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On Generalized Atom–Bond Connectivity Index of Cacti

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ABSTRACT

The generalized atom-bond connectivity index of a graph G is denoted by $ABC_\alpha(G)$ and defined as the sum of weights $\left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)^\alpha$ over all edges $uv \in G$, where $d(u)$ is the degree of the vertex u in G, and α is an arbitrary non-zero real number. A cactus is a graph in which any two cycles have at most one common vertex. In this paper, we compute sharp bounds for ABC_α index for cacti of order n with fixed number of cycles and for cacti of order n with given number of pendant vertices. Furthermore, we identify all the cacti that achieve the bounds.

1. INTRODUCTION

Throughout this paper, all graphs considered are simple and connected. Let G be a graph on n vertices with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, let $N_G(v)$ be the set of all neighbors of v in G. The degree of $v \in V(G)$, denoted by $d_G(v)$ or $d(v)$, is the cardinality of $N_G(v)$. Denote by $\Delta(G)$ be maximum degree of G. A vertex is said to be a pendant vertex if its degree is one, and an edge is said to be a pendant edge if one of its end vertices is a pendant vertex. The graph formed from G by deleting any vertex $v \in V(G)$ (resp. edge $uv \in E(G)$) is denoted by $G - v$ (resp. $G - uv$). Similarly, the graph formed from G by adding an edge uv is denoted by $G + uv$, where u and v are non-adjacent vertices of G. As usual, by C_n, S_n and P_n we denote the cycle, star and path on n vertices, respectively.

Molecular descriptors play a key role in mathematical chemistry. Among them, topological indices, or graph invariant playing an important role. The most studied degree-

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based graph invariant probably is the Randić index [17]. For more degree base topological indices see [22, 23].

For a connected graph G the atom-bond connectivity index (or ABC index for short) introduced by Estrada et al. [11] and defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}},$$

where $d(u)$ is the degree of vertex u in G. In [11] it has been showed that the ABC index correlated well with the heat of formation of alkane, and also they showed a chemical explanation for its descriptive ability. Due to the above (chemical) applications, various mathematical properties of the ABC index, have been extensively investigated, for more details see [3, 4, 6,7, 13,15, 18, 19, 20, 21], and the references cited therein. A cactus is a graph that any block is either a cut edge or a cycle, or equivalently, a graph in which any two cycles have at most one common vertex. Let $\mathbb{C}(n,t)$ denote the class of all cacti of order n with t cycles, and $\mathbb{C}^1(n,r)$ denote the class of all cacti of order n with r pendant vertices. Dong and Wu [8] obtained the maximum value of the ABC index in $\mathbb{C}(n,t)$ and $\mathbb{C}^1(n,r)$. Ashrafi et al. [2] determined the first and second maximum values of the ABC index among all n-vertex cacti. For more studies about cacti one may be referred to [1, 14].

In order to obtain the better correlation abilities of the ABC index for the heat of formation of alkane, Furtula et al. [12] made generalization of the ABC index by replacing 1/2 with an arbitrary non-zero real number α as

$$ABC_\alpha(G) = \sum_{uv\in E(G)} \left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)^\alpha.$$

They showed that $ABC_{-3}(G)$ have a better prediction power than the ABC index in the study of heat of formation for heptane and octanes, which was named as augmented Zagreb index. It was also discussed in [19]. Estrada [9, 10] provided a probabilistic explanation for the capacity of ABC-like indices to describe the energetics of alkanes.

Recently, Chen and Hao [5] obtained graphs with maximum $ABC_\alpha(G)$ index for $\alpha < 0$ among all connected graphs with given order and vertex connectivity, edge connectivity and matching number. Liu et el. [16] determined $ABC_\alpha(G)$ of unicyclic graphs with maximal and second-maximal (resp. minimal and second-minimal) values for $\alpha > 0$ (resp. $-3 \le \alpha < 0$), and bicyclic graphs with maximal and second-maximal (resp. minimal and second-minimal) values for $\alpha > 0$ (resp. $-1 \le \alpha < 0$).

Motivated from [5, 16],in this paper we further explore mathematical properties of ABC_α index for cacti. In the second section, we give some preliminary results for the proof of our main results. In the third section, we obtain sharp upper and lower bounds for $\alpha > 0$ and $-3 \le \alpha < -1$, respectively for the ABC_α index for cacti in $\mathbb{C}(n,t)$, and characterize the corresponding extremal graphs, which generalize some known results in [8, 1]. Finally, in section 4, we give sharp upper and lower bounds for $\alpha > 0$ and $-3 \le \alpha < -1$, respectively for the ABC_α index for cacti in $\mathbb{C}^1(n,r)$, and characterize the corresponding extremal graphs.

2. PRELIMINARIES

In this section we give some preliminary results for the proof of our main results. For any nonzero real number α and $x, y \geq 1$, let $g(x,y,\alpha) = \left(\frac{x+y-2}{xy}\right)^\alpha$. Note that $g(1,1,\alpha) = 0$, and for $x \geq 1$, $g(x,2,\alpha) = \left(\frac{1}{2}\right)^\alpha$.

Lemma 2.1. [16] *For $x \geq 2$, let $g(x,1,\alpha) = \left(\frac{x-1}{x}\right)^\alpha$.*

i. *If $\alpha > 0$, then $g(x,1,\alpha)$ is strictly increasing with x.*
ii. *If $-3 \leq \alpha < 0$, then $g(x,1,\alpha)$ is strictly decreasing with x.*

Lemma 2.2. *Let $G \in \mathbb{C}(n,0)$ of order $n \geq 2$. Then*

$$ABC_\alpha(G)\begin{cases} \leq (n-1)\left(\frac{n-2}{n-1}\right)^\alpha & \alpha > 0, \\ \geq (n-1)\left(\frac{n-2}{n-1}\right)^\alpha & -3 \leq \alpha < 0, \end{cases}$$

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

Proof. Let $G \in \mathbb{C}(n,0)$ of order $n \geq 2$. Then by Lemma 2.1, we have

$$\begin{aligned} ABC_\alpha(G) &= \sum_{uv\in E(G)} \left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)^\alpha \\ &\begin{cases} \leq \sum_{uv\in E(G)} \left(\frac{1+(n-1)-2}{1.(n-1)}\right)^\alpha & \alpha > 0 \\ \geq \sum_{uv\in E(G)} \left(\frac{1+(n-1)-2}{1.(n-1)}\right)^\alpha & -3 \leq \alpha < 0 \end{cases} \\ &= (n-1)\left(\frac{n-2}{n-1}\right)^\alpha, \end{aligned}$$

with equality if and only if $\{d(u), d(v)\} = \{1, n-1\}$ for every edge uv, i.e., $G \cong S_n$. ∎

3. EXTREMAL ABC_α INDEX IN $\mathbb{C}(n,t)$

In this section we compute sharp upper bounds for $\alpha > 0$ and sharp lower bounds for $-3 \leq \alpha < -1$, respectively for the ABC_α index of cacti in $\mathbb{C}(n,t)$, and characterize the corresponding extremal graphs.

A bundle is a cactus in which all cycles have exactly one common vertex. Let $C_{n,t}$ denote the bundle with t triangles having $n-2t-1$ pendant vertices attached to the common vertex.

Lemma 3.1. [16] *Let $G \in \mathbb{C}(n,1)$ of order $n \geq 3$.*

i. *If $\alpha > 0$, then $G \cong C_{n,1}$ is the unique graph having maximal ABC_α index.*
ii. *If $-3 \leq \alpha < 0$, then $G \cong C_{n,1}$ is the unique graph having minimal ABC_α index.*

By direct calculation, we have

$$ABC_\alpha(C_{n,t}) = 3t\left(\frac{1}{2}\right)^\alpha + (n-2t-1)\left(\frac{n-2}{n-1}\right)^\alpha.$$

Let

$$A(n,t,\alpha) = 3t\left(\frac{1}{2}\right)^\alpha + (n-2t-1)\left(\frac{n-2}{n-1}\right)^\alpha.$$

Theorem 3.1. *Let $G \in \mathbb{C}(n,t)$ of order $n \geq 5$. Then*

$$ABC_\alpha(G)\begin{cases} \leq A(n,t,\alpha) & \alpha > 0, \\ \geq A(n,t,\alpha) & -3 \leq \alpha < -1, \end{cases}$$

with equality if and only if $G \cong C_{n,t}$.

Proof. We prove it by induction on n and t. For $t = 0$ and $t = 1$ the result holds due to Lemma 2.2 and Lemma 3.1, respectively. Now, we assume that $n \geq 5$ and $t \geq 2$. For $n = 5$ the result holds due to the fact that there is only one graph which is isomorphic to $C_{5,2}$. Let $G \in \mathbb{C}(n,t)$ where $n \geq 6$ and $t \geq 2$, then we consider the following two possible cases.

Case 1. G has no pendant vertex. In this case, there must exist two edges say uv and uw in some cycle of G such that $d(u) = d(v) = 2$ and $d(w) = d \geq 3$. Here, we consider two subcases to complete the proof.

Subcase 1. $vw \notin E(G)$. Let $G' = G - u + vw$, then $G' \in \mathbb{C}(n-1,t)$. Then by inductive assumption and Lemma 2.1, we have

$$\begin{aligned} ABC_\alpha(G) &= ABC_\alpha(G') + \left(\frac{1}{2}\right)^\alpha \\ &\begin{cases} \leq A(n-1,t,\alpha) + \left(\frac{1}{2}\right)^\alpha & \alpha > 0 \\ \geq A(n-1,t,\alpha) + \left(\frac{1}{2}\right)^\alpha & -3 \leq \alpha < -1 \end{cases} \\ &= A(n,t,\alpha) + \left(\frac{1}{2}\right)^\alpha - (n-2t-1)\left(\frac{n-2}{n-1}\right)^\alpha + (n-2t-2)\left(\frac{n-3}{n-2}\right)^\alpha \\ &= A(n,t,\alpha) + \left(\left(\frac{1}{2}\right)^\alpha - \left(\frac{n-2}{n-1}\right)^\alpha\right) \\ &+ \left((n-2t-2)\left(\frac{n-3}{n-2}\right)^\alpha - (n-2t-2)\left(\frac{n-2}{n-1}\right)^\alpha\right) \\ &\begin{cases} < A(n,t,\alpha) & \alpha > 0, \\ > A(n,t,\alpha) & -3 \leq \alpha < -1. \end{cases} \end{aligned}$$

Subcase 2. $vw \in E(G)$. Let $N_G(w)\backslash\{u,v\} = \{u_1, u_2, \dots, u_{d-2}\}$. Since $\delta(G) \geq 2$, therefore $d(u_i) \geq 2$ for $1 \leq i \leq d-2$. Let $G' = G - u - v$, then $G' \in \mathbb{C}(n-2, t-1)$. Then by inductive assumption and Lemma 2.1, we have

$$ABC_\alpha(G) = ABC_\alpha(G') + 3\left(\tfrac{1}{2}\right)^\alpha + \textstyle\sum_{i=1}^{d-2} [g(d, d(u_i), \alpha) - g(d-2, d(u_i), \alpha)]$$

$$\begin{cases} \leq A(n-2, t-1, \alpha) + 3\left(\tfrac{1}{2}\right)^\alpha \\ + \sum_{i=1}^{d-2} [g(d, d(u_i), \alpha) - g(d-2, d(u_i), \alpha)] \quad if \ \alpha > 0 \\ \geq A(n-2, t-1, \alpha) + 3\left(\tfrac{1}{2}\right)^\alpha \\ + \sum_{i=1}^{d-2} [g(d, d(u_i), \alpha) - g(d-2, d(u_i), \alpha)] \quad if \ -3 \leq \alpha < -1 \end{cases}$$

$$= A(n,t,\alpha) - 3\left(\tfrac{1}{2}\right)^\alpha - (n-2t-1)\left(\tfrac{n-2}{n-1}\right)^\alpha + (n-2t-1)\left(\tfrac{n-4}{n-3}\right)^\alpha$$

$$+ 3\left(\tfrac{1}{2}\right)^\alpha + \textstyle\sum_{i=1}^{d-2} [g(d, d(u_i), \alpha) - g(d-2, d(u_i), \alpha)]$$

$$= A(n,t,\alpha) + (n-2t-1)\left[\left(\tfrac{n-4}{n-3}\right)^\alpha - \left(\tfrac{n-2}{n-1}\right)^\alpha\right]$$

$$+ \textstyle\sum_{i=1}^{d-2} [g(d, d(u_i), \alpha) - g(d-2, d(u_i), \alpha)]$$

$$\begin{cases} \leq A(n,t,\alpha) & \alpha > 0, \\ \geq A(n,t,\alpha) & -3 \leq \alpha < -1, \end{cases}$$

where the last equality holds if and only if all the inequalities become equalities, i.e., $G' \cong C_{n-2,t-1}$, $2t = n-1$ and $d(u_i) = 2$ for $i = 1,2, \dots, d-2$. Thus, $ABC_\alpha(G) = A(n,t,\alpha)$ if and only if $G \cong C_{n,t}$.

Case 2. G has at least one pendant vertex. Let $u_0 \in V(G)$ with $d(u_0) = 1$ and $u_0v_0 \in E(G)$. Let $d(v_0) = d$ and $N_G(v_0)\backslash\{u_0\} = \{v_1, v_2, \dots, v_{d-1}\}$, then $2 \leq d \leq n-1$. Without loss of generality we assume that $d(v_i) = 1$ for $i = 1,2, \dots, z-1$ and $d(v_i) \geq 2$ for $i = z, z+1, \dots, d-1$. Let $G^* = G - u_0 - \sum_{i=1}^{z-1} v_i$, then $G^* \in \mathbb{C}(n-z, t)$. Then by inductive assumption and Lemma 2.1, we have

$$ABC_\alpha(G) = ABC_\alpha(G^*) + z\left(\tfrac{d-1}{d}\right)^\alpha + \textstyle\sum_{i=z}^{d-1} [g(d, d(v_i), \alpha) - g(d-z, d(v_i), \alpha)]$$

$$\begin{cases} \leq ABC_\alpha(G^*) + z\left(\dfrac{d-1}{d}\right)^\alpha & \alpha > 0 \\ \geq ABC_\alpha(G^*) + z\left(\dfrac{d-1}{d}\right)^\alpha & -3 \leq \alpha < -1 \end{cases}$$

$$\begin{cases} \leq A(n-z, t, \alpha) + z\left(\dfrac{d-1}{d}\right)^\alpha & \alpha > 0 \\ \geq A(n-z, t, \alpha) + z\left(\dfrac{d-1}{d}\right)^\alpha & -3 \leq \alpha < -1 \end{cases}$$

$$= A(n,t,\alpha) - (n-2t-1)\left(\tfrac{n-2}{n-1}\right)^\alpha$$

$$+ (n-2t-1-z)\left(\frac{n-z-2}{n-z-1}\right)^{\alpha} + r\left(\frac{d-1}{d}\right)^{\alpha}$$
$$= A(n,t,\alpha) + (n-2t-1-z)\left[\left(\frac{n-z-2}{n-z-1}\right)^{\alpha} - \left(\frac{n-2}{n-1}\right)^{\alpha}\right]$$
$$+ z\left[\left(\frac{d-1}{d}\right)^{\alpha} - \left(\frac{n-2}{n-1}\right)^{\alpha}\right]$$
$$\begin{cases} \leq A(n,t,\alpha) & \alpha > 0, \\ \geq A(n,t,\alpha) & -3 \leq \alpha < -1, \end{cases}$$
and the last equality holds if and only if all the inequalities become equalities, i.e., $G^* \cong C_{n-z,t}$, $2t = n-z-1$ and $d = n-1$. Thus, $ABC_\alpha(G) = A(n,t,\alpha)$ if and only if $G \cong C_{n,t}$. By combining Case 1 and Case 2, the result follows. ∎

4. Extremal ABC_α Index in $\mathbb{C}^1(n,r)$

In this section we determine sharp upper and lower bounds for $\alpha > 0$ and $-3 \leq \alpha < -1$, respectively for the ABC_α index of cacti in $\mathbb{C}^1(n,r)$, and characterize the corresponding extremal graphs. Denote by $S_{1,n-3}$ the tree formed by adding one pendant vertex to a pendant vertex of the star S_{n-1}.

Lemma 4.1. *Let $G \in \mathbb{C}^1(n,n-2)$ of order $n \geq 4$. Then*
$$ABC_\alpha(G)\begin{cases} \leq (n-3)\left(\frac{n-3}{n-2}\right)^{\alpha} + 2\left(\frac{1}{2}\right)^{\alpha} & \alpha > 0, \\ \geq (n-3)\left(\frac{n-3}{n-2}\right)^{\alpha} + 2\left(\frac{1}{2}\right)^{\alpha} & -3 \leq \alpha < -1, \end{cases}$$
with equality if and only if $G \cong S_{1,n-3}$.

Proof. Since G have $n-2$ pendant vertices, G have exactly two vertices say u, v of degree at least 2 and all vertices other than u, v are of degree one and also u, v are adjacent. For any vertex, say w in G other than u, v is either adjacent to u or adjacent to v but not both. Let $d(u) = x \geq 2$ then $d(v) = n-x$. Without loss of generality, we assume that $d(u) \leq d(v)$. We have
$$ABC_\alpha(G) = (x-1)\left(\frac{x-1}{x}\right)^{\alpha} + (n-x-1)\left(\frac{n-x-1}{n-x}\right)^{\alpha} + \left(\frac{n-2}{x(n-x)}\right)^{\alpha} = g(x,n).$$
Then
$$g_x(x,n) = \alpha(x-1)\left(\frac{x-1}{x}\right)^{\alpha-1}\frac{1}{x^2} + \left(\frac{x-1}{x}\right)^{\alpha} - \alpha\left(\frac{n-x-1}{n-x}\right)^{\alpha-1}\frac{1}{n-x} - \left(\frac{n-x-1}{n-x}\right)^{\alpha}$$
$$+ \alpha(n-2)^{\alpha}\left(\frac{1}{x(n-x)}\right)^{\alpha-1}\frac{2x-n}{(x(n-x))^2}.$$
If $\alpha > 0$, then $g_x(x,n) < 0$, i.e., $g(x,n)$ is decreasing with x. If $-3 \leq \alpha < -1$, then $g_x(x,n) > 0$, i.e., $g(x,n)$ is increasing with x. Thus, we have

$$ABC_\alpha(G) = (x-1)\left(\frac{x-1}{x}\right)^\alpha + (n-x-1)\left(\frac{n-x-1}{n-x}\right)^\alpha + \left(\frac{n-2}{x(n-x)}\right)^\alpha$$
$$\begin{cases} \leq (n-3)\left(\frac{n-3}{n-2}\right)^\alpha + 2\left(\frac{1}{2}\right)^\alpha & \alpha > 0, \\ \geq (n-3)\left(\frac{n-3}{n-2}\right)^\alpha + 2\left(\frac{1}{2}\right)^\alpha & -3 \leq \alpha < -1, \end{cases}$$

with equality if and only if $x = 2$, i.e., $G \cong S_{1,n-3}$. ■

Let $C^1_{n,r}$ be the graph formed by adding $\frac{n-r-1}{2}$ independent edges to the star S_n if $n-r$ is odd and adding $\frac{n-r-2}{2}$ independent edges to the star S_{n-1} and then inserting a degree two-vertex in one of the independent edge if $n-r$ is even.

Theorem 4.1. *Let $G \in \mathbb{C}^1(n,r)$, where $n \geq 4$, $3 \leq r \leq n-1$ and $\alpha > 0$.*

i. *If $r = n-1$, then $ABC_\alpha(G) = (n-1)\left(\frac{n-2}{n-1}\right)^\alpha$ and $G \cong S_n$.*
ii. *If $r = n-2$, then $ABC_\alpha(G) \leq (n-3)\left(\frac{n-3}{n-2}\right)^\alpha + 2\left(\frac{1}{2}\right)^\alpha$ with equality if and only if $G \cong S_{1,n-3}$.*
iii. *If $r \leq n-3$, then $ABC_\alpha(G) \leq M(n,r,\alpha)$ with equality if and only if $G \cong C^1_{n,r}$, where*

$$M(n,r,\alpha) = \begin{cases} r\left(\frac{n-2}{n-1}\right)^\alpha + \frac{3(n-r-1)}{2}\left(\frac{1}{2}\right)^\alpha & n-r \text{ is odd}, \\ r\left(\frac{n-3}{n-2}\right)^\alpha + \frac{3(n-r-2)}{2}\left(\frac{1}{2}\right)^\alpha + \left(\frac{1}{2}\right)^\alpha & n-r \text{ is even}. \end{cases}$$

Proof. If $r = n-1$, then by Lemma 2.2, $ABC_\alpha(G) = (n-1)\left(\frac{n-2}{n-1}\right)^\alpha$ and $G \cong S_n$. If $r = n-2$, then G is a tree with $n-2$ pendant vertices. Thus, by Lemma 4.1, $ABC_\alpha(G) \leq (n-3)\left(\frac{n-3}{n-2}\right)^\alpha + 2\left(\frac{1}{2}\right)^\alpha$ with equality if and only if $G \cong S_{1,n-3}$. Suppose that $r \leq n-3$, we prove the result by induction on $n+r$. If $n+r = 4$, then $n = 4$ and $r = 0$, i.e., $G \cong C_4$ and $G \cong C^1_{n,0}$. The result holds in this case. Now, we assume that $n+r \geq 5$, and we consider the following two possible cases.

Case 1. $r = 0$. In this case, there must exist two edges, say uv and uw in some cycle of G such that $d(u) = d(v) = 2$ and $d(w) = d \geq 3$. Here, we consider two subcases to complete the proof.

Subcase 1. $vw \notin E(G)$. Let $G' = G - u + vw$, then $G' \in \mathbb{C}^1(n-1,0)$. If n is odd, then $M(n-1,0,\alpha) = \frac{3(n-3)}{2}\left(\frac{1}{2}\right)^\alpha + \left(\frac{1}{2}\right)^\alpha$ and $M(n,0,\alpha) = \frac{3(n-1)}{2}\left(\frac{1}{2}\right)^\alpha$. If n is even, then $M(n-1,0,\alpha) = \frac{3(n-2)}{2}\left(\frac{1}{2}\right)^{\alpha}$ and $M(n,0,\alpha) = \frac{3(n-2)}{2}\left(\frac{1}{2}\right)^{\alpha} + \left(\frac{1}{2}\right)^{\alpha}$. Then by inductive assumption, we have

$$ABC_{\alpha}(G) = ABC_{\alpha}(G') + \left(\frac{1}{2}\right)^{\alpha} \begin{cases} \leq M(n-1,0,\alpha) < M(n,0,\alpha) + \left(\frac{1}{2}\right)^{\alpha} & n \ is \ odd \\ \leq M(n-1,0,\alpha) + \left(\frac{1}{2}\right)^{\alpha} = M(n,0,\alpha) & n \ is \ even. \end{cases}$$

with equality if and only if $G' \cong C^1_{n-1,0}$. Hence, $ABC_{\alpha}(G) = M(n,0,\alpha)$ holds if and only if $G \cong C^1_{n,0}$ for even n.

Subcase 2. $vw \in E(G)$. Let $N_G(w)\backslash\{u,v\} = \{u_1,u_2,\ldots,u_{d-2}\}$. Since $\delta(G) \geq 2$, $d(u_i) \geq 2$ for $1 \leq i \leq d-2$. If $G' = G-u-v$, then $G' \in \mathbb{C}^1(n-2,0)$. Hence by inductive assumption and Lemma 2.1, we have

$$\begin{aligned} ABC_{\alpha}(G) &= ABC_{\alpha}(G') + 3\left(\frac{1}{2}\right)^{\alpha} + \sum_{i=1}^{d-2} [g(d,d(u_i),\alpha) - g(d-2,d(u_i),\alpha)] \\ &\leq M(n-2,0,\alpha) + 3\left(\frac{1}{2}\right)^{\alpha} + \sum_{i=1}^{d-2} [g(d,d(u_i),\alpha) - g(d-2,d(u_i),\alpha)] \\ &= M(n,0,\alpha) - 3\left(\frac{1}{2}\right)^{\alpha} + 3\left(\frac{1}{2}\right)^{\alpha} \\ &+ \sum_{i=1}^{d-2} [g(d,d(u_i),\alpha) - g(d-2,d(u_i),\alpha)] \\ &\leq M(n,0,\alpha), \end{aligned}$$

and $ABC_{\alpha}(G) = M(n,0,\alpha)$ if and only if all the inequalities become equalities, i.e., $G' \cong C^1_{n-2,0}$, and $d(u_i) = 2$ for $i = 1,2,\ldots,d-2$. Thus, $ABC_{\alpha}(G) = M(n,0,\alpha)$ if and only if $G \cong C^1_{n,0}$.

Case 2. $r \geq 1$. Let $u_0 \in V(G)$ with $d(u_0) = 1$ and $u_0v_0 \in E(G)$. Let $d(v_0) = d$ and $N_G(v_0)\backslash\{u_0\} = \{v_1,v_2,\ldots,v_{d-1}\}$, then $2 \leq d \leq n-1$. Without loss of generality we assume that $d(v_i) = 1$ for $i = 1,2,\ldots,s-1$, and $d(v_i) \geq 2$ for $i = s,s+1,\ldots,d-1$. If $\Delta(G) = n-1$, then $d(v_0) = n-1$ and each block of G is either triangle or an edge, i.e., $G \cong C_{n,\frac{n-r-1}{2}}$, where $n-r-1$ is even. Suppose that $\Delta(G) \leq n-2$. If $G^* = G - u_0 - \sum_{i=1}^{s-1}(v_i)$, then $G^* \in \mathbb{C}^1(n-s,r-s)$. Note that $n-r$ and $n-s-(r-s)$ have same parity. Then by inductive assumption and Lemma 2.1, we have

$$\begin{aligned} ABC_{\alpha}(G) &= ABC_{\alpha}(G^*) + s\left(\frac{d-1}{d}\right)^{\alpha} + \sum_{i=s}^{d-1} [g(d,d(v_i),\alpha) - g(d-s,d(v_i),\alpha)] \\ &\leq ABC_{\alpha}(G^*) + s\left(\frac{d-1}{d}\right)^{\alpha} \\ &\leq M(n-s,r-s,\alpha) + s\left(\frac{d-1}{d}\right)^{\alpha} \end{aligned}$$

$$= \begin{cases} M(n,r,\alpha) - r\left(\frac{n-2}{n-1}\right)^{\alpha} + (r-s)\left(\frac{n-s-2}{n-s-1}\right)^{\alpha} + s\left(\frac{d-1}{d}\right)^{\alpha} & n-r \ is \ odd \\ M(n,r,\alpha) - r\left(\frac{n-3}{n-2}\right)^{\alpha} + (r-s)\left(\frac{n-s-3}{n-s-2}\right)^{\alpha} + s\left(\frac{d-1}{d}\right)^{\alpha} & n-r \ is \ even \end{cases}$$

$$= \begin{cases} M(n,r,\alpha) + (r-s)\left[\left(\frac{n-s-2}{n-s-1}\right)^{\alpha} - \left(\frac{n-2}{n-1}\right)^{\alpha}\right] \\ \quad + s\left[\left(\frac{d-1}{d}\right)^{\alpha} - \left(\frac{n-2}{n-1}\right)^{\alpha}\right] & n-r \ is \ odd \\ M(n,r,\alpha) + (r-s)\left[\left(\frac{n-s-3}{n-s-2}\right)^{\alpha} - \left(\frac{n-3}{n-2}\right)^{\alpha}\right] \\ \quad + s\left[\left(\frac{d-1}{d}\right)^{\alpha} - \left(\frac{n-3}{n-2}\right)^{\alpha}\right] & n-r \ is \ even \end{cases}$$

$$\leq M(n,r,\alpha),$$

with equality if and only if all the inequalities become equalities, i.e., if and only if $d = n-1$, $r = s$ and $G^* \cong C^1_{n-s,r-s}$. Thus, $ABC_\alpha(G) = M(n,r,\alpha)$ if and only if $G \cong C^1_{n,r}$.

By combining Case 1 and Case 2, the result follows. ■

Let $S_n(r_1, r_2)$ be a tree of order n formed from the path on $n - r_1 - r_2$ vertices by attaching r_1 and r_2 pendant vertices to its end vertices respectively, where $2 \leq r_1 \leq r_2$ and $r_1 + r_2 \leq n-3$. Let n_{xy} be the number of edges of a graph G connecting vertices of degrees x and y.

Lemma 4.2. *Let T be a tree of order $n \geq 2$ with r pendant vertices, where $2 \leq r \leq n-3$ and $-3 \leq \alpha < -1$. Then*

$$ABC_\alpha(T) \geq \left\lfloor\frac{r}{2}\right\rfloor\left(\frac{\left\lfloor\frac{r}{2}\right\rfloor}{\left\lfloor\frac{r}{2}\right\rfloor+1}\right)^{\alpha} + \left\lceil\frac{r}{2}\right\rceil\left(\frac{\left\lceil\frac{r}{2}\right\rceil}{\left\lceil\frac{r}{2}\right\rceil+1}\right)^{\alpha} + (n-1-r)\left(\frac{1}{2}\right)^{\alpha},$$

with equality if and only if $T \cong S_n(r_1, r_2)$.

Proof. For $r = 2$, the result holds trivially and so we consider $r \geq 3$. Let $u_1, u_2, \ldots, u_k$ are k vertices of T such that each u_i contains r_i pendant vertices for $1 \leq i \leq k$, and $\sum_{i=1}^{k} r_i = r$. Note that $k \geq 2$ and $r_i \geq 1$ for $1 \leq i \leq k$. Then

$$ABC_\alpha(T) = \sum_{i=1}^{k} r_i g(1, d(u_i), \alpha) + \sum_{2 \leq x \leq y \leq n-1} n_{xy} g(x, y, \alpha). \quad (1)$$

Without loss of generality, we assume that u_1 and u_2 are the neighbours of two terminal vertices of diametrical path P, then we have $d(u_1) = r_1 + 1$ and $d(u_2) = r_2 + 1$. Note that $d(u_i) \geq 2$ for $1 \leq i \leq k$, and $\sum_{i=1}^{k} d(u_i) \leq 2(n-1) - r - 2(n-r-k) = r + 2k - 2$. For $2 \leq i \leq k$, we claim that $d(u_i) \leq r + 2 - d(u_i)$. Otherwise, if $d(u_i) > r + 2 - d(u_i)$

for some $i \neq 1$, then $r + 2k - 2 \geq \sum_{i=1}^{k} d(u_i) > d(u_1) + (r + 2 - d(u_1)) + 2(k-2) = r + 2k - 2$, a contradiction. Therefore, by Lemma 2.1, we have

$$\begin{aligned}\sum_{i=1}^{k} r_i g(1, d(u_i), \alpha) &= r_1 g(1, d(u_1), \alpha) + \sum_{i=2}^{k} r_i g(1, d(u_i), \alpha)\\ &\geq r_1 g(1, d(u_1), \alpha) + \sum_{i=2}^{k} r_i g(1, r + 2 - d(u_1), \alpha)\\ &= r_1 g(1, r_1 + 1, \alpha) + (r - r_1) g(1, r - r_1 + 1, \alpha)\\ &= r_1 \left(\frac{r_1}{r_1+1}\right)^{\alpha} + (r - r_1)\left(\frac{r-r_1}{r-r_1+1}\right)^{\alpha},\end{aligned}$$

with equality if and only if $k = 2$ and $d(u_2) = r - d(u_1) + 2 = r - r_1 + 1$, i.e., $r_1 + r_2 = r$. Moreover, let $g(x) = x\left(\frac{x}{x+1}\right)^{\alpha}$, then $g(x)$ is convex since

$$g''(x) = \alpha\left(\frac{x}{x+1}\right)^{\alpha-1} \frac{1}{(x+1)^2} \frac{1+\alpha}{x+1} > 0.$$

Thus,

$$g(2) + g(r-2) \geq g(3) + g(r-3) \geq \cdots \geq g(\lfloor \tfrac{r}{2} \rfloor) + g(\lceil \tfrac{r}{2} \rceil).$$

We have

$$\begin{aligned}\sum_{i=1}^{k} r_i g(1, d(u_i), \alpha) &= r_1\left(\frac{r_1}{r_1+1}\right)^{\alpha} + (r - r_1)\left(\frac{r-r_1}{r-r_1+1}\right)^{\alpha}\\ &\geq \left\lfloor \frac{r}{2} \right\rfloor \left(\frac{\lfloor \frac{r}{2} \rfloor}{\lfloor \frac{r}{2} \rfloor + 1}\right)^{\alpha} + \left\lceil \frac{r}{2} \right\rceil \left(\frac{\lceil \frac{r}{2} \rceil}{\lceil \frac{r}{2} \rceil + 1}\right)^{\alpha}\end{aligned}$$

and equality holds if and only if $k = 2$, $r_1 = \lfloor \frac{r}{2} \rfloor$ and $r_2 = \lceil \frac{r}{2} \rceil$. On the other hand, by Lemma 2.1, we have

$$n_{xy} \sum_{2 \leq x \leq y \leq n-1} g(x, y, \alpha) \geq n_{xy} \sum_{2 \leq x \leq y \leq n-1} g(2, y, \alpha) = (n - 1 - r)\left(\frac{1}{2}\right)^{\alpha},$$

and equality holds if and only if all edges are pendant or the edges with one end vertex of degree 2. Thus, from (1), we have

$$ABC_{\alpha}(T) \geq \left\lfloor \frac{r}{2} \right\rfloor \left(\frac{\lfloor \frac{r}{2} \rfloor}{\lfloor \frac{r}{2} \rfloor + 1}\right)^{\alpha} + \left\lceil \frac{r}{2} \right\rceil \left(\frac{\lceil \frac{r}{2} \rceil}{\lceil \frac{r}{2} \rceil + 1}\right)^{\alpha} + (n - 1 - r)\left(\frac{1}{2}\right)^{\alpha},$$

with equality if and only if $T \cong S_n(r_1, r_2)$.

Lemma 4.3. [5] *Let G be a simple connected graph with two non adjacent vertices u and v. If $\alpha < 0$, then $ABC_{\alpha}(G + uv) > ABC_{\alpha}(G)$.*

Theorem 4.2. *Let $G \in \mathbb{C}^1(n, r)$, where $n \geq 4$, $3 \leq r \leq n - 1$ and $-3 \leq \alpha < -1$.*

i. *If $r = n - 1$, then $ABC_{\alpha}(G) = (n-1)\left(\frac{n-2}{n-1}\right)^{\alpha}$ and $G \cong S_n$.*

ii. *If $r = n - 2$, then $ABC_{\alpha}(G) \geq (n-3)\left(\frac{n-3}{n-2}\right)^{\alpha} + 2\left(\frac{1}{2}\right)^{\alpha}$ with equality if and only if $G \cong S_{1,n-3}$.*

iii. *If* $r \le n-3$, *then*

$$ABC_\alpha(G) \ge \left\lfloor\frac{r}{2}\right\rfloor\left(\frac{\left\lfloor\frac{r}{2}\right\rfloor}{\left\lfloor\frac{r}{2}\right\rfloor+1}\right)^\alpha + \left\lceil\frac{r}{2}\right\rceil\left(\frac{\left\lceil\frac{r}{2}\right\rceil}{\left\lceil\frac{r}{2}\right\rceil+1}\right)^\alpha + (n-1-r)\left(\frac{1}{2}\right)^\alpha,$$

with equality if and only if $G \cong S_n(r_1, r_2)$.

Proof. If $r = n-1$, then by Lemma 2.2, $ABC_\alpha(G) = (n-1)\left(\frac{n-2}{n-1}\right)^\alpha$ and $G \cong S_n$. If $r = n-2$, then G is tree with $n-2$ pendant vertices. By Lemma 4.1,

$$ABC_\alpha(G) \ge (n-3)\left(\frac{n-3}{n-2}\right)^\alpha + 2\left(\frac{1}{2}\right)^\alpha,$$

with equality if and only if $G \cong S_{1,n-3}$. Note that G is either a tree or a graph having at least one cycle. If G is a tree then the result follows from Lemma 4.2. If G contains cycles, let G' be the graph obtain from G by removing an edge from each cycle of G. Clearly, $G' \in \mathbb{C}^1(n, r)$, by Lemma 4.3, $ABC_\alpha(G) > ABC_\alpha(G')$. By Lemma 4.2, we have

$$ABC_\alpha(G) > ABC_\alpha(G') \ge \left\lfloor\frac{r}{2}\right\rfloor\left(\frac{\left\lfloor\frac{r}{2}\right\rfloor}{\left\lfloor\frac{r}{2}\right\rfloor+1}\right)^\alpha + \left\lceil\frac{r}{2}\right\rceil\left(\frac{\left\lceil\frac{r}{2}\right\rceil}{\left\lceil\frac{r}{2}\right\rceil+1}\right)^\alpha + (n-1-r)\left(\frac{1}{2}\right)^\alpha.$$

This completes the proof. ■

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