k,\ell})$. ■

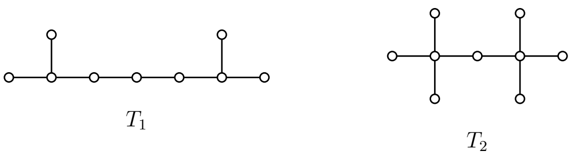

Figure 1. Two trees T_1 and T_2.

For $n \leq 8$, one can easily check that $Sz_3(T) \leq \frac{(n^2-5n+8)(n-1)}{2}$ with equality if and only if $T \cong S_n$ or $T \cong DS(3, 3)$ $(n = 8)$. For $n = 9$, we have $Sz_3(T) \leq 188$ with equality if and only if $T \cong T_1$ or $T \cong T_2$ (see, Fig. 1). We are now ready to give an upper bound on $Sz_3(T)$ in terms of n when $n \geq 10$.

Theorem 9. *Let $S(n_1, n_2, \ldots, n_q)$ be a starlike tree of order $n \geq 10$. Then*

$$Sz_3\Big(S(n_1, n_2, \ldots, n_q)\Big) \leq \sum_{i=1}^{n-1} \left(\binom{i-1}{2} + 1\right)\left(\binom{n-i-1}{2} + 1\right)$$

with equality holding if and only if $S(n_1, n_2, \ldots, n_q) \cong P_n$.

Proof. For $S(n_1, n_2, \ldots, n_q) \cong P_n$,

$$Sz_3\Big(S(n_1, n_2, \ldots, n_q)\Big) = \sum_{i=1}^{n-1} \left(\binom{i-1}{2} + 1\right)\left(\binom{n-i-1}{2} + 1\right)$$

and hence the equality holds. Otherwise, $S(n_1, n_2, \ldots, n_q) \ncong P_n$. We consider the following two cases:

Case 1 : $n_1 = 1$. We have $S(n_1, n_2, \ldots, n_q) \cong S_n$. Since $n \geq 10$, we obtain

$$\begin{aligned}
& Sz_3(P_n) - Sz_3(S_n) \\
= \ & \sum_{i=1}^{n-1} \left(\binom{i-1}{2} + 1\right)\left(\binom{n-i-1}{2} + 1\right) - (n-1)\left(\binom{n-2}{2} + 1\right) \\
= \ & \sum_{i=5}^{n-5} \left[\left(\binom{i-1}{2} + 1\right)\left(\binom{n-i-1}{2} + 1\right) - \left(\binom{n-2}{2} + 1\right)\right] - 2\left[\binom{n-2}{2}\right. \\
& \left. - \binom{n-3}{2}\right] + 2\left[2\binom{n-4}{2} + 1 - \binom{n-2}{2}\right] + 2\left[4\binom{n-5}{2} + 3 - \binom{n-2}{2}\right] \\
= \ & \sum_{i=5}^{n-5} \left[\left(\binom{i-1}{2} + 1\right)\left(\binom{n-i-1}{2} + 1\right) - \left(\binom{n-2}{2} + 1\right)\right] \\
& -2(n-3) + \Big[(n-6)(n-7) - 6\Big] + 3\Big[(n-6)(n-7) - 2\Big] \\
= \ & \sum_{i=5}^{n-5} \left[\left(\binom{i-1}{2} + 1\right)\left(\binom{n-i-1}{2} + 1\right) - \left(\binom{n-2}{2} + 1\right)\right] \\
+ \ & 4\Big[(n-6.5)(n-7) - 5\Big] > 0
\end{aligned}$$

as each term inside the bracket is greater than 0. Hence $Sz_3(P_n) > Sz_3(S_n)$.

Case 2 : $n_1 > 1$. Since $n \geq 10$, by Lemma 12, we obtain $Sz_3\Big(S(n_1, n_2, \ldots, n_q)\Big) < Sz_3\Big(S(n_1+1, n_2, \ldots, n_q - 1)\Big) < \cdots < Sz_3\Big(S(n_1+n_q, n_2, \ldots, n_{q-1}, 0)\Big) < \cdots < Sz_3\Big(S(n - n_2 - 2, n_2, 1, 0, \ldots, 0)\Big) < Sz_3\Big(S(n - n_2 - 1, n_2, 0, 0, \ldots, 0)\Big) = Sz_3(P_n)$. This completes the proof of the theorem. ■

5 Concluding remarks and future work

In this paper we presented some upper and lower bounds on $Sz_k(G)$ and $rSz_k(G)$. The result in Lemma 4 presented among the trees of order n. We believe that the following conjecture is true:

Conjecture 13. *Let G be a connected graph of order n. Then G is a star graph if and only if $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ for any edge $e = uv \in E(G)$.*

Also we obtain Nordhaus-Gaddum-type results on $rSz_k(G) + rSz_k(\overline{G})$ and $Sz_k(G) + Sz_k(\overline{G})$. Moreover, we determined a formula on $rSz_k(G)$ for trees in general. Using this result we proved that S'_n gives the minimum value of Sz_3 among the trees T of order n. Finally, we prove that the path P_n gives the maximum value of Sz_3 among the star-like trees of order $n \geq 10$. So it is natural to ask the following problem:

Problem 14. *Which graph gives the maximum value of $Sz_3(T)$ among the trees T of order n.*

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