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Minimal Value of the Exponential of the Generalized Randić Index Over Trees

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Abstract

The generalized Randić index of a graph G with vertex set $V(G)$ and edge set $E(G)$, is defined as

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

where α is an arbitrary real number, and $d(u)$ denotes the degree of $u \in V(G)$. In this paper we study the exponential of $\chi_\alpha(G)$, defined as

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

More concretely, we show that over the set $\mathcal{T}_n$ of trees with n vertices, the minimal value of e^{χ_α} is attained in the path P_n when $\alpha > 0$, and in the star S_n when $\alpha < 0$.

1 Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Two vertices are called adjacent if they are connected by an edge. If there is an edge from vertex u to vertex v we indicate this by writing uv. For a vertex v of G, the degree of v is denoted by $d(v) = d_G(v)$. We will denote by $m_{i,j} = m_{i,j}(G)$ the number of edges in G joining vertices of degree i and j.

A tree T is a connected acyclic graph. A vertex u of a tree T is called a branching vertex if $d_T(u) \geq 3$ and it is called a leaf if $d_T(u) = 1$. Let $\pi : v_0 v_1 \cdots v_k$ be a path of length k of a tree T such that $d_T(v_i) = 2$ for all $i = 1, \ldots, k-1$. If v_0 and v_k are branching vertices of T then π is an internal path of T; if v_0 is a branching vertex and v_k is a leaf then π is a pendant path of T.

The Randić index $\chi(G)$ is one of the classical topological indices which play an important role in theoretical chemistry, especially in QSPR/QSAR research [11, 15, 16, 26, 27]. It was invented by Milan Randić in 1975 [24] and defined as

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

Later, in 1998 Bollobás and Erdös [3] generalized this index as

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

where α is an arbitrary real number. For a comprehensive survey of its mathematical properties see the surveys [13, 17], and for recent results see the papers [2, 9, 10, 12, 14, 18–20, 25].

The (generalized) Randić index is an important example of what is now known as vertex-degree-based (VDB, for short) topological indices [1, 4, 21, 22, 28, 29], defined for a graph G with n vertices as

$$\varphi(G) = \sum_{(i,j) \in K} m_{i,j}(G)\, \varphi(i,j) ,$$

where $\{\varphi(i,j)\}$ is a set of real numbers, and

$$K = \{(i,j) \in \mathbb{N} \times \mathbb{N} : 1 \leq i \leq j \leq n-1\} .$$

When $\varphi(i,j) = (ij)^\alpha$, we recover χ_α.

The exponential of a VDB topological index was recently introduced in [23], and defined as

$$e^\varphi(G) = \sum_{(i,j) \in K} m_{i,j}(G)\, e^{\varphi(i,j)} .$$

For further results see [4–8]. Our main concern in this paper is to study the exponential of the generalized Randić index. For a graph G with n vertices, the exponential of the generalized Randić index χ_α is defined as

$$e^{\chi_\alpha}(G) = \sum_{(i,j) \in K} m_{i,j}(G)\, e^{(ij)^\alpha} ,$$

where $\alpha \in \mathbb{R}$. We are particularly interested in $\mathcal{T}_n$, the set of trees with n vertices. Let $T \in \mathcal{T}_n$, where $n \geq 3$. Since a tree is a connected acyclic graph, then $m_{1,1}(T) = 0$, $m_{i,j}(T) = 0$ for any $1 \leq i \leq j \leq n-1$ such that $i + j > n$ and

$$\sum_{(i,j)\in K} m_{i,j}(T) = n - 1. \tag{1}$$

Hence, for every $T \in \mathcal{T}_n$

$$e^{\chi_\alpha}(T) = \sum_{(i,j)\in L} m_{i,j}(T) e^{(ij)^\alpha}, \tag{2}$$

where L is the subset of K defined as

$$L = \{(i,j) \in K : i + j \leq n, (i,j) \neq (1,1)\}.$$

We say that T is a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$ if $e^{\chi_\alpha}(T) \leq e^{\chi_\alpha}(S)$ for all $S \in \mathcal{T}_n$. We will show in this paper that if $\alpha > 0$ (resp. $\alpha < 0$) then, the path P_n (resp. the star S_n) on n vertices is a tree with minimum e^{χ_α} over $\mathcal{T}_n$.

2 Minimal value of e^{χ_α} in trees when $\alpha > 0$

We show in this section that if $\alpha > 0$ then, P_n is the unique minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$. First we need a technical lemma.

Lemma 2.1 *Let $\alpha > 0$.*

1. *The function $h(q) = e^{(3q)^\alpha} - e^{(2q)^\alpha}$ is increasing in $[2, +\infty)$;*
2. *$e^{6^\alpha} - e^{4^\alpha} > e^{4^\alpha} + e^{2^\alpha} - 2e^{3^\alpha}$;*
3. *$2e^{6^\alpha} - 2e^{4^\alpha} > e^{4^\alpha} - e^{3^\alpha}$.*

Proof. 1. For all $q \in [2, +\infty)$, the derivative

$$\frac{d}{dq} h(q) = \alpha q^{\alpha-1}\left(3^\alpha e^{(3q)^\alpha} - 2^\alpha e^{(2q)^\alpha}\right) > 0,$$

for all $q \geq 2$, since $q^{\alpha-1} > 0$, $3^\alpha > 2^\alpha$ and $e^{(3q)^\alpha} > e^{(2q)^\alpha}$.

2. We will first show that

$$6^\alpha - 4^\alpha > 4^\alpha - 3^\alpha. \tag{3}$$

In fact, the function $g(\alpha) = \frac{3^\alpha}{2^\alpha} + \frac{3^\alpha}{2^{2\alpha}} - 2$ is strictly increasing in $[0, +\infty)$ since

$$\begin{aligned} \frac{d}{d\alpha} g(\alpha) &= \left(\frac{3}{2}\right)^\alpha \ln\left(\frac{3}{2}\right) + \left(\frac{3}{4}\right)^\alpha \ln\left(\frac{3}{4}\right) \geq \left(\frac{3}{4}\right)^\alpha \ln\left(\frac{3}{2}\right) + \left(\frac{3}{4}\right)^\alpha \ln\left(\frac{3}{4}\right) \\ &= \left(\frac{3}{4}\right)^\alpha \left[\ln\left(\frac{3}{2}\right) + \ln\left(\frac{3}{4}\right)\right] > 0 . \end{aligned}$$

Hence

$$6^\alpha + 3^\alpha - 2\left(4^\alpha\right) = 2^{2\alpha} g\left(\alpha\right) > 2^{2\alpha} g\left(0\right) = 0.$$

Now from (3) we deduce that

$$\begin{aligned} e^{6^\alpha} - e^{4^\alpha} &= e^{4^\alpha}\left(e^{6^\alpha - 4^\alpha} - 1\right) > e^{3^\alpha}\left(e^{4^\alpha - 3^\alpha} - 1\right) \\ &= e^{4^\alpha} - e^{3^\alpha} > \left(e^{4^\alpha} - e^{3^\alpha}\right) + \left(e^{2^\alpha} - e^{3^\alpha}\right) = e^{4^\alpha} + e^{2^\alpha} - 2e^{3^\alpha}. \end{aligned}$$

3. Using (3),

$$2e^{6^\alpha} - 2e^{4^\alpha} = 2e^{4^\alpha}\left(e^{6^\alpha - 4^\alpha} - 1\right) > e^{3^\alpha}\left(e^{4^\alpha - 3^\alpha} - 1\right) = e^{4^\alpha} - e^{3^\alpha}.$$

■

Proposition 2.2 *Let $n \geq 5$ and $\alpha > 0$. Consider the trees T and T' with n vertices shown in Figure 1. If $p \geq 3$ then, $e^{\chi_\alpha}(T) > e^{\chi_\alpha}(T')$.*

Proof. Let $q = d_T(u)$. Then

$$\begin{aligned} \Delta &= e^{\chi_\alpha}(T) - e^{\chi_\alpha}(T') = e^{(pq)^\alpha} + (p-1)\, e^{p^\alpha} - e^{(2q)^\alpha} - (p-2)\, e^{4^\alpha} - e^{2^\alpha} \\ &= \left(e^{(pq)^\alpha} - e^{(2q)^\alpha}\right) + (p-2)\left(e^{p^\alpha} - e^{4^\alpha}\right) + \left(e^{p^\alpha} - e^{2^\alpha}\right). \end{aligned}$$

If $p \geq 4$, then each of the summands is non-negative since $\alpha > 0$. Consequently, $\Delta > 0$. Now assume that $p = 3$. Then

$$\Delta = \left(e^{(3q)^\alpha} - e^{(2q)^\alpha}\right) + \left(e^{3^\alpha} - e^{4^\alpha}\right) + \left(e^{3^\alpha} - e^{2^\alpha}\right).$$

Note that $q \geq 2$ since $n \geq 5$. It follows from parts **1.** and **2.** of Lemma 2.1 that

$$e^{(3q)^\alpha} - e^{(2q)^\alpha} \geq h\left(2\right) = e^{6^\alpha} - e^{4^\alpha} > e^{4^\alpha} + e^{2^\alpha} - 2e^{3^\alpha},$$

which implies that $\Delta > 0$. ■

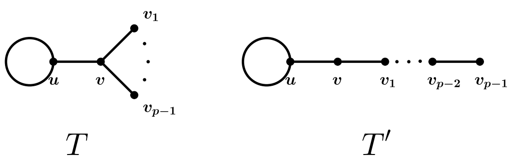

Figure 1. Trees used in the proof of Proposition 2.2.

Proposition 2.3 *Let $\alpha > 0$. Suppose that T is a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$. If v is a vertex of T adjacent to a leaf u of T, then $d_T(v) = 2$.*

Proof. Assume that $d_T(v) = d$ and let π be a largest path of T that contains v. Let s be an end-vertex of π and r a vertex in π adjacent to s. By Proposition 2.2, $d_T(r) = 2$. Let T' be the tree obtained from T by deleting the leaf u and adding an edge incident to s (see Figure 2). Let $q_1, \ldots, q_{d-1}$ be the degrees of the adjacent vertices of v different from u. Clearly,

$$\Delta = e^{\chi_\alpha}(T) - e^{\chi_\alpha}(T') = \sum_{i=1}^{d-1}\left(e^{(dq_i)^\alpha} - e^{((d-1)q_i)^\alpha}\right) + e^{d^\alpha} - e^{4^\alpha}. \tag{4}$$

We consider two cases:

1. $d \geq 4$. It follows easily from (4) that $\Delta > 0$, since $\alpha > 0$.

2. $d = 3$. Let v_1 and v_2 be the adjacent vertices to v (different from u), such that $d_T(v_1) = p$ and $d_T(v_2) = q$. It follows from Proposition 2.2 that $p \geq 2$ and $q \geq 2$. Then

$$\Delta(p,q) = e^{(3p)^\alpha} - e^{(2p)^\alpha} + e^{(3q)^\alpha} - e^{(2q)^\alpha} + e^{3^\alpha} - e^{4^\alpha}.$$

Since $\alpha > 0$, then

$$\frac{\partial \Delta(p,q)}{\partial p} = \frac{\alpha}{p}\left(e^{(3p)^\alpha}(3p)^\alpha - e^{(2p)^\alpha}(2p)^\alpha\right) > 0,$$

and

$$\frac{\partial \Delta(p,q)}{\partial q} = \frac{\alpha}{q}\left(e^{(3q)^\alpha}(3q)^\alpha - e^{(2q)^\alpha}(2q)^\alpha\right) > 0.$$

Hence by part **3.** of Lemma 2.1,

$$\Delta(p,q) \geq \Delta(2,2) = 2e^{6^\alpha} - 2e^{4^\alpha} + e^{3^\alpha} - e^{4^\alpha} > 0,$$

which contradicts the fact that T is minimal. ■

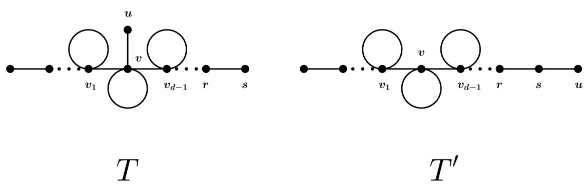

Figure 2. Trees used in the proof of Proposition 2.3.

We need one more techincal lemma to prove the main result of this section.

Lemma 2.4 *Let* $\alpha > 0$. *Then*

$$e^{x^{2\alpha}}\left(1+2\alpha x^{2\alpha}\right)+2e^{2^{\alpha}}-3e^{4^{\alpha}}>0,$$

for all $x \geq 2$.

Proof. Since $\alpha > 0$ and $x \geq 2$,

$$1+2\alpha x^{2\alpha} \geq 1+2\alpha 2^{2\alpha}=1+\alpha 2^{2\alpha+1}. \tag{5}$$

On the other hand, $e^{x} \geq 1+x$ for all $x \in \mathbb{R}$. In particular,

$$e^{2^{\alpha}-4^{\alpha}} \geq 1+2^{\alpha}-4^{\alpha}. \tag{6}$$

From (5) and (6) we deduce,

$$\begin{aligned} e^{x^{2\alpha}}\left(1+2\alpha x^{2\alpha}\right)+2e^{2^{\alpha}}-3e^{4^{\alpha}} &\geq e^{2^{2\alpha}}\left(1+\alpha 2^{2\alpha+1}\right)+2e^{2^{\alpha}}-3e^{4^{\alpha}} \\ &= 2e^{2^{2\alpha}}\left(\alpha 2^{2\alpha}+e^{2^{\alpha}-4^{\alpha}}-1\right) \\ &\geq 2e^{2^{2\alpha}}\left(\alpha 2^{2\alpha}+2^{\alpha}-4^{\alpha}\right) \\ &= 2^{2\alpha+1}e^{2^{2\alpha}}\left(\alpha+\frac{1}{2^{\alpha}}-1\right). \end{aligned} \tag{7}$$

Moreover, the function $p(\alpha)=\alpha+\frac{1}{2^{\alpha}}-1$ is strictly increasing in $\left(\frac{\ln(\ln 2)}{(\ln 2)},+\infty\right)$, since

$$\frac{d}{d\alpha}p(\alpha)=1-\frac{\ln 2}{2^{\alpha}}>0,$$

for all $\alpha \geq \frac{\ln(\ln 2)}{(\ln 2)} \approx -0.528\,77$. Consequently,

$$\alpha+\frac{1}{2^{\alpha}}-1>p\left(0\right)=0,$$

and by (7),

$$e^{x^{2\alpha}}\left(1+2\alpha x^{2\alpha}\right)+2e^{2^{\alpha}}-3e^{4^{\alpha}}>0.$$

■

Recall that L is the subset of K defined as

$$L=\left\{(i,j)\in K : i+j\leq n, (i,j)\neq(1,1)\right\}.$$

Define the function

$$f\left(i,j\right)=\frac{ij}{i+j}\left(e^{(ij)^{\alpha}}+2e^{2^{\alpha}}-3e^{4^{\alpha}}\right),$$

where $(i,j) \in L$. Note that

$$f(1,2) = f(2,2) = 2\left(e^{2^\alpha} - e^{4^\alpha}\right).$$

It can be easily deduced from [4, Theorem 2.1] that if $T \in \mathcal{T}_n$ then,

$$e^{\chi_\alpha}(T) = e^{\chi_\alpha}(P_n) + \sum_{(i,j)\in L} [f(i,j) - f(1,2)] \frac{i+j}{ij} m_{i,j}(T), \tag{8}$$

for every $\alpha \in \mathbb{R}$. Consider the extension of L to the compact set

$$\widehat{L} = \{(x,y) \in \mathbb{R} \times \mathbb{R} : 1 \leq x \leq y \leq n-1,\ x+y \leq n,\ y \geq 2\}.$$

Theorem 2.5 *Let $\alpha > 0$ and $n \geq 5$. The path P_n is the unique minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$.*

Proof. Let T_0 be a tree with minimal value of χ_α over $\mathcal{T}_n$. By Proposition 2.3, $m_{1,j}(T_0) = 0$ for all $j \geq 3$. Let

$$M = \{(i,j) \in L : i \geq 2\}.$$

Then by (8),

$$\begin{aligned} e^{\chi_\alpha}(T_0) &= e^{\chi_\alpha}(P_n) + \sum_{(i,j)\in L} [f(i,j) - f(1,2)] \frac{i+j}{ij} m_{i,j}(T_0) \\ &= e^{\chi_\alpha}(P_n) + \sum_{(i,j)\in M} [f(i,j) - f(1,2)] \frac{i+j}{ij} m_{i,j}(T_0). \end{aligned} \tag{9}$$

Let

$$\widehat{M} = \left\{(x,y) \in \widehat{L} : x \geq 2\right\}$$

and

$$f(x,y) = \frac{xy}{x+y}\left(e^{(xy)^\alpha} + 2e^{2^\alpha} - 3e^{4^\alpha}\right),$$

defined over $\widehat{M}$. We will show that $\min_{(i,j)\in\widehat{M}} f(i,j) = f(2,2)$. By Lemma 2.4 and the fact that $\alpha > 0$,

$$\begin{aligned} \frac{\partial}{\partial y} f(x,y) &= x\frac{xe^{(xy)^\alpha} + 2xe^{2^\alpha} - 3xe^{4^\alpha} + x\alpha e^{(xy)^\alpha}(xy)^\alpha + y\alpha e^{(xy)^\alpha}(xy)^\alpha}{(x+y)^2} \\ &\geq x\frac{xe^{x^{2\alpha}} + 2xe^{2^\alpha} - 3xe^{4^\alpha} + x\alpha e^{x^{2\alpha}} x^{2\alpha} + x\alpha e^{x^{2\alpha}} x^{2\alpha}}{(x+y)^2} \\ &= \frac{x^2}{(x+y)^2}\left(e^{x^{2\alpha}}\left(1 + 2\alpha x^{2\alpha}\right) + 2e^{2^\alpha} - 3e^{4^\alpha}\right) > 0, \end{aligned}$$

for all $(x, y) \in \widehat{M}$, and

$$\frac{\partial}{\partial x} f(x, x) = \frac{1}{2}\left(e^{x^{2\alpha}}\left(1 + 2\alpha x^{2\alpha}\right) + 2e^{2^{\alpha}} - 3e^{4^{\alpha}}\right) > 0,$$

for all $x \geq 2$. This clearly implies that the minimum value of f over $\widehat{M}$ is $f(2, 2) = f(1, 2)$.

Finally, if $T \in \mathcal{T}_n$ then by (9) we deduce

$$e^{\chi_\alpha}(T) \geq e^{\chi_\alpha}(T_0) \geq e^{\chi_\alpha}(P_n) \ .$$

■

3 Minimal value of e^{χ_α} in trees when $\alpha < 0$

In this section we prove that the star S_n attains the minimal value of e^{χ_α} over $\mathcal{T}_n$, when $\alpha < 0$.

Proposition 3.1 *Let $\alpha < 0$ and $T \in \mathcal{T}_n$ be a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$. Then T has no pendent paths of length greater than one.*

Proof. Suppose T a minimal tree with respect to e^{χ_α} and it contains a pendent path of length $k \geq 3$. Then T has the form depicted in Figure 3, where S is a subtree of T and $x = d_T(u) \geq 3$. Consider the tree T' in the same figure and let $x_i = d_T(u_i)$, where $u_1, \ldots, u_{x-1}$ are the vertices adjacent to u in S. Then

$$\begin{aligned} e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) &= \sum_{i=1}^{x-1}\left[e^{x_i^\alpha (x+k-2)^\alpha} - e^{x_i^\alpha x^\alpha}\right] + \left[e^{2^\alpha (x+k-2)^\alpha} - e^{2^\alpha x^\alpha}\right] \\ &\quad + (k-2)\left[e^{(x+k-2)^\alpha} - e^{4^\alpha}\right] < 0. \end{aligned}$$

and we get a contradiction.

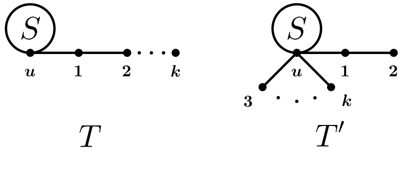

Figure 3. Trees used in the proof of Proposition 3.1 for $k \geq 3$.

Now suppose T is a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$ and it contains a pendent path of length $k = 2$. Then T has the form depicted in Figure 4, where S is a subtree of

T and $x = d_T(u) \geq 3$. Consider the tree T' in the same figure and let $x_i = d_T(u_i)$, where $u_1, \ldots, u_{x-1}$ are the vertices adjacent to u in S. Then

$$\begin{aligned} e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) &= \sum_{i=1}^{x-1} \left[e^{x_i^\alpha (x+1)^\alpha} - e^{x_i^\alpha x^\alpha} \right] + 2e^{(x+1)^\alpha} - e^{2^\alpha x^\alpha} - e^{2^\alpha} \\ &< 2e^{(x+1)^\alpha} - e^{(2x)^\alpha} - e^{2^\alpha} = f_1(x). \end{aligned}$$

$f_1(x)$ is a real continuosly differentiable function defined for $x \geq 1$. The derivative of f_1

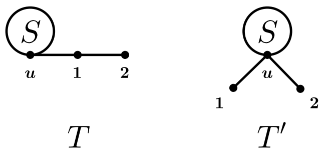

Figure 4. Trees used in the proof of Proposition 3.1 for $k = 2$.

is

$$\frac{d}{dx} f_1(x) = 2\alpha \left[e^{(x+1)^\alpha} (x+1)^{\alpha-1} - e^{(2x)^\alpha} (2x)^{\alpha-1} \right]$$

Note that since $\alpha < 0$, $\frac{d}{dx} f_1(x) < 0$ for $x > 1$ and $\frac{d}{dx} f_1(1) = 0$. Then $f_1(x)$ attains its maximum at $x = 1$. Then

$$e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) < f_1(x) \leq f_1(1) = 0$$

and we get a contradiction. ■

Proposition 3.2 *Let $\alpha < 0$ and $T \in \mathcal{T}_n$ be a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$. Then T has no internal paths of length greater than 1.*

Proof. Suppose T is a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$ and contains an internal path of length $k+1$ with $k \geq 2$ (see Figure 5) and consider the tree T' depicted in Figure 5, where U and V are subtrees of T. Assume that $x = d_T(u) \geq 3$, $y = d_T(v) \geq 3$, and $x_i = d_T(u_i)$, where $u_1, \ldots, u_{x-1}$ are the vertices adjacent to u in U. Then

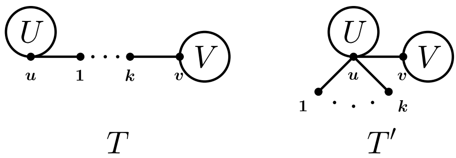

Figure 5. Trees used in the proof of Proposition 3.2 for $k \geq 2$.

$$\begin{aligned} e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) &= \sum_{i=1}^{x-1}\left[e^{x_i^\alpha (x+k)^\alpha} - e^{x_i^\alpha x^\alpha}\right] + (k-1)\left[e^{(x+k)^\alpha} - e^{4^\alpha}\right] + \\ &\quad \left[e^{(x+k)^\alpha y^\alpha} - e^{2^\alpha y^\alpha}\right] + e^{(x+k)^\alpha} - e^{2^\alpha x^\alpha} \\ &< (k-1)\left[e^{(x+k)^\alpha} - e^{4^\alpha}\right] + e^{(x+k)^\alpha} - e^{2^\alpha x^\alpha} \\ &\leq \left[e^{(x+k)^\alpha} - e^{4^\alpha}\right] + e^{(x+k)^\alpha} - e^{2^\alpha x^\alpha} \\ &= 2e^{(x+k)^\alpha} - e^{4^\alpha} - e^{2^\alpha x^\alpha} \\ &\leq 2e^{(x+2)^\alpha} - e^{4^\alpha} - e^{2^\alpha x^\alpha} = f_2(x). \end{aligned}$$

$f_2(x)$ is a real continuosly differentiable function defined for $x \geq 2$. The derivative of f_2 is

$$\frac{d}{dx}f_2(x) = 2\alpha\left[e^{(x+2)^\alpha}(x+2)^{\alpha-1} - (2x)^{\alpha-1}e^{(2x)^\alpha}\right].$$

Note that since $\alpha < 0$, $\frac{d}{dx}f_2(x) < 0$ for $x > 2$ and $\frac{d}{dx}f_2(2) = 0$. Then $f_2(x)$ attains its maximum at $x = 2$. Then

$$e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) < f_2(x) \leq f_2(2) = 0.$$

and we get a contradiction.

Suppose now that T is a minimal tree with respect to e^{χ_α} and contains an internal path of length $k = 2$ (see Figure 6) and consider the tree T' depicted in Figure 6, where U and V are subtrees of T. Assume that $x = d_T(u) \geq 3$, $y = d_T(v) \geq 3$, $x_i = d_T(u_i)$, where $u_1, \ldots, u_{x-1}$ are the vertices adjacent to u in U and $y_i = d_T(v_i)$, where $v_1, \ldots, v_{y-1}$ are the vertices adjacent to v in V. Then

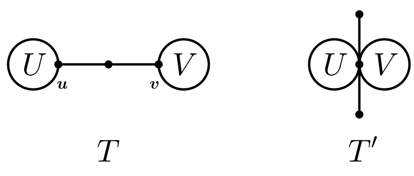

Figure 6. Trees used in the proof of Proposition 3.2 for $k = 1$.

$$
\begin{aligned}
e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) &= \sum_{i=1}^{x-1}\left[e^{x_i^\alpha (x+y)^\alpha} - e^{x_i^\alpha x^\alpha}\right] + \sum_{i=1}^{y-1}\left[e^{y_i^\alpha (x+y)^\alpha} - e^{y_i^\alpha y^\alpha}\right] \\
&\quad + 2e^{(x+y)^\alpha} - e^{2^\alpha x^\alpha} - e^{2^\alpha y^\alpha} \\
&< 2e^{(x+y)^\alpha} - e^{2^\alpha x^\alpha} - e^{2^\alpha y^\alpha} \\
&= f_3(x+y) - f_3(2x) + f_3(x+y) - f_3(2y)
\end{aligned}
$$

where $f_3(z) = e^{z^\alpha}$ is a real continuosly differentiable function for $z > 0$.
If $x = y$, $f_3(x+y) - f_3(2x) + f_3(x+y) - f_3(2y) = 0$ and

$$
e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) < f_3(x+y) - f_3(2x) + f_3(x+y) - f_3(2y) = 0.
$$

If $x < y$, then $2x < x+y < 2y$. By the mean value Theorem, there exists two points $2x < z_1 < x+y < z_2 < 2y$ such that

$$
\begin{aligned}
e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) &< f_3(x+y) - f_3(2x) + f_3(x+y) - f_3(2y) \\
&= \left(f_3'(z_1) - f_3'(z_2)\right)(y-x) \\
&= \alpha(y-x)\left[z_1^{\alpha-1}e^{z_1^\alpha} - z_2^{\alpha-1}e^{z_2^\alpha}\right] < 0
\end{aligned}
$$

If $x > y$, similarly one can prove that $e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) < 0$ and we get a contradiction.

■

Let T be a tree with at least one branching vertex v of degree $k \geq 3$. The tree T can be viewed as the coalescence of k subtrees $T_1, \ldots, T_k$ of T at the vertex v. These subtrees are called branches of T at v (see Figure 7). A branching vertex v of T is an outer branching vertex of T if all branches of T at v (except for possibly one) are paths [5].

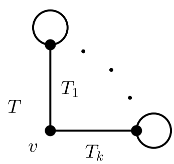

Figure 7. Branches of the tree T at branching vertex v.

Proposition 3.3 *Let $\alpha < 0$ and $T \in \mathcal{T}_n$ be a minimal tree with respect to e^{χ_α}. Then T has at most one branching vertex.*

Proof. Suppose T is a minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$. By Propositions 3.1 and 3.2, T has no internal paths of length greater than one and all pendent paths are of length one. Suppose T has more than one branching vertex, then T has the form depicted in Figure 8 where u is a branching vertex and v is an outer branching vertex of degree $k+1$ for $k \geq 2$. Consider the tree T' depicted in Figure 8, where U is a subtree of T. Assume that $x = d_T(u) \geq 3$ and $x_i = d_T(u_i)$, where $u_1, \ldots, u_{x-1}$ are the vertices adjacent to u in U. Then

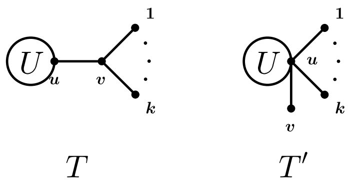

Figure 8. Trees used in the proof of Proposition 3.3.

$$\begin{aligned} e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) &= \sum_{i=1}^{x-1} \left[e^{x_i^\alpha (x+k)^\alpha} - e^{x_i^\alpha x^\alpha} \right] \\ &\quad + (k+1) e^{(x+k)^\alpha} - k e^{(k+1)^\alpha} - e^{x^\alpha (k+1)^\alpha} \\ &< (k+1) e^{(x+k)^\alpha} - k e^{(k+1)^\alpha} - e^{x^\alpha (k+1)^\alpha} = f_4(x). \end{aligned}$$

$f_4(x)$ is a real continuosly differentiable function defined for $x \geq 1$. The derivative of f_4 is

$$\frac{d}{dx} f_4(x) = \alpha (k+1) \left[e^{(k+x)^\alpha} (k+x)^{\alpha-1} - (x(k+1))^{\alpha-1} e^{(x(k+1))^\alpha} \right]$$

Note that since $\alpha < 0$, $\frac{d}{dx} f_4(x) < 0$ for $x > 1$ and $\frac{d}{dx} f_4(1) = 0$. Then $f_4(x)$ attains its maximum at $x = 1$. Consequently,

$$e^{\chi_\alpha}(T') - e^{\chi_\alpha}(T) < f_4(x) \leq f_4(1) = 0$$

and we get a contradiction. ■

Theorem 3.4 *Let $\alpha < 0$. For $n \geq 5$, the minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$ is the star S_n.*

Proof. By Proposition 3.3, the minimal tree with respect to e^{χ_α} over $\mathcal{T}_n$ has at most one branching vertex. The only tree with no branching vertices is the path P_n and the only tree, satisfying Propositions 3.1 and 3.2, with exactly one branching vertex, is the star S_n. Then,

$$\begin{aligned} e^{\chi_\alpha}(S_n) - e^{\chi_\alpha}(P_n) &= (n-1)\, e^{(n-1)^\alpha} - (n-3)\, e^{4^\alpha} - 2e^{2^\alpha} \\ &= (n-3)\left(e^{(n-1)^\alpha} - e^{4^\alpha}\right) + 2\left(e^{(n-1)^\alpha} - e^{2^\alpha}\right) < 0. \end{aligned}$$

■

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