Trees with a given order and matching number that have maximum general sum-connectivity index

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Abstract. The general sum-connectivity index is defined as $\chi_{\alpha}(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^{\alpha}$. Let $\mathcal{T}(n,\beta)$ be the class of trees of order n with given matching number β . In this paper, we characterize the structure of the trees with a given order and matching number that have maximum general sum-connectivity index for $0 < \alpha < 1$ and give sharp upper bound for $\alpha \ge 1$.

Keywords: general sum-connectivity index; tree; matching

AMS subject classification: 05C69, 05C05

1. Introduction

Let G = (V(G), E(G)) be a connected simple graph with |V(G)| = n and |E(G)| = m. If m = n + c - 1, then G is called a c-cyclic graph. Specially, if c = 0 or 1, then G is called a tree or a unicyclic graph, respectively. Let $N_G(v)$ denote the neighbor set of vertex v in G, then $d_G(v) = |N_G(v)|$ is named the degree of v in G. Let $\Delta(G)$ be the maximum degree of G. Let P_n and S_n be respectively the path and the star with n vertices. A pendent path in G is a path having one end-vertex of degree at least 3, the other is of degree 1 and the intermediate vertices are of degree 2. An internal path of G is defined as a walk $v_0v_1 \dots v_s(s \ge 1)$ such that the vertices v_0, v_1, \dots, v_s are distinct, $d_G(v_0) > 2$, $d_G(v_s) > 2$ and $d_G(v_i) = 2$, whenever 0 < i < s. For a path P_n , denote by $|P_n|$ the length of P_n . A matching M of the graph G is a subset of E(G) such that no two edges in M share a common vertex. A matching M of G is said to be maximum, if for any other matching M' of G, $|M'| \le |M|$. The matching number G of G is the number of edges of a maximum matching in G. If G is a matching

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of a graph G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be M-saturated, otherwise be M-unsaturated.

The well-known Randić connectivity index R(G) of G, is defined as: $R(G) = \sum_{uv \in E(G)} (d_G(u)d_G(v))^{-\frac{1}{2}}$, which is proposed by Randić in 1975 [1], has received intensive attention since its successful applications in QSPR and QSAR [2]. Its mathematical properties as well as those of its generalizations have been studied extensively as summarized in the books [3, 4]. Recently, a closely related variant of Randić connectivity index called the sum-connectivity index [5], denoted by $\chi(G)$, is defined as: $\chi(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^{-\frac{1}{2}}$.

It has been found that the sum-connectivity index and the Randić connectivity index correlate well among themselves and with π -electronic energy of benzenoid hydrocarbons [5]. The ordinary Randić connectivity index has been extended to the general Randić connectivity index [4] defined as: $R_{\alpha}(G) = \sum_{uv \in E(G)} (d_G(u)d_G(v))^{\alpha}$, where α is a real number. Motivated by this, the general sum-connectivity index [6] is defined as: $\chi_{\alpha}(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^{\alpha}$.

Some properties of $\chi_{\alpha}(G)$, such as for trees and unicyclic graphs, have already been established [6, 7]. But by the results of experiments, B. Zhou and N. Trinajstić [7] have pointed out that the optimum exponent of the sum-connectivity index depends on the property considered and the properties of the general sum-connectivity index warrant further studies. In this paper, we will study the trees of order n with given matching number β , and characterize the structure of the trees which have maximal general sum-connectivity index for $0 < \alpha < 1$ and give sharp upper bound for $\alpha \ge 1$ in $\mathcal{F}(n,\beta)$, where $\mathcal{F}(n,\beta)$ is the class of trees of order n with given matching number β .

2. Trees with maximal general sum-connectivity index in $\mathcal{T}(n,\beta)$

For convenience, let T^* be the extremal tree in $\mathcal{T}(n,\beta)$ which has maximal general sum-connectivity index for $\alpha>0$, $V^*=\{v\in V(T^*),d(v)\geq 3\}$, and M^* a fixed maximum matching of T^* . Note that if $\beta=1$, then $T^*\cong S_n$; if $\beta=2, n=4, T^*\cong P_4$. Hence we can only consider the case for $\beta\geq 2$ and $n\geq 5$ in the following discussion. Note that we have $\Delta(T^*)\geq 3$. Otherwise, if $\Delta(T^*)\leq 2$, then T^* must be a path. Let $T^*=v_0v_1\ldots v_{n-1}$ and $T'=T^*-\{v_1v_2\}+\{v_1v_3\}$, it is easy to see that T' and T have the same matching number and $\chi_{\alpha}(T')-\chi_{\alpha}(T^*)=5^{\alpha}-3^{\alpha}>0$, for n=5,

and for $n \ge 6 \ \chi_{\alpha}(T') - \chi_{\alpha}(T^*) = 2 \cdot 5^{\alpha} - 2 \cdot 4^{\alpha} > 0$, it is contradict to maximality of T^* .

Lemma 2.1. Let P be a pendent path of T^* , then $|P| \leq 2$.

Proof. Assume to the contrary that $P=v_0v_1\dots v_l$ $(l\geq 3)$ is a pendent path of T^* with $d(v_0)=t$ $(t\geq 3)$, $d(v_l)=1$, $d(v_1)=\dots=d(v_{l-1})=2$. Denote $N_0=N_{T^*}(v_0)\setminus\{v_1\}$. Let $T'=T^*-\{v_{l-2}v_{l-1}\}+\{v_0v_l\}$. Note that if $v_{l-1}v_l\in M^*$, it must have $v_{l-2}v_{l-1}\notin M^*$, then M^* is also a maximal matching of T'. If $v_{l-1}v_l\notin M^*$, it must have $v_{l-2}v_{l-1}\in M^*$, then $M^*-\{v_{l-2}v_{l-1}\}+\{v_{l-1}v_l\}$ is a maximal matching of T'. Hence $T'\in \mathcal{T}(n,\beta)$.

Case 1. If $l \geq 4$, then $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > [(t+3)^{\alpha} - 4^{\alpha}] - [4^{\alpha} - 3^{\alpha}] \geq [6^{\alpha} - 4^{\alpha}] - [4^{\alpha} - 3^{\alpha}]$. By the Lagrange mean-value theorem, we have $[6^{\alpha} - 4^{\alpha}] - [4^{\alpha} - 3^{\alpha}] = \alpha(2 \cdot \eta_{1}^{\alpha - 1} - \eta_{2}^{\alpha - 1})$, where $\eta_{1} \in (4,6), \eta_{2} \in (3,4)$. If $\alpha \geq 1$, it is obvious that $2 \cdot \eta_{1}^{\alpha - 1} - \eta_{2}^{\alpha - 1} > 0$. If $\alpha \in (0,1), 2 \cdot \eta_{1}^{\alpha - 1} - \eta_{2}^{\alpha - 1} > 2 \cdot 6^{\alpha - 1} - 3^{\alpha - 1}$, and $\frac{2 \cdot 6^{\alpha - 1}}{3^{\alpha - 1}} = \frac{2}{2^{1 - \alpha}} > 1$, then $2 \cdot \eta_{1}^{\alpha - 1} - \eta_{2}^{\alpha - 1} > 0$. Hence $\chi_{\alpha}(T') > \chi_{\alpha}(T^*)$, a contradiction.

Case 2. If l=3, then

$$\chi_{\alpha}(T') - \chi_{\alpha}(T^{*}) = \sum_{u \in N_{0}} (t+1+d(u))^{\alpha} + (t+3)^{\alpha} + (t+2)^{\alpha} - \left[\sum_{u \in N_{0}} (t+d(u))^{\alpha} + (t+2)^{\alpha} + 4^{\alpha}\right] > 0,$$

also a contradiction. This completes the proof.

Lemma 2.2. Let P be an internal path of T^* , then $|P| \leq 1$.

Proof. Assume to the contrary that $P = v_0 v_1 \dots v_l (l \ge 2)$ is an internal path of T^* with $d(v_0) = t(t \ge 3)$, $d(v_l) = s(s \ge 3)$, $d(v_1) = \dots = d(v_{l-1}) = 2$. Let $N_0 = N_{T^*}(v_0) \setminus \{v_1\}$ and $N_1 = N_{T^*}(v_l) \setminus \{v_{l-1}\}$.

Case 1. l = 2.

Subcase 1.1. If v_1 is M^* -unsaturated, then v_0 and v_2 are both M^* -saturated. Let $T' = T^* - \{v_1v_2\} + \{v_0v_2\}$, we have $T' \in \mathcal{T}(n,\beta)$ (as shown in Figure 1).

$$\chi_{\alpha}(T') - \chi_{\alpha}(T^{*})$$

$$= \sum_{u \in N_{0}} (t+1+d(u))^{\alpha} + (t+2)^{\alpha} + (t+s+1)^{\alpha} + \sum_{u \in N_{1}} (s+d(u))^{\alpha}$$

$$- [\sum_{u \in N_{0}} (t+d(u))^{\alpha} + (t+2)^{\alpha} + (s+2)^{\alpha} + \sum_{u \in N_{1}} (s+d(u))^{\alpha}] > 0,$$

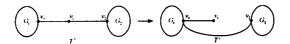


Figure 1: The graphs T^* and T' in Subcase 1.1.

a contradiction.

Subcase 1.2. If v_1 is M^* -saturated, without loss of generality, let $v_0v_1 \in M^*$. Using the same transformation as in subcase 1.1, it is contradict to the assumption of T^* .

Case 2. l = 3.

Subcase 2.1. If $v_1v_2 \in M^*$, let $T' = T^* - \{v_2v_3\} + \{v_0v_3\}$, we have $T' \in \mathcal{T}(n,\beta)$ (as shown in Figure 2).

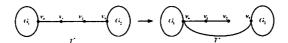


Figure 2: The graphs T^* and T' in Subcase 2.1.

$$\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > [(t+s+1)^{\alpha} - (s+2)^{\alpha}] - [4^{\alpha} - 3^{\alpha}]$$

= $\alpha \cdot [(t-1)\eta_1^{\alpha-1} - \eta_2^{\alpha-1}],$

where $\eta_1 \in (s+2, s+t+1), \eta_2 \in (3, 4)$. If $\alpha \geq 1$, $(t-1)\eta_1^{\alpha-1} - \eta_2^{\alpha-1} > 0$ since $s, t \geq 3$. If $\alpha \in (0, 1)$, $(t-1)\eta_1^{\alpha-1} - \eta_2^{\alpha-1} > (t-1)(s+t+1)^{\alpha-1} - 3^{\alpha-1} > 2 \cdot 7^{\alpha-1} - 3^{\alpha-1} > 2 \cdot 6^{\alpha-1} - 3^{\alpha-1} > 0$ since $s, t \geq 3$. Then $\chi_{\alpha}(T') > \chi_{\alpha}(T^*)$, a contradiction.

Subcase 2.2. If $v_1v_2 \notin M^*$, let $T' = T^* - \{v_1v_2\} + \{v_0v_3\}$, we have $T' \in \mathcal{T}(n,\beta)$ and $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > 0$, a contradiction.

Case 3. l = 4.

Subcase 3.1. If v_2 is M^* -unsaturated, then v_1 and v_3 must be M^* -saturated. Let $T' = T^* - \{v_1v_2, v_2v_3\} + \{v_0v_2, v_1v_3\}$, we have $T' \in \mathcal{T}(n, \beta)$ (as shown in Figure 3). $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) = [\sum_{u \in N_0} (t+1+d(u))^{\alpha} - (t+1+d(u))^{\alpha}]$

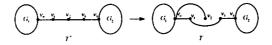


Figure 3: The graphs T^* and T' in Subcase 3.1.

 $\sum_{u\in N_0} (t+d(u))^{\alpha} + [(t+3)^{\alpha} - 4^{\alpha}] > 0$, since $t\geq 3$, a contradiction.

Subcase 3.2. If v_2 is M^* -saturated, without loss of generality, let $v_1v_2 \in M^*$, let $T' = T^* - \{v_2v_3\} + \{v_0v_3\}$, we have $T' \in \mathcal{T}(n,\beta)$. $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > [(t+3)^{\alpha} - 4^{\alpha}] - [4^{\alpha} - 3^{\alpha}] > [6^{\alpha} - 4^{\alpha}] - [4^{\alpha} - 3^{\alpha}] > 0$, since $t \geq 3$, a contradiction.

Case 4. $l \geq 5$. Let $T' = T^* - \{v_1v_2, v_3v_4\} + \{v_0v_2, v_1v_4\}$, we have $T' \in \mathcal{F}(n,\beta)$ (as shown in Figure 4), we also have $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > 0$, a contradiction.

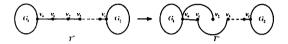


Figure 4: The graphs T^* and T' in Case 4.

Lemma 2.3. $|V^*| \le 2$.

Proof. Assume that $|V^*| \geq 3$, then by Lemma 2.2, there exist $v_0, v_1, v_2 \in V^*$ such that $v_0v_1, v_1v_2 \in E(T^*)$. Let $d(v_0) = r, d(v_1) = s, d(v_2) = t$. Let $N_0 = N_{T^*}(v_0) \setminus \{v_1\}, N_1 = N_{T^*}(v_1) \setminus \{v_0, v_2\}$ and $N_2 = N_{T^*}(v_2) \setminus \{v_1\}$, respectively.

Case 1. Only one vertex of $\{v_0, v_1, v_2\}$ is M^* -saturated. Then it must be v_1 . Let $T' = T^* - \bigcup_{v \in N_2} \{vv_2\} + \bigcup_{v \in N_0} \{vv_1\}$, obviously, M^* is also a maximum matching of T'. $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > (r+s+t-1)^{\alpha} - (r+s)^{\alpha} > 0$, a contradiction.

Case 2. Exactly two vertices of $\{v_0, v_1, v_2\}$ are M^* -saturated.

Subcase 2.1. If v_0, v_1 are M^* -saturated, then every vertex in N_2 is M^* -saturated. Let $T' = T^* - \bigcup_{v \in N_2} \{vv_2\} + \bigcup_{v \in N_2} \{vv_1\}$, obviously, M^* is also a maximum matching of T'. Similar to Case 1, we also obtain a contradiction.

Subcase 2.2. If v_0, v_2 are M^* -saturated, assume $v_2x \in M^*$. Let $T' = T^* - \bigcup_{v \in N_2} \{vv_2\} + \bigcup_{v \in N_2} \{vv_1\}$, obviously, $M^* - \{v_2x\} + \{v_1v_2\}$ is also a maximum matching of T'. Similar to Case 1, we also have a contradiction.

Subcase 2.3. If v_1, v_2 are M^* -saturated, then every vertex in N_0 is M^* -saturated. Let $T' = T^* - \bigcup_{v \in N_0} \{vv_2\} + \bigcup_{v \in N_0} \{vv_1\}$, obviously, M^* is also a maximum matching of T'. $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > (r+s+t-1)^{\alpha} - (s+t)^{\alpha} > 0$, a contradiction.

Case 3. $\{v_0, v_1, v_2\}$ are all M^* -saturated.

Subcase 3.1. $v_0v_1 \in M^*$ or $v_1v_2 \in M^*$. Without loss of generality, let $v_0v_1 \in M^*$, then there exists $w \in V(T^*) \setminus \{v_0, v_1\}$ such that $v_2w \in M^*$.

let $T' = T^* - \bigcup_{v \in N_0} \{vv_0\} + \bigcup_{v \in N_0} \{vv_1\}$, obviously, M^* is also a maximum matching of T'. Similar to Subcase 2.3, a contradiction to the assumption of T^* .

Subcase 3.2. $v_0v_1, v_1v_2 \notin M^*$. Then there exist $x \in N_0, y \in N_1, z \in N_2$ such that $v_0x, v_1y, v_2z \in M^*$. If $d(x) \geq 3$, we choose x, v_0, v_1 instead of v_0, v_1, v_2 for consideration, and back to Subcase 1.1, we get a contradiction. If d(x) = 2, by Lemma 2.1, we know that the degree of the vertex which is adjacent to x other than v_0 is 1. It is easy to see that $M^* - \{v_0x\} + \{ux\}$ is a maximum matching of T^* . At the same time, there are exactly two vertices of $\{v_0, v_1, v_2\}$ that are saturated by $M^* - \{v_0x\} + \{ux\}$. then back to Case 1, we also get a contradiction. So we have d(x) = 1, d(y) = 1, d(z) = 1. Let $T' = T^* - \bigcup_{v \in (N_0 - x)} \{vv_0\} - \bigcup_{v \in (N_2 - z)} \{vv_2\} + \bigcup_{v \in (N_0 - x) \cup (N_2 - z)} \{vv_1\}$.

$$\chi_{\alpha}(T') - \chi_{\alpha}(T^{*}) > (r+s+t-3)^{\alpha} + 2(r+s+t-2)^{\alpha} + 2 \cdot 3^{\alpha} - [(r+1)^{\alpha} + (s+1)^{\alpha} + (t+1)^{\alpha} + (r+s)^{\alpha} + (s+t)^{\alpha}].$$

Let $F(r,s,t)=(r+s+t-3)^{\alpha}+2(r+s+t-2)^{\alpha}+2\cdot 3^{\alpha}-[(r+1)^{\alpha}+(s+1)^{\alpha}+(t+1)^{\alpha}+(r+s)^{\alpha}+(s+t)^{\alpha}]$. If $\alpha=1$, it is easy to see that F(r,s,t)=r+t-2>0, a contradiction. If $\alpha>1$, we have $\frac{\partial F(r,s,t)}{\partial r}, \frac{\partial F(r,s,t)}{\partial s}, \frac{\partial F(r,s,t)}{\partial t}>0$. Hence, $F(r,s,t)\geq F(3,3,3)>0$, where $\eta_1\in(6,7)$ and $\eta_2\in(3,4)$, also a contradiction.

If $0 < \alpha < 1$, without loss of generality, let $r \le s \le t$ and $T' = T^* - \nu_0 x + xy$. $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) > [(r+s-1)^{\alpha} - (r+s)^{\alpha}] + [3^{\alpha} - (r+1)^{\alpha}] - [(s+1)^{\alpha} - (s+2)^{\alpha}] \ge \alpha(\eta_1^{\alpha-1} + \eta_2^{\alpha-1} - \eta_3^{\alpha-1})$, where $\eta_1 \in (r+s-1, r+s), \eta_2 \in (3, r+1)$ and $\eta_3 \in (s+1, s+2)$. Obviously, $\eta_2 < \eta_3$, then $\eta_2^{\alpha-1} - \eta_3^{\alpha-1} > 0$. Hence $\chi_{\alpha}(T') > \chi_{\alpha}(T^*)$, it is a contradiction. This completes the proof.

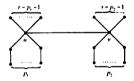


Figure 5: The structure of the graph in Theorem 2.4 (ii).

By Lemmas 2.1-2.3, we have the following theorem.

Theorem 2.4. Let T^* be the extremal tree in $\mathcal{F}(n,\beta)$ which has maximal general sum-connectivity index for $\alpha > 0$, $V^* = \{v \in V(T^*), d(v) \geq 3\}$.

(i) If $|V^*| = 1$ and $V^* = \{w\}$, then the attached parts of w are either pendent paths of length 1 or pendent paths of length 2;

(ii) If $|V^*| = 2$ and $V^* = \{u, v\}$, then $uv \in E(T^*)$. Besides u and v, the attached parts of u and v are either pendent paths of length 1 or pendent paths of length 2 (as shown in Figure 5).

Lemma 2.5. If $V^* = \{u, v\}$, let $d_{T^*}(u) = r, d_{T^*}(v) = s(r, s \geq 3)$, then there exist pendent vertices in $N_{T^*}(u)$ and $N_{T^*}(v)$, respectively.

Proof. We prove it by contradiction. Without loss of generality, suppose there are no pendent vertices in $N_{T^*}(u)$. Let t be the number of pendent paths of length 2 attached at v, and $T' = T^* - \sum_{w \in (N_{T^*}(v) - \{u\})} vw + \sum_{w \in (N_{T^*}(v) - \{u\})} uw$, obviously, $T' \in \mathcal{F}(n,\beta)$. $\chi_{\alpha}(T') - \chi_{\alpha}(T^*) = (r-1)[(r+s+1)^{\alpha} - (r+2)^{\alpha}] + t[(r+s+1)^{\alpha} - (s+2)^{\alpha}] + (s-t-1)[(r+s)^{\alpha} - (s+1)^{\alpha}] > 0$, since $r, s \geq 3$. It is contradict to the maximality of T^* . \square

Lemma 2.6. If $\alpha \geq 1$, $|V^*| = 1$.

Proof. Suppose to the contrary that $V^*=\{u,v\}$. Assume $d_{T^*}(u)=r,d_{T^*}(v)=s$ and $r\geq s\geq 3$. Let p_1 be the number of paths of length 2 attached at u and p_2 the number of paths of length 2 attached at v. By Lemma 2.5, there exists $z\in N_{T^*}(v)$ with $d_{T^*}(z)=1$, and $r-p_1-1\geq 1$. Let $T'=T^*-\sum_{w\in (N_{T^*}(v)-\{u,z\})}wv+\sum_{w\in (N_{T^*}(v)-\{u,z\})}wu$. Then $\chi_{\alpha}(T')-\chi_{\alpha}(T^*)\geq (r+s-1)^{\alpha}-(r+1)^{\alpha}+3^{\alpha}-(s+1)^{\alpha}$. Let $F(r,s)=(r+s-1)^{\alpha}-(r+1)^{\alpha}+3^{\alpha}-(s+1)^{\alpha}$. If $\alpha\geq 1$, we have $\frac{\partial F(r,s)}{\partial r},\frac{\partial F(r,s)}{\partial s}>0$. Then $F(r,s)\geq F(3,3)=(5^{\alpha}-4^{\alpha})-(4^{\alpha}-3^{\alpha})=\eta_1^{\alpha-1}-\eta_2^{\alpha-1}>0$, since $\eta_1\in (4,5)$ and $\eta_2\in (3,4)$. Hence $\chi_{\alpha}(T')>\chi_{\alpha}(T^*)$, it is contradict to the maximality of T^* .

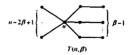


Figure 6: The graph $T(n, \beta)$.

Theorem 2.7. For $\alpha \geq 1$, let $T \in \mathcal{T}(n,\beta)$, then we have $\chi_{\alpha}(T) \leq (\beta - 1)(n-\beta+2)^{\alpha} + (\beta-1)3^{\alpha} + (n-2\beta+1)(n-\beta+1)^{\alpha}$. The equality holds if and only if T has the structure of Figure 6.

Proof. If $n=2\beta$ or $n\geq 2\beta+2$, by Theorem 2.4 and Lemma 2.6, the structure of extremal tree T^* is unique and showed in Figure 6.

$$\chi_{\alpha}(T^*) = (\beta - 1)(n - \beta + 2)^{\alpha} + (\beta - 1)3^{\alpha} + (n - 2\beta + 1)(n - \beta + 1)^{\alpha}.$$

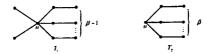


Figure 7: The graphs T_1 and T_2 .

If $n = 2\beta + 1$, then there are two possible structures of extremal trees showed in Figure 7. By direct calculation, we have

$$\chi_{\alpha}(T_1) = (\beta - 1)(\beta + 3)^{\alpha} + 2(\beta + 2)^{\alpha} + (\beta - 1)3^{\alpha},$$

$$\chi_{\alpha}(T_2) = \beta(\beta + 2)^{\alpha} + \beta \cdot 3^{\alpha},$$

then,

$$\chi_{\alpha}(T_1) - \chi_{\alpha}(T_2) = (\beta - 2)[(\beta + 3)^{\alpha} - (\beta + 2)^{\alpha}] + (\beta + 3)^{\alpha} - 3^{\alpha} > 0.$$

This completes the proof.

Remark: For $T \in \mathcal{F}(n,\beta)$ $(n \geq 5, \beta \geq 2)$, if $\alpha \geq 1$, we have obtained the maximum value of the general sum-connectivity index and characterized the corresponding extremal tree. But for the case $0 < \alpha < 1$, it is rather complicated, we only have characterized the structure of the corresponding extremal trees in Theorem 2.4. It would be interesting to find the exact extremal graphs for $0 < \alpha < 1$.

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