MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **88** (2022) 643–658
ISSN: 0340–6253
doi: 10.46793/match.88-3.643R

On General Sum–Connectivity Index of Trees of Fixed Maximum Degree and Order

Zahid Raza[a], Selvaraj Balachandran[b], Suresh Elumalai[c], Akbar Ali[d,*]

[a]*Department of Mathematics, College of Sciences, University of Sharjah, Sharjah, UAE*

[b]*Department of Mathematics, School of Arts, Sciences and Humanities, SASTRA Deemed University, Thanjavur, India*

[c]*Department of Mathematics, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpet 603 203, India*

[d]*Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia*

zraza@sharjah.ac.ae, bala_maths@rediffmail.com, sureshkako@gmail.com, akbarali.maths@gmail.com

(Received March 18, 2022)

Abstract

The general sum-connectivity index is a molecular descriptor introduced within the field of mathematical chemistry about a decade ago. For an arbitrary real number α, the general sum-connectivity index of a graph G is denoted $\chi_\alpha(G)$ and is defined as the sum of the numbers $(d(u)+d(v))^\alpha$ over all edges uv of G, where $d(u)$ and $d(v)$ denote the degrees of the vertices u and v, respectively. This paper characterizes the trees attaining the extremum values of χ_α over the class of all trees of order n and maximum degree Δ for $\alpha < 0$ as well as for $\alpha > 1$, where $3 \le \lceil n/2 \rceil \le \Delta \le n-2$.

*Corresponding author.

1 Introduction

In graph theory, a graph invariant is a function I defined on the set of all graphs such that the equation $I(G) = I(G')$ holds if and only if G is isomorphic to G'; provided that the codomain of I contains the extended real numbers. A graph invariant may be a set of numbers (for example, the spectrum of a graph), a numerical value (for example, diameter of a graph), a polynomial (for example, the characteristic polynomial of a graph), etc. In chemical graph theory, numerical graph invariants are usually referred to as topological indices [27]. The connectivity index, proposed by Randić [21] in 1975, (nowadays, known as the Randić index [18]) is one of the most studied and applied topological indices [11, 16]; this index for a graph G is defined as the sum of the numbers $[d(u)d(v)]^{-1/2}$ over all edges uv of G, where $d(w)$ denotes the degree of any vertex w of G. The connectivity index was generalized in [7] by replacing the exponent "$-1/2$" with an arbitrary real number. Most of the detail about the mathematical properties of the connectivity index and general connectivity index, as well as about their chemical applicability, can be found in the survey paper [18], books [14, 17] and in the related references cited therein. The present study is motivated from the paper [19] concerning the general connectivity/Randić index.

Motivated from the success of the connectivity index, Zhou and Trinajstić [28, 29] proposed the sum-connectivity index χ and the general sum-connectivity index χ_α; these indices for a graph G are defined as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}$$

and

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha ,$$

where $E(G)$ is the edge set of G and α is a real number. It was found that the sum-connectivity index and the connectivity index correlate well between themselves and with the π-electron energy of benzenoid hydrocarbons [20].

In the study of topological indices, it is often of interest to find extremum values of a given topological index of graphs under certain constraints. Along this line, extremum values of the general sum-connectivity index have been extensively explored. Zhou and Trinajstić [29] determined the minimum general sum-connectivity index χ_α of trees of fixed order for every $\alpha \neq 0$ and they found the maximum general sum-connectivity index χ_α of trees of fixed order for every non-zero value of α satisfying the inequality $\alpha > \alpha_0 \approx -1.4094$. Du et al. [13] found the maximum general sum-connectivity index χ_α of trees of fixed order for $\alpha < \alpha_1 \approx -4.3586$. Tomescu and Kanwal [26], and Cui and Zhong [10] studied the minimum and maximum general sum-connectivity index χ_α, respectively, of trees of fixed order with a given number of pendent vertices for $-1 \leq \alpha < 0$. Additional results along these lines concerning the general sum-connectivity index can be found in the survey [6], articles [2–5,12,24,25], and related references cited therein. This paper is concerned with the following extremal problem.

Problem 1. *Characterize graphs attaining the extremum values of the general sum-connectivity index χ_α over the class of all trees of maximum degree Δ and order n, for all non-zero α.*

Rasi et al. [23] solved the maximal part of Problem 1 for $\alpha = -1$. Jamil and Tomescu [15] generalized the main result reported in [23] and hence solved the maximal part of Problem 1 for $-1.7036 \leq \alpha < 0$; the same result for $-1 \leq \alpha < 0$ was also proved in [1] independently. The minimal part of Problem 1 for $\alpha = -1$ was attacked in [22]. In the present paper, Problem 1 is solved for the case when $3 \leq \lceil n/2 \rceil \leq \Delta \leq n-2$ for $\alpha < 0$ as well as for $\alpha > 1$.

2 Preliminaries

In this section, we recall some graph-theoretical terminology, notation, and two elementary lemmas that are needed in the remaining part of this paper. The set of vertices and the set of edges of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree $d(u)$ of a vertex u of a graph

G is the number of vertices adjacent to u; if there are at least two graphs under consideration then the notation $d_G(u)$ will be used instead of $d(u)$ for the degree of u in G. A vertex of degree one in a graph is called a pendent vertex. We use Δ to denote the maximum degree of G. For an edge $uv \in E(G)$, the vertices u, v are called neighbors of each other. The set of all neighbors of a vertex $u \in V(G)$ is denoted by $N_G(u)$, or simply by $N(u)$ when there is no danger of confusion. A path $P = v_0v_1 \cdots v_l$ of length at least 1 in a graph G is said to be a pendent path if one of the two vertices v_0, v_l is pendent and the other has degree at least 3, and every other vertex (if exists) of P has degree 2. The (chemical) graph theoretical terminology and notation used in this paper, without defining them here, can be found in the relevant books, like [8,9,27].

Lemma 1. *If $\alpha < 0$ or $\alpha > 1$ then the function f defined by*

$$f(x) = (x+1)^{\alpha} - x^{\alpha}$$

is strictly increasing for $x \geq 1$.

Lemma 2. *The function f defined by*

$$f(x) = x(x+2)^{\alpha} + (x-2)x^{\alpha} - 2(x-1)(x+1)^{\alpha}$$

is a positive-valued function for $x \geq 2$ and $\alpha \geq 1$.

Proof. We observe that $f(x) > 0$ for $\alpha = 1$. In what follows, we assume that $x \geq 2$. Let us take $f_1(x) = (x-1)(x+1)^{\alpha} - (x-2)x^{\alpha}$. Then $f(x) = f_1(x+1) - f_1(x)$. The second derivative of f_1 is given as

$$f_1''(x) = \alpha(x+1)^{\alpha-2}[\alpha x - \alpha + x + 3] - \alpha x^{\alpha-2}[\alpha x - 2\alpha + x + 2]. \quad (1)$$

If $\alpha \geq 2$ then from Equation (1) it follows that

$$\begin{aligned} f_1''(x) &\geq \alpha x^{\alpha-2}[\alpha x - \alpha + x + 3] - \alpha x^{\alpha-2}[\alpha x - 2\alpha + x + 2] \\ &= \alpha x^{\alpha-2}[\alpha + 1] > 0. \end{aligned}$$

If $1 < \alpha < 2$ then one has

$$1 + \frac{\alpha + 1}{\alpha x - 2\alpha + x + 2} > 1 + \frac{1}{x} > \left(1 + \frac{1}{x}\right)^{2-\alpha},$$

which implies that

$$\left(1 + \frac{\alpha + 1}{\alpha x - 2\alpha + x + 2}\right)\left(1 + \frac{1}{x}\right)^{\alpha-2} > 1,$$

that is equivalent to

$$(x+1)^{\alpha-2}(\alpha x - \alpha + x + 3) > x^{\alpha-2}(\alpha x - 2\alpha + x + 2),$$

which together with Equation (1) confirm that $f_1''(x) > 0$.

Hence, f_1' is strictly increasing for $x \geq 2$ and $\alpha > 1$. Therefore,

$$f'(x) = f_1'(x+1) - f_1'(x) > 0,$$

which implies that f is strictly increasing for $x \geq 2$ and $\alpha > 1$, and hence $f(x) \geq f(2) = 2(4^\alpha - 3^\alpha) > 0$. ■

3 Results Concerning the Maximum χ_α

Lemma 3. *Let G be a graph, and let $u, v \in V(G)$ with $d_G(u), d_G(v) \geq 3$. Suppose that $u_0 u$ and $v_0 v_1 \cdots v_l$ $(v_l = v)$ are the pendent paths of G with end vertices u, v, respectively, where $l \geq 3$. Set $G^* = G - v_0 v_1 + u_0 v_0$. If $\alpha < 0$ or $\alpha > 1$, then $\chi_\alpha(G^*) > \chi_\alpha(G)$.*

Proof. Let $d_G(u) = t$. Then $t \geq 3$. By Lemma 1, we have

$$\begin{aligned}\chi_\alpha(G^*) - \chi_\alpha(G) &= (t+2)^\alpha + (2+1)^\alpha - (t+1)^\alpha - (2+2)^\alpha \\ &= (t+2)^\alpha - (t+1)^\alpha + 3^\alpha - 4^\alpha \\ &> (5^\alpha - 4^\alpha) - (4^\alpha - 3^\alpha) > 0,\end{aligned}$$

and hence the lemma holds. ■

Lemma 4. *Suppose that G is a graph and $u, v \in V(G)$ with $d_G(u) > d_G(v) \geq 2$. Let $uu_0, vv_0 \in E(G)$ where u_0 is a pendent vertex and $N_G(v_0) \setminus \{v\} := \{v_1, v_2, \cdots v_s\}$ $(s \geq 1)$ and v_0 being not on the path connecting u to v. Set $G' = G - v_0v_1 - \cdots - v_0v_s + u_0v_1 + \cdots + u_0v_s$. If $\alpha < 0$ or $\alpha > 1$, then $\chi_\alpha(G') > \chi_\alpha(G)$. Also, if $0 < \alpha < 1$, then $\chi_\alpha(G') < \chi_\alpha(G)$*

Proof. If $\alpha < 0$ or $\alpha > 1$ then we have

$$\begin{aligned}\chi_\alpha(G') - \chi_\alpha(G) &= (s + 1 + d_G(u))^\alpha - (s + 1 + d_G(v))^\alpha \\ &\quad - [(d_G(u) + 1)^\alpha - (d_G(v) + 1)^\alpha] \\ &\geq [(2 + d_G(u))^\alpha - (d_G(u) + 1)^\alpha] \\ &\quad - [(2 + d_G(v))^\alpha - (d_G(v) + 1)^\alpha] \\ &> 0.\end{aligned}$$

Similarly, the inequality $\chi_\alpha(G') - \chi_\alpha(G) < 0$ holds for $0 < \alpha < 1$. ■

Lemma 5. *Let G be a connected graph. Let $u_0, v_0 \in V(G)$ be two pendent neighbors of a vertex $v \in V(G)$ of degree at least 3. Set $G^* = G - vu_0 + u_0v_0$. Then, for $\alpha < 0$, $\chi_\alpha(G^*) > \chi_\alpha(G)$.*

Proof. Simple calculations yield

$$\begin{aligned}\chi_\alpha(G^*) - \chi_\alpha(G) &= \sum_{u \in N_G(v) \setminus \{v_0, u_0\}} \Big[(d_G(u) + d_G(v) - 1)^\alpha \\ &\quad - (d_G(u) + d_G(v))^\alpha \Big] + 3^\alpha - (d_G(v) + 1)^\alpha \\ &> 3^\alpha - (d_G(v) + 1)^\alpha > 0.\end{aligned}$$

■

For $2\Delta \geq n$, denote by $S_{n,\Delta}$ the tree of order n formed from the star $S_{\Delta+1}$ by attaching a pendent vertex to each of $n - \Delta - 1$ pendent vertices of $S_{\Delta+1}$. Let $\mathcal{T}_{n,\Delta}$ be the class of all trees of order n and maximum degree Δ.

Theorem 2. *Let $T \in \mathcal{T}_{n,\Delta}$ and $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n - 2$. Then*

$$\chi_\alpha(T) \leq (2\Delta - n + 1)(\Delta + 1)^\alpha + (n - \Delta - 1)3^\alpha + (n - \Delta - 1)(\Delta + 2)^\alpha$$

for $\alpha < 0$ and equality holds if and only if $T \cong S_{n,\Delta}$.

Proof. We note that if $T \cong S_{n,\Delta}$, then

$$\chi_\alpha(T) = (2\Delta - n + 1)(\Delta + 1)^\alpha + (n - \Delta - 1)3^\alpha + (n - \Delta - 1)(\Delta + 2)^\alpha.$$

Next, we choose $T \in \mathcal{T}_{n,\Delta}$ such that $\chi_\alpha(T)$ is as large as possible. Let $w \in V(T)$ with $d_T(w) = \Delta \geq 3$. The assumption $\Delta \geq \lceil \frac{n}{2} \rceil$ implies that at least one of the neighbors of w is pendent (for otherwise, every component of $T - w$ contains at least two vertices and hence one has $n \geq 2\Delta + 1$, a contradiction). Let $u_0 \in V(T)$ be a pendent neighbor of w. We will show three facts.

By Lemma 3, the following fact holds.

Fact 1. Every pendent path of T has length at most 2.

Fact 2. Let $v_0 v_1 \cdots v_l$ be a pendent path of T, where v_l is a branching vertex and v_0 is a pendent vertex. If $v_l \neq w$, then $l = 1$.

Proof of the Fact 2. Contrarily, assume that $l \geq 2$. Then by Fact 1, $l = 2$. Since $\Delta \geq \lceil \frac{n}{2} \rceil$ and $v_l \neq w$, we have

$$d_T(v_l) \leq n - \Delta - 1 \leq \left\lfloor \frac{n}{2} \right\rfloor - 1 < \Delta = d_T(w).$$

Set $T' = T - v_0 v_1 + u_0 v_0$. Then $T' \in \mathcal{T}_{n,\Delta}$. By Lemma 4, $\chi_\alpha(T') > \chi_\alpha(T)$, a contradiction with our choice of T.

Fact 3. For every vertex $v \in V(T) \setminus \{w\}$, it holds that $d_T(v) \leq 2$.

Proof of Fact 3. Assume that $d_T(v) \geq 3$ for some $v \in V(T) \setminus \{w\}$. We choose v such that $d_T(w, v)$ is as large as possible. From Fact 2, it follows that T has at least two pendent neighbors. Let $u', v' \in V(T)$ be two pendent neighbors of v. Set $T' = T - u'v + u'v'$. Then $T' \in \mathcal{T}_{n,\Delta}$. By Lemma 5, we have $\chi_\alpha(T') > \chi_\alpha(T)$, a contradiction with our choice of T.

By Fact 3, the proof of the theorem is now complete. ■

Lemma 6. *Let $Q_{s,t}$ be the graph as shown in Figure 1. If $s \geq t \geq 2$ then, for $\alpha \geq 1$, $\chi_\alpha(Q_{s,t}) < \chi_\alpha(Q_{s+1,t-1})$.*

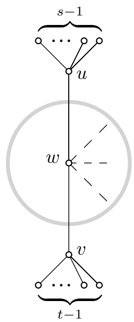

Figure 1. The graph $Q_{s,t}$ used in Lemma 6.

Proof. Set $d_G(w) = p$. Then, we note that

$$\begin{aligned}\chi_\alpha(Q_{s+1,t-1}) - \chi_\alpha(Q_{s,t}) &= s(s+2)^\alpha + (s+p+1)^\alpha + (t-2)t^\alpha \\ &\quad + (t+p-1)^\alpha - (s-1)(s+1)^\alpha \\ &\quad - (s+p)^\alpha - (t-1)(t+1)^\alpha - (t+p)^\alpha\end{aligned}$$

If $\alpha = 1$, then $\chi_1(Q_{s+1,t-1}) - \chi_1(Q_{s,t}) = 2(s-t+1) > 0$. If $\alpha > 1$, then by keeping in mind the assumption $s \geq t \geq 2$, we get

$$\begin{aligned}\chi_\alpha(Q_{s+1,t-1}) - \chi_\alpha(Q_{s,t}) &= [s(s+2)^\alpha - (s-1)(s+1)^\alpha] \\ &\quad + [(s+p+1)^\alpha - (s+p)^\alpha] \\ &\quad + [(t-2)t^\alpha - (t-1)(t+1)^\alpha] \\ &\quad + [(t+p-1)^\alpha - (t+p)^\alpha] \\ &> [t(t+2)^\alpha - (t-1)(t+1)^\alpha] \\ &\quad + [(t+p+1)^\alpha - (t+p)^\alpha] \\ &\quad + [(t-2)t^\alpha - (t-1)(t+1)^\alpha] \\ &\quad + [(t+p-1)^\alpha - (t+p)^\alpha] \\ &= [t(t+2)^\alpha + (t-2)t^\alpha - 2(t-1)(t+1)^\alpha] \\ &\quad + [(t+p+1)^\alpha + (t+p-1)^\alpha - 2(t+p)^\alpha] \\ &> 0. \end{aligned} \tag{2}$$

The last inequality in (2) holds because of the following facts: From Lemma

2 it follows that

$$t(t+2)^\alpha + (t-2)t^\alpha - 2(t-1)(t+1)^\alpha > 0.$$

Since the function ϕ defined by $\phi(x) = x^\alpha$ is strictly convex for $x > 0$ and $\alpha > 1$, hence by Jensen's inequality, it holds that

$$\begin{aligned}(t+p+1)^\alpha + (t+p-1)^\alpha - 2(t+p)^\alpha &= \phi(t+p+1) + \phi(t+p-1) \\ &\quad - 2\phi(t+p) > 0\ .\end{aligned}$$

■

Denote by $DS_{n-\Delta-1,\Delta-1}$ the double star formed by attaching $\Delta - 1$ pendent vertices to one of the vertices of the path P_2 and $n-\Delta-1$ pendent vertices to the other vertex of P_2.

Theorem 3. *Let T be a tree of order n and maximum degree Δ such that $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$. Then*

$$\chi_\alpha(T) \leq (\Delta-1)(\Delta+1)^\alpha + (n-\Delta-1)(n-\Delta+1)^\alpha + n^\alpha \qquad (3)$$

for $\alpha > 1$ and equality holds if and only if $T \cong DS_{n-\Delta-1,\Delta-1}$.

Proof. First, we note that if $T \cong DS_{n-\Delta-1,\Delta-1}$, then equality in (3) holds.

In what follows, we assume that T is a tree of order n and maximum degree Δ such that $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$ and that $\chi_\alpha(T)$ is as large as possible. Take $w \in V(T)$ with $d_T(w) = \Delta \geq 3$. The assumption $\Delta \geq \lceil \frac{n}{2} \rceil$ implies that at least one of the neighbors of w is pendent (for otherwise, every component of $T-w$ contains at least two vertices and hence one has $n \geq 2\Delta + 1$, a contradiction). Let $u_0 \in V(T)$ be a pendent neighbor of w. We first show two facts.

Fact 1. Every non-pendent neighbor of w has only one non-pendent neighbor (namely w).

Proof of Fact 1. Contrarily, assume that $u \in N_T(w)$ is a non-pendent vertex having a non-pendent neighbor u' different from w. Take $N_T(u') \setminus \{u\} = \{u_1, \ldots, u_s\}$, where $s \geq 1$. Since T contains at least Δ pendent vertices and $\Delta \geq \lceil \frac{n}{2} \rceil$, one has $d_T(u) \leq n - \Delta - 1 \leq \lfloor \frac{n}{2} \rfloor - 1 < \Delta = d_T(w)$. Set $T' = T - u'u_1 - \cdots - u'u_s + u_0u_1 + \cdots + u_0u_s$. Observe that T' has order n and maximum degree Δ. However, from Lemma 4, it follows that $\chi_\alpha(T') > \chi_\alpha(T)$, which is a contradiction with the choice of T.

Fact 2. The vertex w has only one non-pendent neighbor.

Proof of Fact 2. Suppose to the contrary that $u, v \in N_T(w)$ such that $d_T(u) = s \geq 2$ and $d_T(v) = t \geq 2$. Without loss of generality, we assume that $s \geq t$. By Fact 1, each of the sets $N_T(u)$ and $N_T(v)$ contains only one non-pendent neighbor, namely w. Note that $T \cong Q_{s,t}$ (see Lemma 6) and hence $\chi_\alpha(Q_{s+t-1,1}) > \cdots > \chi_\alpha(Q_{s+1,t-1}) > \chi_\alpha(Q_{s,t}) = \chi_\alpha(T)$ by Lemma 6. On the other hand, observe that $(s-1) + (t-1) + (\Delta+1) \leq n$, which together with the assumption $\Delta \geq \lceil \frac{n}{2} \rceil$ implies that $s + t - 1 \leq n - \Delta \leq \lfloor \frac{n}{2} \rfloor \leq \Delta$. Thus, the graph $Q_{s+t-1,1}$ has order n and maximum degree Δ with $\chi_\alpha(Q_{s+t-1,1}) > \chi_\alpha(T)$, which is again a contradiction with our choice of T.

By Facts 1 and 2, the proof of the theorem is complete. ■

4 Results Concerning the Minimum χ_α

Lemma 7. *Suppose that G is a graph and $v, w \in V(G)$ with $d_G(w) > d_G(v) \geq 2$. Let $wu, vv_0 \in E(G)$ where v_0 is pendent and u does not lie on the w-v path. Let $N_G(u) \setminus \{w\} := \{u_1, u_2, \cdots, u_s\}$, with $s \geq 1$. Set $G' = G - uu_1 - \cdots - uu_s + v_0u_1 + \cdots + v_0u_s$. If $\alpha < 0$ or $\alpha > 1$, then $\chi_\alpha(G') < \chi_\alpha(G)$. Also, if $0 < \alpha < 1$ then $\chi_\alpha(G') > \chi_\alpha(G)$.*

Proof. If $\alpha < 0$ or $\alpha > 1$ then

$$\begin{aligned}
\chi_\alpha(G') - \chi_\alpha(G) &= (s + d_G(v) + 1)^\alpha - (s + d_G(u) + 1)^\alpha \\
&\quad + (d_G(u) + 1)^\alpha - (d_G(v) + 1)^\alpha \\
&\leq (d_G(v) + 2)^\alpha - (d_G(v) + 1)^\alpha \\
&\quad - [(d_G(u) + 2)^\alpha - (d_G(u) + 1)^\alpha] < 0 \, .
\end{aligned}$$

In a similar way, one gets $\chi_\alpha(G') - \chi_\alpha(G) > 0$ for $0 < \alpha < 1$. ■

Theorem 4. *If T is a tree of order n and maximum degree Δ such that $3 \le \lceil \frac{n}{2} \rceil \le \Delta \le n-2$, then*

$$\chi_\alpha(T) \ge (\Delta-1)(\Delta+1)^\alpha + (n-\Delta-1)(n-\Delta+1)^\alpha + n^\alpha \qquad (4)$$

and equality holds if and only if $T \cong DS_{n-\Delta-1,\Delta-1}$ for $\alpha < 0$.

Proof. We choose T such that $\chi_\alpha(T)$ is as small as possible. Take $w \in V(T)$ with $d_T(w) = \Delta \ge 3$. The assumption $\Delta \ge \lceil \frac{n}{2} \rceil$ implies that at least one of the neighbors of w is pendent (for otherwise, every component of $T-w$ contains at least two vertices and hence one has $n \ge 2\Delta+1$, a contradiction). Let $u_0 \in V(T)$ be a pendent neighbor of w. We first show two facts.

Fact 1. The vertex w has only one non-pendent neighbor.
Proof of Fact 1. Let $v \in V(T) \setminus \{w\}$ be a non-pendent vertex adjacent to a pendent vertex $v_0 \in V(T)$. Suppose to the contrary that w has at least two non-pendent neighbors. Then, there exists at least one non-pendent vertex $u \in N_T(w)$ such that u does not lie on the w-v path. Take $N_T(u) \setminus \{w\} := \{u_1, \cdots, u_s\}$, where $s \ge 1$. Since T contains at least Δ pendent vertices and $\Delta \ge \lceil \frac{n}{2} \rceil$, it holds that $d_T(v) \le n-\Delta-1 \le \lfloor \frac{n}{2} \rfloor - 1 \le \Delta - 1 < d_T(w)$. Set $T' = T - uu_1 - \cdots - uu_s + v_0u_1 + \cdots + v_0u_s$. Observe that T' has order n and Δ. But, by Lemma 7, we have $\chi_\alpha(T') < \chi_\alpha(T)$, a contradiction with the choice of T.

By Fact 1, $T-w$ contains only one non-trivial component; denote this unique non-trivial component of $T-w$ by C.

Fact 2. The component C of $T-w$ is a star.
Proof of Fact 2. Contrarily, assume that C is not a star. Then there exists at least one pair of non-pendent adjacent vertices $v', v \in V(T) \setminus \{w\}$. Take $d_T(v) = t \ge 2$ and $d_T(v') = s \ge 2$. We choose $v'v$ in such a way that the distance $d_T(w, v)$ is as large as possible. Then v has only one non-pendent neighbor. Let $v_1, v_2, \cdots, v_{t-1}$ be the all pendent neighbors of v. If $T' = T - vv_1 - vv_2 - \cdots - vv_{t-1} + v'v_1 + v'v_2 + \cdots + v'v_{t-1}$, then we

have

$$\chi_\alpha(T) - \chi_\alpha(T') = (t-1)[(t+1)^\alpha - (s+t)^\alpha] + \sum_{x \in N_T(v')\setminus\{v\}} [(d_T(x)+s)^\alpha - (d_T(x)+s+t-1)^\alpha] > (t-1)[(t+1)^\alpha - (s+t)^\alpha] > 0\,,$$

a contradiction to the choice of T.

By Facts 1 and 2, the proof of the theorem is complete. ■

Denote by $S^*_{n,\Delta}$ the tree of order n formed from the path $P_{n-\Delta+1}$ by attaching $\Delta - 1$ pendent vertices to only one of the pendent vertices of $P_{n-\Delta+1}$. Recall that a vertex (in a tree) of degree at least 3 is known as a branching vertex.

Theorem 5. *If T is a tree of order n and maximum degree Δ such that $3 \le \lceil \frac{n}{2} \rceil \le \Delta \le n-2$, then*

$$\chi_\alpha(T) \ge (\Delta-1)(\Delta+1)^\alpha + (\Delta+2)^\alpha + (n-\Delta-2)4^\alpha + 3^\alpha \tag{5}$$

for $\alpha > 1$ and equality holds if and only if $T \cong S^*_{n,\Delta}$.

Proof. Simple calculations yield

$$\chi_\alpha(S^*_{n,\Delta}) = (\Delta-1)(\Delta+1)^\alpha + (\Delta+2)^\alpha + (n-\Delta-2)4^\alpha + 3^\alpha$$

Next, let T be a tree of order n and maximum degree Δ such that $3 \le \lceil \frac{n}{2} \rceil \le \Delta \le n-2$ and that $\chi_\alpha(T)$ is as small as possible. Take $w \in V(T)$ with $d_T(w) = \Delta \ge 3$. By an argument similar to the proof of Theorem 4, we conclude that the vertex w has $\Delta - 1$ pendent neighbors.

We claim that the unique non-trivial component of $T - w$ is a path. In what follows, we prove this claim. Suppose to the contrary that the mentioned claim is not true. Then, there exists at least one branching vertex of T different from w. Let u be the unique non-pendent neighbor of w. Let $v \in V(T)$ be a branching vertex such that the distance $d_T(u,v)$ is as large as possible. Let $v_0v_1 \cdots v_{l-1}v$ be a pendent path of T. Take

$N_T(v) = \{x_1, \cdots, x_{s-2}, v', v_{l-1}\}$, where each of the vertices $x_1, \cdots, x_{s-2}$ does not lie on the w-v_{l-1} path and v' lies on the w-v_{l-1} path. Take $d_T(x_i) = a_i$ for $i = 1, 2, \cdots, s-2$, and $d_T(v') = b$. Certainly, $b \geq 2$ and $s \geq 3$. The vertices u and v may or may not be the same (if $u = v$ then $v' = w$). Set $T' = T - vx_1 - \cdots - vx_{s-2} + v_0x_1 + \cdots + v_0x_{s-2}$. Observe that T has order n and maximum degree Δ.
If $l = 1$, then

$$\begin{aligned}\chi_\alpha(T) - \chi_\alpha(T') &= \sum_{i=1}^{s-2}[(a_i + s)^\alpha - (a_i + (s-1))^\alpha] + (s+b)^\alpha - (b+2)^\alpha \\ &\geq (s-2)[(1+s)^\alpha - s^\alpha] + (s+2)^\alpha - 4^\alpha > 0 \ .\end{aligned}$$

If $l \geq 2$, then

$$\begin{aligned}\chi_\alpha(T) - \chi_\alpha(T') &= \sum_{i=1}^{s-2}[(a_i + s)^\alpha - (a_i + (s-1))^\alpha] + (s+b)^\alpha - (b+2)^\alpha \\ &\quad + [(s+2)^\alpha - (s+1)^\alpha] - [4^\alpha - 3^\alpha] \\ &> [(s+2)^\alpha - (s+1)^\alpha] - [4^\alpha - 3^\alpha] \\ &\geq 5^\alpha - 3^\alpha > 0 \ .\end{aligned}$$

Therefore, for $\alpha \geq 1$, we have $\chi_\alpha(T) > \chi_\alpha(T')$, a contradiction to the choice of T. Thus, we conclude that the unique non-trivial component of $T - w$ is a path and hence $T = S^*_{n,\Delta}$. By the choice of T, we deduce that $\chi_\alpha(T^\star) \geq \chi_\alpha(T) = \chi_\alpha(S^*_{n,\Delta})$ for any tree $T^\star$ of order n and maximum degree Δ, where $3 \leq \left\lceil \frac{n}{2} \right\rceil \leq \Delta \leq n-2$ and the equation $\chi_\alpha(T^\star) = \chi_\alpha(S^*_{n,\Delta})$ holds if and only if $T^\star = S^*_{n,\Delta}$. ■

***Acknowledgment*:** Zahid Raza has been funded during the work on this paper by the University of Sharjah under Project #2102144098 and #1802144068 and MASEP Research Group.

References

[1] S. Ahmed, On the maximum general sum-connectivity index of trees with a fixed order and maximum degree, *Discr. Math. Algor. Appl.* **13** (2021) #2150042.

[2] S. Akhter, M. Imran, Z. Raza, On the general sum-connectivity index and general Randić index of cacti, *J. Ineq. Appl.* **2016** (2016) #300.

[3] A. Ali, An alternative but short proof of a result of Zhu and Lu concerning general sum-connectivity index, *Asian-European J. Math.* **11** (2018) #1850030.

[4] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, *Discr. Appl. Math.* **238** (2018) 32–40.

[5] A. Ali, D. Dimitrov, Z. Du, F. Ishfaq, On the extremal graphs for general sum- connectivity index (χ_α) with given cyclomatic number when $\alpha > 1$, *Discr. Appl. Math.* **257** (2019) 19–30.

[6] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalization: Extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 249–311.

[7] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Comb.* **50** (1998) 225–233.

[8] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[9] G. Chartrand, L. Lesniak, P. Zhang, *Graphs & Digraphs*, CRC Press, Boca Raton, 2016.

[10] Q. Cui, L. Zhong, On the general sum-connectivity index of trees with given number of pendent vertices, *Discr. Appl. Math.* **222** (2017) 213–221.

[11] J. Devillers, A.T. Balaban, *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.

[12] Z. Du, B. Zhou, N. Trinajstić, Minimum general sum-connectivity index of unicyclic graphs, *J. Math. Chem.* **48** (2010) 697–703.

[13] Z. Du, B. Zhou, N. Trinajstić, On the general sum-connectivity index of trees, *Appl. Math. Lett.* **24** (2011) 402–405.

[14] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.

[15] M. K. Jamil, I. Tomescu, General sum-connectivity index of trees and unicyclic graphs with fixed maximum degree, *Proc. Rom. Acad. Ser. A* **20** (2019) 11–17.

[16] L. B. Kier, L. H. Hall, *Molecular Connectivity in Structure–Activity Analysis*, Wiley, New York, 1986.

[17] X. Li, I. Gutman, *Mathematical Aspects of Randić–Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.

[18] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[19] H. Liu, X. Yan, Z. Yan, Bounds of the general Randić index of trees with a given maximum degree, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 155–166.

[20] B. Lučić, N. Trinajstić, B. Zhou, Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons, *Chem. Phys. Lett.* **475** (2009) 146–148.

[21] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[22] R. Rasi, S. M. Sheikholeslami, The smallest harmonic index of trees with given maximum degree, *Discuss. Math. Graph Theory* **38** (2018) 499–513.

[23] R. Rasi, S. M. Sheikholeslami, I. Gutman, On Harmonic index of trees, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 405–416.

[24] R. M. Tache, I. Tomescu, General sum-connectivity index with $\alpha \geq 1$ for trees and unicyclic graphs with k pendents, in: *17th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing*, Timisoara, 2015, pp. 307–311.

[25] Y. Tang, D.B. West, B. Zhou, Extremal problems for degree-based topological indices, *Discr. Appl. Math.* **203** (2016) 134–143.

[26] I. Tomescu, S. Kanwal, Ordering trees having small general sum-connectivity index, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 535–548.

[27] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, 2018.

[28] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.

[29] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.