

Article

The smallest sum-connectivity index on trees with n vertices and k pendant vertices

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Abstract: For a given connected graph G and a real number α , denote by $d(u)$ the degree of vertex u of G , and denote by $\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha$ the general sum-connectivity index of G . In the present note, we determine the smallest general sum-connectivity index of trees (resp., chemical trees) together with corresponding extremal trees among all trees (resp., chemical trees) with n vertices and k pendant vertices for $0 < \alpha < 1$.

Keywords: General sum-connectivity index, chemical trees, extremal trees.

MSC: 05C05, 05C12, 05C50.

1. Introduction

Let $G = (V, E)$ be a connected undirected simple graph. If G contains exactly n vertices and $n - 1$ edges, then G is called a *tree*. For a vertex u of G , denote by $N(u)$ and $d(u)$ the neighborhood set and degree of u , that is, $d(u) = |N(u)|$. If $d(u) = k$, then we call u as a k -vertex. Specially, a 1-vertex is called a *pendant vertex*, while a k -vertex with $k \geq 2$ will be referred as a *non-pendant vertex*. A *pendant edge* is an edge incident with a pendant vertex. Hereafter, n_k defines the number of k -vertices. Denote by $\Delta(G)$ the maximum degree of G . As usual, S_n and P_n define the star and path with n vertices, respectively.

Let $G - uv$ be the resultant graph obtained after removing the edge uv from the edge set of G . Let $E_2(G) = \{uv : uv \in E(G) \text{ with } d(u) = d(v) = 2\}$. We write $A := B$ to indicate that B is the same as A .

The *first Zagreb index* $M_1(G)$ and *second Zagreb index* $M_2(G)$ [1] are two famous topological indices among all the vertex-degree-based graph invariants, where

$$M_1(G) = \sum_{v \in V(G)} (d(v))^2, \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

In what follows, α denotes a real number. As a generalization of $M_1(G)$, Li and Zheng [2] introduced the notation of *zeroth-order general Randić index* $R_\alpha^0(G)$, where

$$R_\alpha^0(G) = \sum_{v \in V(G)} (d(v))^\alpha.$$

Since $\sum_{uv \in E(G)} (d(u) + d(v)) = \sum_{v \in V(G)} (d(v))^2$, as another extension to $M_1(G)$, the *general sum-connectivity index* [3] $\chi_\alpha(G)$ of G is constructed as

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

Recently, the extremal problems of general sum-connectivity index among different categories of graphs have attracted more and more attention. In this field, Cui *et al.* [4] obtained the largest general sum-connectivity indices of trees and chemical trees with their corresponding extremal trees among all tree and chemical trees with n vertices and k pendant vertices for $-1 \leq \alpha < 0$; Tomescu *et al.* [5] identified

the smallest general sum-connectivity index of unicyclic graphs with n vertices and pendant vertices for $-1 \leq \alpha < 0$ and characterized the corresponding extremal graphs; Tomescu *et al.* [6] determined the smallest general sum-connectivity index of trees with fixed diameter, n vertices and k pendant vertices for $-1 \leq \alpha < 0$, respectively.

In what follows, by following the idea of [4], we will demonstrate the smallest general sum-connectivity index with its corresponding extremal trees in the class of trees and chemical trees with n vertices and k pendant vertices for $0 < \alpha < 1$, respectively.

2. Preliminaries

This section is dedicated to some lemmas, which will be used to prove our main result in the next section. For this aim, we need to introduce more notations. It is easily checked that any tree has at least two pendant vertices and the star is the unique tree with $n - 1$ pendant vertices and n vertices. For $2 \leq k \leq n - 1$, denote by $\mathcal{T}_{n,k}$ (resp., $\mathcal{CT}_{n,k}$) the set of trees (resp., chemical trees) with n vertices and k pendant vertices. If $T \in \mathcal{T}_{n,k}$ and every non-pendant vertex of T is a 3-vertex, then T is called a $(k, 3)$ -tree. It can be straightly checked that every $(k, 3)$ -tree has $2k - 2$ vertices, among which there is exactly k pendant vertices.

Let $\mathcal{T}_{n,k}^* = \{T : T \text{ is obtained from a } (k, 3)\text{-tree } H \text{ by adding } n - 2k + 2 \text{ new 2-vertices to } H \text{ such that every pendant edge of } H \text{ is inserted at least one new 2-vertex}\}$. For every tree T of $\mathcal{T}_{n,k}^*$, from the definition of $\mathcal{T}_{n,k}^*$ we can conclude that $|V(T)| = n$, $\Delta(T) = 3$ and each neighbor vertex of a 3-vertex is either a 3-vertex or a 2-vertex. This implies that $n_1(T) = k$, $n_2(T) = n - 2k + 2$ and $n_3(T) = k - 2$. For example, there are exactly trees in the class of $\mathcal{T}_{12,4}^*$, which are shown in Figure 1. Combining with $\mathcal{T}_{n,2} = \mathcal{CT}_{n,2} = \{P_n\}$, $\mathcal{T}_{n,n-1} = \{S_n\}$ and $\mathcal{CT}_{n,n-1} = \{S_n \mid 3 \leq n \leq 5\}$, we only take $3 \leq k \leq n - 2$ into consideration in what follows.

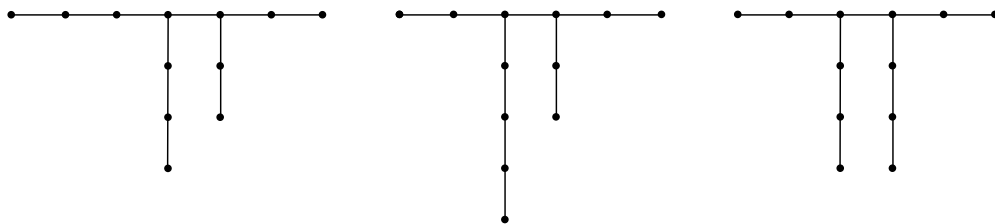


Figure 1. The elements of the set $\mathcal{T}_{12,4}^*$.

The following three transformations on a tree T with n vertices were firstly constructed by Zhang *et al.* [7], they will play an important role in the proof of our main result.

(i) For a fixed edge uv of the tree T with n vertices, denote by T_{uv} the tree obtained from T via identifying the two vertices of $T - uv$, that is, T_{uv} is a tree with $n - 1$ vertices obtained from T by contracting the edge uv of T . Hereafter, we say that T_{uv} is obtained from T by **Transformation I**.

(ii) Let $v \in V(T)$ with $N(v) = V' \cup V''$ satisfying $V' \cap V'' = \emptyset$, $|V'| = q_1 \geq 1$ and $|V''| = q_2 \geq 1$. Denote by $T_{v \rightarrow (q_1, q_2)}$ the tree with $n + 1$ vertices constructed from the tree T via splitting the vertex v into two new vertices v' and v'' , adding one edge between v' and v'' , joining v' and all vertices of V' , and then joining v'' and all vertices of V'' . In the sequel, $T_{v \rightarrow (q_1, q_2)}$ will be referred to be obtained from T by **Transformation II**.

(iii) Let v be a q -vertex of the tree T , where $q \geq 4$. Denote by $T_{v \rightarrow (3-reg)}$ the graph with $n + q - 3$ vertices obtained from T via replacing the vertex v of T with a $(q, 3)$ -tree H such that every vertex of $N(v)$ and every pendant vertex of H are identified individually. In what follows, we say that $T_{v \rightarrow (3-reg)}$ is obtained from T by **Transformation III**.

Let T be the tree with eight vertices as shown in Figure 2. The readers can refer to Figure 2 for illustrated examples to the above three transformations, where $V' = \{u\}$ and $V'' = \{v_1, v_2, v_3\}$.

Lemma 1. If $k \geq 1$ and $0 < \alpha < 1$, then $\varphi(x) = (x + k)^\alpha - x^\alpha$ is a strictly decreasing function for $x \geq 1$.

Proof. It is easy to see that $\varphi'(x) = \alpha \left((x + k)^{\alpha-1} - x^{\alpha-1} \right) < 0$ for $k \geq 1$ and $0 < \alpha < 1$. Consequently, the result holds. □

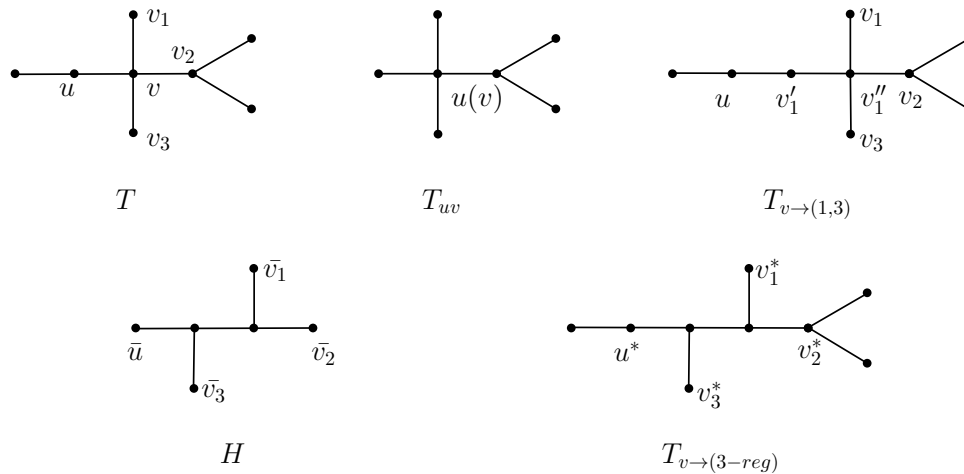


Figure 2. The example of three transformations.

Lemma 2. Let T be a tree of $\mathcal{T}_{n,k}$ and w be a 2-vertex of T . If the two neighbor vertices of w are both non-pendant vertices and $0 < \alpha < 1$, then there is a tree T^* of $\mathcal{T}_{n,k}$ such that $\chi_\alpha(T) \geq \chi_\alpha(T^*)$, with equality iff w is adjacent to at least one 2-vertex.

Proof. Suppose that $N(w) = \{u, v\}$ with $d(u) = s \geq 2$ and $d(v) = t \geq 2$. Let y be a pendant vertex with $xy \in E(G)$ and $d(x) = r \geq 2$. By Transformation I, we can construct T_{uv} from T . Let T^* be the tree obtained from T_{uv} via adding a new pendant edge adjacent to x . Now, it is easily checked that T^* is also a tree of $\mathcal{T}_{n,k}$ such that

$$\begin{aligned} \chi_\alpha(T) - \chi_\alpha(T^*) &= (s + 2)^\alpha + (t + 2)^\alpha + (r + 1)^\alpha - (s + t)^\alpha - (r + 2)^\alpha - 3^\alpha \\ &= \left((s + 2)^\alpha + (t + 2)^\alpha - (s + t)^\alpha \right) - \left((r + 2)^\alpha - (r + 1)^\alpha \right) - 3^\alpha. \end{aligned}$$

Let $\psi(s, t) = (s + 2)^\alpha + (t + 2)^\alpha - (s + t)^\alpha$ with $s, t \geq 2$. Combining with $0 < \alpha < 1$, we have

$$\frac{\partial \psi(s, t)}{\partial s} = \alpha \left((s + 2)^{\alpha-1} - (s + t)^{\alpha-1} \right) \geq 0, \text{ and } \frac{\partial \psi(s, t)}{\partial t} = \alpha \left((t + 2)^{\alpha-1} - (s + t)^{\alpha-1} \right) \geq 0,$$

this implies that $\psi(s, t)$ is increasing for both s and t with $s, t \geq 2$. In view of Lemma 1 (the case of $k = 1$), it follows that

$$\chi_\alpha(T) - \chi_\alpha(T^*) = \psi(s, t) - \varphi(r + 1) - 3^\alpha \geq \psi(2, 2) - \varphi(3) - 3^\alpha = 0.$$

So the assertion of the lemma holds. □

Lemma 3. Let T be a tree of $\mathcal{T}_{n,k}$ and xy be an edge of T with $d(x) = q \geq 3$ and $d(y) = 1$. If $0 < \alpha < 1$ and $E_2(T) \neq \emptyset$, then there is a tree T^* of $\mathcal{T}_{n,k}$ with $\chi_\alpha(T) > \chi_\alpha(T^*)$.

Proof. Note that $E_2(T) \neq \emptyset$. Thus, we can construct a new tree T^* with $n - 1$ vertices from T by contracting an arbitrary edge of $E_2(T)$ and then inserting another new vertex to the pendant edge xy . Now, T^* is also a tree of $\mathcal{T}_{n,k}$. By Lemma 1 (the case of $k = 1$), it follows that

$$\begin{aligned} \chi_\alpha(T) - \chi_\alpha(T^*) &= 4^\alpha + (q + 1)^\alpha - (q + 2)^\alpha - 3^\alpha \\ &= (4^\alpha - 3^\alpha) - \left((q + 2)^\alpha - (q + 1)^\alpha \right) \\ &= \varphi(3) - \varphi(q + 1) > 0. \end{aligned}$$

This finishes the proof of the lemma. □

Lemma 4. Let T be a tree of $\mathcal{T}_{n,k}$ and u be a 4-vertex of T . Let v_1, v_2, v_3 and v_4 be four neighbor vertices of u such that $d(v_4) \leq 5$ and $d(v_1) \leq d(v_2) \leq d(v_3) \leq 3$. If $0 < \alpha < 1$ and $E_2(T) \neq \emptyset$, then there is tree T^* of $\mathcal{T}_{n,k}$ with $\chi_\alpha(T) > \chi_\alpha(T^*)$.

Proof. Note that $E_2(T) \neq \emptyset$. Thus, we can construct a new tree T' with $n - 1$ tree from T via contracting an arbitrary edge of $E_2(T)$. By Transformation III, we can construct another tree $T^* := T_{v \rightarrow (3-reg)}^*$ from T' such that $T^* \in \mathcal{T}_{n,k}$. Since $d(v_1) \leq d(v_2) \leq d(v_3) \leq 3, d(v_4) \leq 5$ and in view of Lemma 1 (the case of $k = 1$), it follows that

$$\begin{aligned} \chi_\alpha(T) - \chi_\alpha(T^*) &= 4^\alpha + \sum_{i=1}^4 \left((4 + d(v_i))^\alpha - (3 + d(v_i))^\alpha \right) - 6^\alpha \\ &\geq 4^\alpha + 3(7^\alpha - 6^\alpha) + (9^\alpha - 8^\alpha) - 6^\alpha \\ &= 4^\alpha - 4 \cdot 6^\alpha + 3 \cdot 7^\alpha - 8^\alpha + 9^\alpha. \end{aligned}$$

Let $\phi(\alpha) = 4^\alpha - 4 \cdot 6^\alpha + 3 \cdot 7^\alpha - 8^\alpha + 9^\alpha$ with $0 < \alpha < 1$. It can be easily checked that $\phi(\alpha) > 0$ for $0 < \alpha < 1$ by applying *MATLAB*, see Figure 3 (Actually, Figures 3-5 are all drawn by *MATLAB*). □

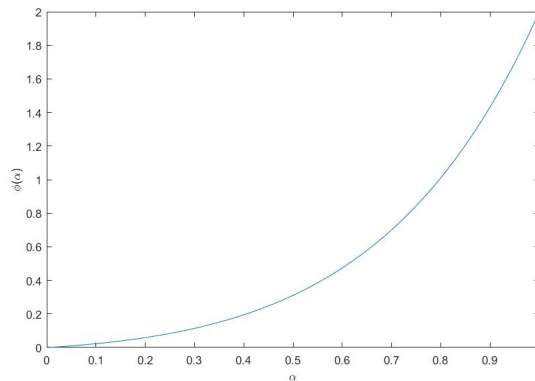


Figure 3. The function $\phi(\alpha)$ in Lemma 4.

Lemma 5. Let T be a tree of $\mathcal{T}_{n,k}$ and u be a q -vertex of T , where $q \geq 4$. Suppose that $|E_2(T)| \geq q - 3$ and $N(u) = \{v_1, v_2, \dots, v_q\}$ with $d(v_1) \leq d(v_2) \leq \dots \leq d(v_q)$. If $0 < \alpha < 1$ and T satisfies either (i) or (ii), then there is a tree T^* of $\mathcal{T}_{n,k}$ with $\chi_\alpha(T) > \chi_\alpha(T^*)$, where (i) $d(v_{q-1}) \leq 3$ and $q \geq 5$; and (ii) $d(v_{q-1}) \leq 4$ and $q \geq 8$.

Proof. Let $d(v_{q-1}) = p$. Note that $|E_2(T)| \geq q - 3$. Thus, we can construct a new tree T' with $n + 3 - q$ vertices obtained from T by contracting $q - 3$ arbitrary edges of $E_2(T)$. Taking Transformation III into consideration, we can construct another tree $T^* := T_{v \rightarrow (3-reg)}^*$ from T' . Now, T^* is also a tree of $\mathcal{T}_{n,k}$. Since $q \geq 4, 0 < \alpha < 1$ and in view of Lemma 1 (the case of $k = q - 3 \geq 1$), we have

$$\begin{aligned} \chi_\alpha(T) - \chi_\alpha(T^*) &= (q - 3)4^\alpha + \sum_{i=1}^q \left((d(v_i) + q)^\alpha - (d(v_i) + 3)^\alpha \right) - (q - 3)6^\alpha \\ &\geq (q - 3)(4^\alpha - 6^\alpha) + (q - 1) \left((p + q)^\alpha - (p + 3)^\alpha \right) \\ &\quad + \left((d(v_q) + q)^\alpha - (d(v_q) + 3)^\alpha \right) \\ &> (q - 3)(4^\alpha - 6^\alpha) + (q - 1) \left((p + q)^\alpha - (p + 3)^\alpha \right). \end{aligned} \tag{1}$$

Let $\phi(p, q) = (q - 3)(4^\alpha - 6^\alpha) + (q - 1) \left((p + q)^\alpha - (p + 3)^\alpha \right)$, where $p \geq 1, q \geq 4$ and $0 < \alpha < 1$. By Lemma 1 (the case of $k = q - 3 \geq 1$), $\phi(p, q)$ is a strictly decreasing function on p . Since $0 < \alpha < 1$, then

$$\frac{\partial \phi(p, q)}{\partial q} = \left((p + q)^\alpha - (p + 3)^\alpha \right) + \alpha(q - 1)(p + q)^{\alpha - 1} + (4^\alpha - 6^\alpha),$$

$$\begin{aligned} \frac{\partial^2 \phi(p, q)}{\partial q^2} &= \alpha(p+q)^{\alpha-2} \left((\alpha-1)(q-1) + 2(p+q) \right) \\ &\geq \alpha(p+q)^{\alpha-2} (2p+q+1) > 0. \end{aligned}$$

Thus, $\frac{\partial \phi(p, q)}{\partial q}$ is a strictly increasing function on q .

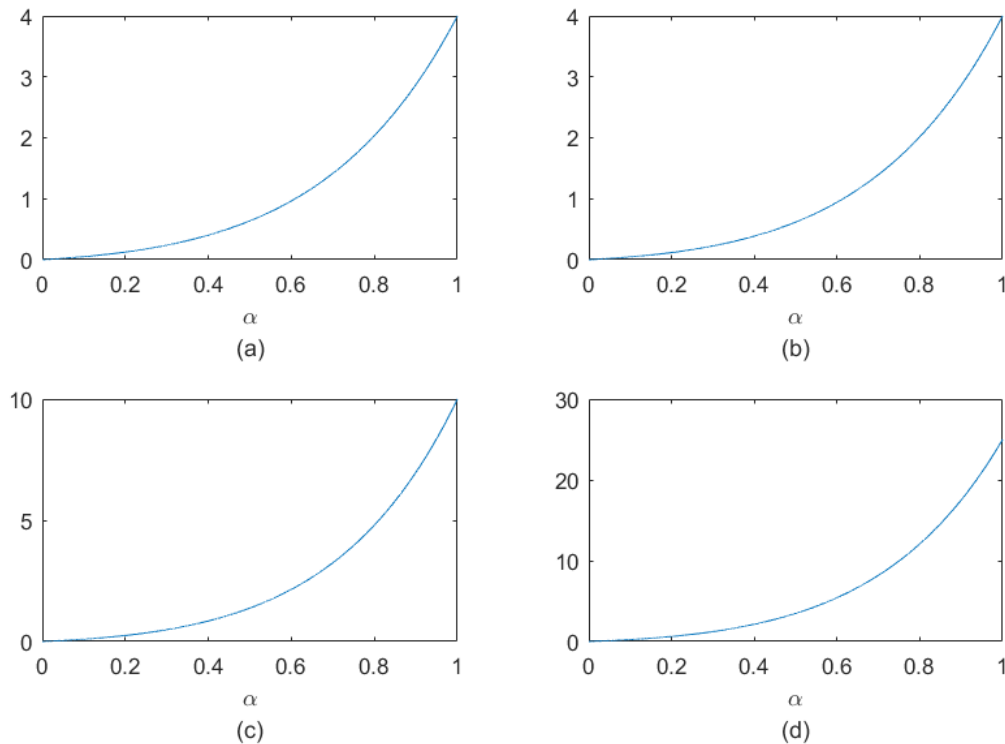


Figure 4. The four functions of α in Lemma 5.

We consider the following two cases:

Case 1. T satisfies (i). In this case, we have $q \geq 5$ and $p \leq 3$, and so $\phi(p, q) \geq \phi(3, q)$. This implies that

$$\begin{aligned} \frac{\partial \phi(3, q)}{\partial q} &\geq \frac{\partial \phi(3, q)}{\partial q} \Big|_{q=5} \\ &= 4\alpha 8^{\alpha-1} + (4^\alpha - 6^\alpha) + (8^\alpha - 6^\alpha) = (8 + 4\alpha)8^{\alpha-1} + 4^\alpha - 2 \cdot 6^\alpha > 0, \end{aligned}$$

where Figure 4 (a) implies the last strictly inequality. Therefore, $\phi(3, q)$ is a strictly increasing function on $q \geq 5$. Combining this with inequality (1), we obtain that

$$\begin{aligned} \chi_\alpha(T) - \chi_\alpha(T^*) &> \phi(p, q) \geq \phi(3, q) \geq \phi(3, 5) \\ &= 4(8^\alpha - 6^\alpha) + 2(4^\alpha - 6^\alpha) = 4 \cdot 8^\alpha + 2 \cdot 4^\alpha - 6^{\alpha+1} > 0, \end{aligned}$$

where Figure 4 (b) implies the last strictly inequality.

Case 2. T satisfies (ii). In this case, we have $q \geq 8$ and $p \leq 4$, and so $\phi(p, q) \geq \phi(4, q)$. This implies that

$$\begin{aligned} \frac{\partial \phi(4, q)}{\partial q} &\geq \frac{\partial \phi(4, q)}{\partial q} \Big|_{q=8} \\ &= 7\alpha 12^{\alpha-1} + (4^\alpha - 6^\alpha) + (12^\alpha - 7^\alpha) \\ &= (12 + 7\alpha)12^{\alpha-1} + 4^\alpha - 6^\alpha - 7^\alpha > 0, \end{aligned}$$

where Figure 4 (c) implies the last strictly inequality. Thus, $\phi(4, q)$ is a strictly increasing function on $q \geq 8$. By (1), we can conclude that

$$\chi_\alpha(T) - \chi_\alpha(T^*) > \phi(p, q) \geq \phi(4, q) \geq \phi(4, 8) = 7(12^\alpha - 7^\alpha) + 5(4^\alpha - 6^\alpha) > 0,$$

where Figure 4 (d) implies the last strictly inequality. □

Let $P = u_0u_1 \dots u_q$ be a path of graph G . If u_0 is a pendant vertex of G and $d(u_1) = d(u_2) = \dots = d(u_{q-1}) = 2 < 3 \leq d(u_q)$ unless $q = 1$, then we call P as a *pendant path* of G . Hereafter, denote by $\mathcal{P}(G)$ the set of all pendant paths of G .

Lemma 6. [7] *Let T be a tree of $\mathcal{T}_{n,k}$. If $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$ and $E_2(T) \subseteq E(\mathcal{P}(T))$, then*

$$|E_2(T)| \geq n_4 + 2n_5 + \dots + (\Delta(T) - 3)n_{\Delta(T)}.$$

3. Main results

Now, we are ready to state the main result of this paper, that is,

Theorem 7. *Let T be a tree of $\mathcal{T}_{n,k}$. If $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$ and $0 < \alpha < 1$, then*

$$\chi_\alpha(T) \geq k(3^\alpha + 5^\alpha) + (n - 3k + 2)4^\alpha + (k - 3)6^\alpha,$$

with the equality iff $T \in \mathcal{T}_{n,k}^*$.

Proof. Throughout this proof, we suppose that $T^* \in \mathcal{T}_{n,k}$ has the smallest general sum-connectivity index. Since $k \geq 3$, then $\Delta(T^*) \geq 3$. Next, we prove some claims.

Claim 1. Every 2-vertex of T^* is on a pendant path.

Proof of the Claim 1. By contradiction, assume that u_0 is not on any pendant path of T^* with $d(u_0) = 2$. In this case, each neighbor vertex of u_0 is a non-pendant vertex. In view of Lemma 2, $\mathcal{T}_{n,k}$ contains a tree T_1 such that $\chi_\alpha(T^*) \geq \chi_\alpha(T_1)$, with equality iff u_0 is adjacent to at least one 2-vertex.

By applying the transformations in the proof of Lemma 2 repeatedly, a set of trees $\{T_i \mid i \geq 0\}$ belonging to $\mathcal{T}_{n,k}$ with $T_0 := T^*$ and a set of vertices $\{u_i \mid i \geq 0\}$ can be constructed such that each u_i is a 2-vertex not on any pendant path of T_i and $\chi_\alpha(T_i) \geq \chi_\alpha(T_{i+1})$ for each $i \geq 0$.

Since the number of 2-vertices not on pendant paths of T_{i+1} is one less than that of T_i , the above transformation will end after finite steps. That is, there is an integer $q \geq 0$ such that each 2-vertex of T_{q+1} is on a pendant path. Therefore, u_q is the unique 2-vertex of T_q not on any pendant path, and hence u_q is adjacent to two vertices with degrees at least 3 in T_q . Thus, we have $\chi_\alpha(T_0) \geq \chi_\alpha(T_1) \geq \dots \geq \chi_\alpha(T_q) > \chi_\alpha(T_{q+1})$, which is contrary with the choice of T^* . □

By Claim 1, it follows that $E_2(T^*) \subseteq E(\mathcal{P}(T^*))$. Next we shall prove that

$$\Delta(T^*) = 3. \tag{2}$$

By contradiction, we assume that (2) does not hold, that is, $\Delta(T^*) \geq 4$. From Lemma 6, it follows that

$$|E_2(T^*)| \geq n_4 + 2n_5 + \dots + (\Delta(T^*) - 3)n_{\Delta(T^*)} \geq \Delta(T^*) - 3 \geq 1.$$

Suppose that $v_0 \in T^*$ with $d(v_0) = \Delta(T^*) \geq 4$, and let $P := v_0v_1 \dots v_t$ be a path of T^* with $d(v_t) \geq 4$. We may assume that the length of P is as large as possible. If $t = 0$, then Lemmas 4 and 5 (i) imply that $\mathcal{T}_{n,k}$ contains a tree with smaller general sum-connectivity index than T^* , but this contradicts the definition of T^* . Thus, $t \geq 1$. By Claim 1, we have $\min \{d(v_i) : 1 \leq i \leq t - 1\} \geq 3$ when $t \geq 2$.

Let $N^*(v_{t-1}) := N(v_{t-1})$ when $t = 1$, and let $N^*(v_{t-1}) := N(v_{t-1}) \setminus \{v_{t-2}\}$ when $t \geq 2$. It is not difficult to see that $v_t \in N^*(v_{t-1})$.

Claim 2. The degree of each vertex of $N^*(v_{t-1})$ in T^* is at most 4 and $d(v_t) = 4$.

Proof of Claim 2. Let $z \in N^*(v_{t-1})$ and let $N(z) = \{z_1, z_2, \dots, z_q\}$ with $d(z_1) \leq d(z_2) \leq \dots \leq d(z_q)$. Clearly, $|E_2(T^*)| \geq \Delta(T^*) - 3 \geq q - 3$. Recall that the length of P is as large as possible. Thus, $d(z_{q-1}) \leq 3$. Since $d(v_{t-1}) = \Delta(T^*) \geq 4 > d(z_{q-1})$ when $t = 1$ (in this case, $v_{t-1} = v_0$) and $d(v_{t-1}) \geq 3 \geq d(z_{q-1})$ when $t \geq 2$, we may suppose that $z_q = v_{t-1}$. By the choice of T^* and in view of Lemma 5 (i), we deduce that $d(z) \leq 4$. Note that $v_t \in N^*(v_{t-1})$ and $d(v_t) \geq 4$, we have $d(v_t) = 4$. This completes the proof of Claim 2. \square

Now, we consider the vertex v_{t-1} . On the one hand, in view of Claim 2, all vertices of $N(v_{t-1})$ except v_{t-2} (when $t \geq 2$) have degrees at most 4 in T^* . Since Lemma 5 (ii) and in view of the choice of T^* , we can conclude that $d(v_{t-1}) \leq 7$. On the other hand, by the proof of Claim 2 we can deduce that the degree of each vertex of $N(v_t)$ except v_{t-1} in T^* is at most 3. Now, in view of $d(v_t) = 4$ and bearing in mind the choice of T^* , Lemma 4 implies that $d(v_{t-1}) \geq 6$. Consequently, we know that $6 \leq d(v_{t-1}) \leq 7$.

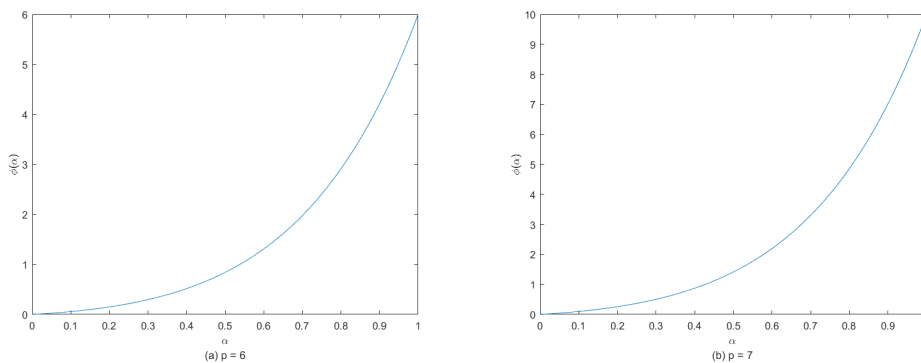


Figure 5. The function $\phi(\alpha)$ in Theorem 7.

Let $d(v_{t-1}) = p$ and let $N(v_{t-1}) = \{w_1, w_2, \dots, w_p\}$ with $w_p := v_{t-2}$ when $t \geq 2$. In view of Claim 2, it follows that $d(w_i) \leq 4$ for $1 \leq i \leq p - 1$. Since $|E_2(T^*)| \geq 1$, we can construct a new tree \bar{T} obtained after contracting an edge of $E_2(T^*)$ from T^* . By Transformation II, we can construct another tree $T' := \bar{T}_{v_{t-1} \rightarrow (3,p-3)}$ of $\mathcal{T}_{n,k}$ from \bar{T} . By Combining with $0 < \alpha < 1, 6 \leq p \leq 7$ and Lemma 1 (the case of $k = p - 4 > 1$ and $k = 2$, respectively), we have

$$\begin{aligned} \chi_\alpha(T^*) - \chi_\alpha(T') &= 4^\alpha + \sum_{i=1}^3 \left((d(w_i) + p)^\alpha - (d(w_i) + 4)^\alpha \right) \\ &\quad + \sum_{i=4}^p \left((d(w_i) + p)^\alpha - (d(w_i) + p - 2)^\alpha \right) - (p + 2)^\alpha \\ &\geq 4^\alpha + 3 \left((p + 4)^\alpha - 8^\alpha \right) + (p - 4) \left((p + 4)^\alpha - (p + 2)^\alpha \right) \\ &\quad + \left((d(w_p) + p)^\alpha - (d(w_p) + p - 2)^\alpha \right) - (p + 2)^\alpha \\ &> 4^\alpha + 3 \left((p + 4)^\alpha - 8^\alpha \right) + (p - 4) \left((p + 4)^\alpha - (p + 2)^\alpha \right) - (p + 2)^\alpha \\ &= (p - 1)(p + 4)^\alpha + 4^\alpha - 3 \cdot 8^\alpha - (p - 3)(p + 2)^\alpha. \end{aligned}$$

Let $\phi(\alpha) = (p - 1)(p + 4)^\alpha + 4^\alpha - 3 \cdot 8^\alpha - (p - 3)(p + 2)^\alpha$, where $0 < \alpha < 1$. If $p = 6$, then $\phi(\alpha) > 0$, where Figure 5 (a) implies the inequality. If $p = 7$, then $\phi(\alpha) > 0$, where Figure 5 (b) implies the inequality. Now, we can conclude that $\chi_\alpha(T^*) - \chi_\alpha(T') > 0$ whenever $6 \leq p \leq 7$, a contradiction. So, (2) holds.

By (2), we have $n_1 + n_2 + n_3 = n$ and $n_1 + 2n_2 + 3n_3 = 2(n - 1)$. Note that $n_1 = k$ and $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$. Thus, $n_2 = n - 2k + 2 \geq k$. Now, in view of Claim 1 and (2), to finish our proof, it suffices to show that each pendant vertex is adjacent to a 2-vertex. By contradiction, we assume that there is a pendant vertex u of T^* such that u is adjacent to a 3-vertex. Since $n_2 \geq k$ and in view of Claim 1, we have $E_2(T^*) \neq \emptyset$. By the choice of T^* and in view of Lemma 3, it will deduce a contradiction. Thus, every pendant vertex of T^* must be adjacent to a 2-vertex. By a simple calculation, we have

$$\chi_\alpha(T^*) = k(3^\alpha + 5^\alpha) + (n - 3k + 2)4^\alpha + (k - 3)6^\alpha.$$

This completes the proof of the theorem. □

In view of Theorem 7 and since $\mathcal{T}_{n,k}^* \subseteq \mathcal{CT}_{n,k} \subseteq \mathcal{T}_{n,k}$, we can deduce the following result for chemical trees immediately.

Theorem 8. *Let T be a tree of $\mathcal{CT}_{n,k}$. If $0 < \alpha < 1$ and $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$, then*

$$\chi_\alpha(T) \geq k(3^\alpha + 5^\alpha) + (n - 3k + 2)4^\alpha + (k - 3)6^\alpha,$$

with the equality iff $T \in \mathcal{T}_{n,k}^*$.

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