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On zeroth-order general Randić index of conjugated unicyclic graphs

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Let G be a graph and d_v denote the degree of the vertex v in G. The zeroth-order general Randić index of a graph is defined as $R_\alpha^0(G) = \sum_{v \in V(G)} {d_v}^\alpha$ where α is an arbitrary real number. In this paper, we investigate the zeroth-order general Randić index $R_\alpha^0(G)$ of conjugated unicyclic graphs G (i.e., unicyclic graphs with a perfect matching) and sharp lower and upper bounds are obtained for $R_\alpha^0(G)$ depending on α in different intervals.

KEY WORDS: conjugated tree, conjugated unicyclic graph, zeroth-order general Randić index

1. Introduction

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$, respectively. For any $v \in V(G)$, we denote the neighbors of v as $N(v)$. By $n(G)$ and $\triangle(G)$ we denote, respectively, the order and maximum degree of graph G. The Randić index of G defined in [16] is

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2},$$

where $d_v = d_G(v)$ denotes the degree of the vertex v in G. Randić showed that his index is well correlated with a variety of Physic–Chemical properties of an alkane. The index $R(G)$ has become one of the most popular molecular descriptors, the interesting reader is referred to [1, 3, 4, 14–17]. The zeroth-order Randić index $R^0(G)$ of G defined by Kier and Hall [10] is $R^0(G) = \sum_{v \in V(G)} {d_v}^{-\frac{1}{2}}$.

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Pavlović [14] determined the unique graph with largest value of $R^0(G)$. In [6], Lielal investigated the same problem for the topological index $M_1(G)$, also known as Zagreb index [17], which is defined as $M_1(G) = \sum_{v \in V(G)} {d_v}^2$. Li and Zheng [13] defined the zeroth-order general Randić index as $R^0_\alpha(G) = \sum_{v \in V(G)} {d_v}^\alpha$. Li and Zhao [11] characterized the trees with the first three largest and smallest zeroth-order general Randić index with α being equal to m, $-m$, $\frac{1}{m}$, $-\frac{1}{m}$ where $m \geqslant 2$ is an integer.

In [8], Hu et al. investigated the molecular graphs having the smallest and largest zeroth-order general Randić index. Hua and Deng [9] gave sharp lower and upper bounds for zeroth-order general Randić index among all unicyclic graphs.

All graphs considered here are both finite and simple. We denote, respectively, by S_n, P_n, and C_n the star, path, and cycle with n vertices.

Let (G_1, v_1) and (G_2, v_2) be two graphs rooted at v_1 and v_2, respectively, then $G = (G_1, v_1) \bowtie (G_1, v_2)$ denote the graph obtained by identifying v_1 with v_2 as one common vertex. Let $\mathfrak{U}_k(n)$ denote the set of all unicyclic graphs of order n and with k as its length of cycle. By $\mathfrak{U}_k(2m, m)$ we denote the set of conjugated unicyclic graphs of order $n = 2m$ in which the length of its unique cycle is k, where m is the number of matchings in G. For any graph G in $\mathfrak{U}_k(2m, m)$, we denote the unique cycle of length k in G as C_k. Other notations and terminology not defined here will conform to those in [11].

For any graph in $\mathfrak{U}_k(2m, m)$ with $n = 2m = k$ or $n = 2m = k + 1$, its zeroth-order general Randić index can be uniquely determined. So we will always assume that $n = 2m \geqslant k + 2$ throughout this paper.

In this paper, we investigate the zeroth-order general Randić index for the conjugated unicyclic graphs (unicyclic graphs having a perfect matching). For any graph $G \in \mathfrak{U}_k(2m, m)$, we give sharp lower and upper bounds for $R^0_\alpha(G)$ depending on α in different intervals.

2. The zeroth-order general Randić index of conjugated trees

For convenience, we introduce some notations in the following.

Let $T(n, m)$ denote all n-vertex trees with an m-matching. Let n and m be positive integers such that $n \geqslant 2m$. A tree $T^0(n, m)$ is defined as follows: $T^0(n, m)$ is obtained from the star S_{n-m+1} by attaching a pendent edge to each of certain $m - 1$ non-central vertices of S_{n-m+1}, then T is a tree with an $m-$matching. In particular, when $n = 2m$, the tree $T^0(2m, m)$ has a perfect matching.

The following two lemmas due to Hou and Li in [7], which will be helpful to the proofs of our main results.

Lemma 2.1. Let T be a n-vertex tree ($n \geqslant 3$) with a perfect matching, then T has at least two pendent vertices such that each are adjacent to vertices of degree two.

Lemma 2.2. Let T be a n-vertex tree ($n \geqslant 3$) with an m – matching where $n > 2m$, then there is an m – matching M and a pendent vertex v such that M does not saturate v.

It is easy to get the following trivial results:

When $\alpha = 0$, $R_\alpha^0(T) = \sum_{v \in V(T)} d_v{}^\alpha = n$, where n is the order of the tree T.

When $\alpha = 1$, $R_\alpha^0(T) = \sum_{v \in V(T)} d_v{}^\alpha = 2m$, where m is the number of edges of the tree T.

So, we need only to consider the two cases $\alpha \in (0, 1)$ and $\alpha \in (-\infty, 0) \bigcup (1, +\infty)$.

For all trees T in $T(2m, m)$ and $\alpha \in (-\infty, 0) \bigcup (1, +\infty)$, sharp lower and upper bounds for $R_\alpha^0(T)$ are obtained in the following theorem.

Theorem 2.3. Let $\alpha > 1$ or $\alpha < 0$ and T be any tree in $T(2m, m)$ where $m \geqslant 1$, then $2 + (2m - 2)2^\alpha \leqslant R_\alpha^0(T) \leqslant m^\alpha + (m - 1)2^\alpha + m$ with left equality holds if and only if $T \cong P_{2m}$ and with right equality holds if and only if $T \cong T^0$ $(2m, m)$.

Proof. We divide the proof of theorem into two parts.

First, we will show $R_\alpha^0(T) \leqslant m^\alpha + (m - 1)2^\alpha + m$.

Let T be a tree in $T(2m, m)$. If $T \cong T^0(2m, m)$, then $R_\alpha^0(T) = R_\alpha^0(T^0(2m, m))$. Otherwise, let u be a vertex in T such that $d(u) = \triangle(T)$, then $d(u) \geqslant 2$. By lemma 2.1, there exists a pair of adjacent vertices, say x_1 and y_1 in T such that $d(x_1) = 1$ and $d(y_1) = 2$. Let $N(y_1) - \{x_1\} = \{z_1\}$.

Set $T^{(1)} = T - y_1z_1 + uy_1$, then $T^{(1)} \in T(2m, m)$. Note that

$$\begin{aligned} R_\alpha^0(T^{(1)}) - R_\alpha^0(T) &= [(d_u + 1)^\alpha - d_u^\alpha] + [d_{z_1}^\alpha - (d_{z_1} - 1)^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $d_{z_1} - 1 < \eta < d_{z_1} \leqslant d_u < \xi < d_u + 1$.

Then $R_\alpha^0(T^{(1)}) > R_\alpha^0(T)$ since $\alpha > 1$ or $\alpha < 0$.

Let $T' = T^{(1)} - \{x_1, y_1\}$, then $T' \in T(2(m-1), m-1)$. Once again by lemma 2.1, there exists a pair of adjacent vertices x_2 and y_2 in T' with $d(x_2) = 1$ and $d(y_2) = 2$. Let $N(y_2) - \{x_2\} = \{z_2\}$. Set $T'' = T' - y_2z_2 + uy_2$, obviously $d_{T'}(u) = \triangle(T) = \triangle(T')$. Similarly, we have $R_\alpha^0(T'') > R_\alpha^0(T')$.

Denote $T^{(2)} = T^{(1)} - y_2z_2 + uy_2$, then

$$\begin{aligned} R_\alpha^0(T^{(2)}) &= d_{x_1}^\alpha + d_{y_1}^\alpha + (d_u + 2)^\alpha - (d_u + 1)^\alpha + R_\alpha^0(T'') \\ &= 1 + 2^\alpha + (d_u + 2)^\alpha - (d_u + 1)^\alpha + R_\alpha^0(T'') \\ &>^* 1 + 2^\alpha + (d_u + 1)^\alpha - d_u^\alpha + R_\alpha^0(T') \\ &= R_\alpha^0(T^{(1)}). \end{aligned}$$

The inequality $(*)$ holds due to the fact that $(d_u + 2)^\alpha - (d_u + 1)^\alpha > (d_u + 1)^\alpha - d_u^\alpha$ when $\alpha > 1$ or $\alpha < 0$ and $R_\alpha^0(T'') > R_\alpha^0(T')$.

Repeating the above process in many times, we finally get a sequence of trees $T^{(1)}, T^{(2)}, \dots T^{(l)}, \dots$ such that $R^0_\alpha(T) < R^0_\alpha(T^{(1)}) < R^0_\alpha(T^{(2)}) < \cdots < R^0_\alpha(T^{(l)}) < \dots$. There must exist some positive integer s such that $T^{(s)} \cong T^{(s+1)}$, and then $T^{(s)} \cong T^0(2m, m)$. So $R^0_\alpha(T) < R^0_\alpha(T^0(2m, m))$ and then $R^0_\alpha(T) \leqslant R^0_\alpha(T^0(2m, m)) = m^\alpha + (m-1)2^\alpha + m$ with equality holds if and only if $T \cong T^0(2m, m)$.

Second, we will show that $R^0_\alpha(T) \geqslant 2 + (2m-2)2^\alpha$.

If $T \cong P_{2m}$, then $R^0_\alpha(T) = R^0_\alpha(P_{2m})$. Otherwise, let P_{2m} be operated as above, we have $R^0_\alpha(P_{2m}) < R^0_\alpha(T^{(1)}) < R^0_\alpha(T^{(2)}) < \cdots < R^0_\alpha(T^{(l)}) < \cdots$. There must exist some positive integer $j \geqslant 1$ such that $T \cong T^{(j)}$, so $R^0_\alpha(T) = R^0_\alpha(T^{(j)}) > R^0_\alpha(P_{2m})$. Therefore, $R^0_\alpha(T) \geqslant R^0_\alpha(P_{2m}) = 2 + (2m-2)2^\alpha$ with equality holds if and only if $T \cong P_{2m}$. □

When $0 < \alpha < 1$, the following theorem follows immediately from the proof of theorem 2.3.

Theorem 2.4. Let $0 < \alpha < 1$ and T be any n-vertex tree in $T(2m, m)$ where $m \geqslant 1$, we have $m^\alpha + (m-1)2^\alpha + m \leqslant R^0_\alpha(T) \leqslant 2 + (2m-2)2^\alpha$ with left equality holds if and only if $T \cong T^0(2m, m)$ and with right equality holds if and only if $T \cong P_{2m}$.

3. The zeroth-order general Randić index of conjugated unicyclic graphs

In this section, we will give sharp lower and upper bounds for $R^0_\alpha(G)$ among all conjugated unicyclic graphs in $\mathcal{U}_k(2m, m)$ according to α in different intervals.

First, we will establish some lemmas which will be useful to the proofs of our main results.

Lemma 3.1. If T is a tree in $T(2m+1, m)$, then there exists at least one pendent vertex u in T such that u is adjacent to a vertex of degree two.

Proof. Let T be a tree in $T(2m+1, m)$ and M an maximal matching of T. There must exist a vertex, say u, in T such that u is not saturated by M.

Since $T \in T(2m+1, m)$, then $T - \{u\} \in T(2m, m)$ and M is a perfect matching of $T - \{u\}$. By lemma 2.1, there exist two pendent vertices in $T - \{u\}$ such that each is adjacent to a vertex of degree two.

Hence T has at least one pendent vertex such that it is adjacent to a vertex of degree two. This completes the proof. □

Lemma 3.2. Let $\alpha > 1$ or $\alpha < 0$ and T be any tree in $T(2m+1, m)$ $(m \geqslant 1)$, then $R^0_\alpha(T) \geqslant R^0_\alpha(P_{2m+1})$ with equality holds if and only if $T \cong P_{2m+1}$.

Proof. Let T be a tree in $T(2m+1, m)$. By lemma 2.2, there exists a pendent vertex v in T such that v is not saturated by some maximal matching M of T. Since $T \in T(2m+1, m)$, all vertices in $T - \{v\}$ are saturated by M. So $T - \{v\} \in T(2m, m)$. Let $N(v) = \{w\}$. Note that $R_\alpha^0(T) = R_\alpha^0(T - \{v\}) + d_w^\alpha - (d_w - 1)^\alpha + d_v^\alpha = R_\alpha^0(T - \{v\}) + d_w^\alpha - (d_w - 1)^\alpha + 1$. Hence, from theorem 2.3 it follows that

$$\begin{aligned} R_\alpha^0(T) &\geqslant R_\alpha^0(P_{2m}) + d_w^\alpha - (d_w - 1)^\alpha + 1 \\ &= 2 + (2m-2).2^\alpha + d_w^\alpha - (d_w - 1)^\alpha + 1 \\ &\geqslant^{**} 2 + (2m-1).2^\alpha \\ &= R_\alpha^0(P_{2m+1}). \end{aligned}$$

To show $(**)$ holds, it suffices to prove that $d_w^\alpha - (d_w - 1)^\alpha + 1 - 2^\alpha \geqslant 0$.

If $d_w = 2$, then $d_w^\alpha - (d_w - 1)^\alpha + 1 - 2^\alpha = 0$. Otherwise $d_w \geqslant 3$, then $d_w^\alpha - (d_w - 1)^\alpha + 1 - 2^\alpha = \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) > 0$ since $\alpha > 1$ or $\alpha < 0$, where $1 < \eta < 2 \leqslant d_w - 1 < \xi < d_w$.

Consequently, $R_\alpha^0(T) \geqslant R_\alpha^0(P_{2m+1})$. It is not difficult to see that the above equality holds if and only if $R_\alpha^0(T - \{v\}) = R_\alpha^0(P_{2m})$ and $d_w = 2$, which implies that $T \cong P_{2m+1}$ by theorem 2.3. □

Lemma 3.3. Let $\alpha > 1$ or $\alpha < 0$ and T be any tree in $T(2m+1, m)(m \geqslant 1)$, then $R_\alpha^0(T) \leqslant R_\alpha^0(T^0(2m+1, m))$ with equality holds if and only if $T \cong T^0(2m+1, m)$.

Proof. Let T be a tree in $T(2m+1, m)$. If $T \cong T^0(2m+1, m)$, then $R_\alpha^0(T) = R_\alpha^0(T^0(2m+1, m))$, otherwise by lemma 2.2, there exists a pendent vertex v in T such that v is not saturated by some maximal matching M of T. Let $N(v) = \{w\}$ and $d_u = \triangle(T)$. Set $T' = T - vw + uv$, then $T' - \{v\} \in T(2m, m)$. By theorem 2.3, we have $R_\alpha^0(T' - v) \leqslant R_\alpha^0(T^0(2m, m))$. So we have

$$\begin{aligned} R_\alpha^0(T') &= R_\alpha^0(T' - v) + d_v^\alpha + (d_u + 1)^\alpha - d_u^\alpha \\ &\leqslant 1 + R_\alpha^0(T^0(2m, m)) + (d_u + 1)^\alpha - d_u^\alpha \\ &<^{***} 1 + R_\alpha^0(T^0(2m, m)) + (m+1)^\alpha - m^\alpha \\ &= 1 + m^\alpha + (m-1).2^\alpha + m + (m+1)^\alpha - m^\alpha \\ &= (m+1)^\alpha + (m-1).2^\alpha + m + 1 \\ &= R_\alpha^0(T^0(2m+1, m)). \end{aligned}$$

To show $(***)$ holds, it suffices to prove that $(d_u + 1)^\alpha - (d_u)^\alpha < (m+1)^\alpha - m^\alpha$. Since $\triangle(T^0(2m, m)) = m$ and $T \ncong T^0(2m+1, m)$, then $d(u) \leqslant m$. If $d(u) = m$, then $[(m+1)^\alpha - m^\alpha] - [(d_u + 1)^\alpha - d_u^\alpha] = 0$. Otherwise, $[(m+1)^\alpha - m^\alpha] - [(d_u + 1)^\alpha - d_u^\alpha] = \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) > 0$, since $d_u < \eta < d_u + 1 \leqslant m < \xi < m + 1$ and $\alpha > 1$or $\alpha < 0$.

Hence $R_\alpha^0(T) < R_\alpha^0(T') < R_\alpha^0(T^0(2m+1, m))$ and then $R_\alpha^0(T) \leqslant R_\alpha^0(T^0(2m+1, m))$ with equality holds if and only if $T \cong T^0(2m+1, m)$. □

The following two lemmas are obvious.

Lemma 3.4. Let $0 < \alpha < 1$ and T be any tree in $T(2m+1, m)$ $(m \geqslant 1)$, then $R_\alpha^0(T) \leqslant R_\alpha^0(P_{2m+1})$ with equality holds if and only if $T \cong P_{2m+1}$.

Lemma 3.5. Let $0 < \alpha < 1$ and T be any tree in $T(2m+1, m)(m \geqslant 1)$, then $R_\alpha^0(T) \geqslant R_\alpha^0(T^0(2m+1, m))$ with equality holds if and only if $T \cong T^0(2m+1, m)$.

Let $S = \{v_i \in V(C_k) | d(v_i) \geqslant 3\}$. For any $v_i \in S$, by $T(v_i)$ we denote the connected component containing v_i of the graph $G - \{v_{i-1}v_i, v_i v_{i+1}\}$.

Lemma 3.6. Let G be a graph in $\mathfrak{U}_k(2m, m)$, then, for each $v_i \in S$, we have that $T(v_i)$ belongs either to $T(n_i, \frac{n_i}{2})$ or to $T(n_i, \frac{n_i-1}{2})$.

Proof. Since $G \in \mathfrak{U}_k(2m, m)$, there exists a perfect matching M of G such that every vertex in G is saturated by M.

For each $v_i \in S$, let $M' = M \bigcap E(T(v_i))$, then M' is also an matching of $T(v_i)$.

If $v_{i-1}v_i \in M$ or $v_i v_{i+1} \in M$, then v_i is not saturated by M', but all other vertices in $T(v_i) - \{v_i\}$ are saturated by M' since $G \in \mathfrak{U}_k(2m, m)$. So $T(v_i) \in T(n_i, \frac{n_i-1}{2})$.

If $v_{i-1}v_i \notin M$ and $v_i v_{i+1} \notin M$, then v_i is saturated by M' as well as all other vertices in $T(v_i) - \{v_i\}$, so $T(v_i) \in T(n_i, \frac{n_i}{2})$. □

For any $G \in \mathfrak{U}_k(2m, m)$, the following several lemmas will give necessary conditions on which $R_\alpha^0(G)$ attains extremal values.

Lemma 3.7. Let $\alpha > 1$ or $\alpha < 0$ and G be a graph in $\mathfrak{U}_k(2m, m)$ such that $R_\alpha^0(G)$ is as small as possible, then $T(v_i) \cong P_{n_i}$ for each $v_i \in S$ where $n_i = n(T(v_i))$. Moreover, v_i is one pendent vertex of P_{n_i}.

Proof. Let G be a graph in $\mathfrak{U}_k(2m, m)$ such that $R_\alpha^0(G)$ is as small as possible and v_i a vertex in S. Let v_{i-1} and v_{i+1} denote the two neighbors of v_i along the cycle C_k. We write $A = [d_{v_i}^\alpha - (d_{v_i} - 2)^\alpha] + [d_{v_{i+1}}^\alpha - (d_{v_{i+1}} - 1)^\alpha] + [d_{v_{i-1}}^\alpha - (d_{v_{i-1}} - 1)^\alpha]$. Let G_1 denote the connected component not containing v_i of the graph $G - \{v_{i-1}v_i, v_i v_{i+1}\}$. Then $R_\alpha^0(G) = R_\alpha^0(G_1) + A + R_\alpha^0(T(v_i))$. By lemma 3.6, $T(v_i)$ belongs either to $T(n_i, \frac{n_i}{2})$ or to $T(n_i, \frac{n_i-1}{2})$. In either cases, we have

$$R_\alpha^0(G) \geqslant R_\alpha^0(G_1) + A + R_\alpha^0(P_{n_i})$$

by theorem 2.3 and lemma 3.2. Moreover, the above equality holds if and only if $T(v_i)) \cong P_{n_i}$.

In the following, we will show that v_i is one pendent vertex of P_{n_i}, that is $d(v_i) = 3$. Assume that $d(v_i) \neq 3$, then $d(v_i) = 4$ since $T(v_i)) \cong P_{n_i}$. Let $N(v_i) -$

$\{v_{i-1}, v_{i+1}\} = \{x, y\}$ and M be a perfect matching of G. Then there were at least one of two edges $v_i x$ and $v_i y$ which does not belong to M. Without loss of generality, we assume that $v_i x \notin M$. Let $P(y) = y_1 \dots y_p (p \geqslant 2)$ denote the path with $y_1 = y$ as one of its pendent vertex.

Set $G' = G - v_i x + y_p x$, then $G' \in \mathcal{U}_k(2m, m)$ and

$$R_\alpha^0(G') - R_\alpha^0(G) = (2^\alpha - 1) - (4^\alpha - 3^\alpha).$$

Since $\alpha > 1$ or $\alpha < 0$, we have $R_\alpha^0(G') < R_\alpha^0(G)$, contradicting the choice of G. Consequently, the desired result follows. □

Lemma 3.8. Let $\alpha > 1$ or $\alpha < 0$ and G be a graph in $\mathcal{U}_k(2m, m)$ such that $R_\alpha^0(G)$ is as great as possible, then for each $v_i \in S$, we have $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$ or $T(v_i) \cong T^0(n_i, \frac{n_i - 1}{2})$. Moreover, if $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$, then $d(v_i) - 2 = \triangle(T^0(n_i, \frac{n_i}{2}))$; if $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$, then v_i is one pendent vertex of $T^0(n_i, \frac{n_i-1}{2})$ which is adjacent to the maximum-degree vertex of $T^0(n_i, \frac{n_i-1}{2})$.

Proof. Let G be a graph in $\mathcal{U}_k(2m, m)$ such that $R_\alpha^0(G)$ is large enough. Let v_i be a vertex in S. Let v_{i-1} and v_{i+1} denote the two neighbors of v_i along the cycle C_k. We write $A = [d_{v_i}^\alpha - (d_{v_i} - 2)^\alpha] + [d_{v_{i+1}}^\alpha - (d_{v_{i+1}} - 1)^\alpha] + [d_{v_{i-1}}^\alpha - (d_{v_{i-1}} - 1)^\alpha]$. Let G_1 denote the connected component not containing v_i of the graph $G - \{v_{i-1}v_i, v_i v_{i+1}\}$. Then $R_\alpha^0(G) = R_\alpha^0(G_1) + A + R_\alpha^0(T(v_i))$. Combining theorem 2.3, lemmas 3.3 and 3.6, we obtain

$$R_\alpha^0(G) \leqslant R_\alpha^0(G_1) + A + R_\alpha^0\left(T^0\left(n_i, \frac{n_i}{2}\right)\right)$$

if n_i is even or

$$R_\alpha^0(G) \leqslant R_\alpha^0(G_1) + A + R_\alpha^0\left(T^0\left(n_i, \frac{n_i - 1}{2}\right)\right)$$

if n_i is odd.

The above two equalities hold if and only if $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$ and $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$, respectively.

In the following, we will show that (i) if $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$, then $d(v_i) - 2 = \triangle(T^0(n_i, \frac{n_i}{2}))$;(ii) if $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$, then v_i is one pendent vertex of $T^0(n_i, \frac{n_i-1}{2})$ which is adjacent to the maximum-degree vertex of $T^0(n_i, \frac{n_i-1}{2})$.

First, we show (i) holds.

Suppose that $d(v_i) - 2 < \triangle(T^0(n_i, \frac{n_i}{2}))$.

Let u be a vertex in $T(v_i)$ such that $d(u) = \triangle(T^0(n_i, \frac{n_i}{2}))$ and G' denote the graph obtained by replacing two edges $v_{i-1}v_i$ and $v_{i+1}v_i$ of G by $v_{i-1}u$ and $v_{i+1}u$. Then $G' \in \mathcal{U}_k(2m, m)$ and

$$R_\alpha^0(G') - R_\alpha^0(G) = [(d_u + 2)^\alpha - d_u^\alpha] - [d_v^\alpha - (d_v - 2)^\alpha].$$

If $d_v \geqslant d_u$, then

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(d_u+2)^\alpha - d_u^\alpha] - [d_v^\alpha - (d_v-2)^\alpha] \\ &= [(d_u+2)^\alpha - d_v^\alpha] - [d_u^\alpha - (d_v-2)^\alpha] \\ &= (d_u + 2 - d_v)\alpha(\xi_1^{\alpha-1} - \eta_1^{\alpha-1}), \end{aligned}$$

where $d_v - 2 < \eta_1 < d_u \leqslant d_v < \xi_1 < d_u + 2$. Since $\alpha > 1$ or $\alpha < 0$, then $R_\alpha^0(G') > R_\alpha^0(G)$, contradicting the choice of G.

If $d_v < d_u$, then

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(d_u+2)^\alpha - d_u^\alpha] - [d_v^\alpha - (d_v-2)^\alpha] \\ &= 2\alpha(\xi_2^{\alpha-1} - \eta_2^{\alpha-1}), \end{aligned}$$

where $d_v - 2 < \eta_2 < d_v < d_u < \xi_1 < d_u + 2$. Since $\alpha > 1$ or $\alpha < 0$, then $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction to the maximality of $R_\alpha^0(G^)$ once again. So the desired result holds.

To show (ii) holds, we need only to prove that $d(v_i) = 3$ and $d(u) = \triangle(T(v_i))$, where $u = N(v_i) - \{v_{i-1},\ v_{i+1}\}$.

Since $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$ and $G \in \mathcal{U}_k(2m, m)$, then $d(v_i) - 2 < \triangle(T^0(n_i, \frac{n_i-1}{2}))$. Note that for any vertex $w \in T^0(n_i, \frac{n_i-1}{2})$, if $d(w) < \triangle(T^0(n_i, \frac{n_i-1}{2}))$, then $d(w) = 1$ or $d(w) = 2$.

If $d(v_i) - 2 = 2$, there must exist a vertex in $T^0(n_i, \frac{n_i-1}{2})$ such that it can not be saturated by some maximal matching M of G, a contradiction. So $d(v_i) - 2 = 1$, that is $d(v_i) = 3$.

If $d(u) < \triangle(T^0(n_i, \frac{n_i-1}{2}))$, then we still have a vertex in $T^0(n_i, \frac{n_i-1}{2})$ such that it can't be saturated by some maximal matching M of G, a contradiction once again.

Therefore the proof is completed. □

The following two lemmas can be obtained easily, so we omitted their proofs here.

Lemma 3.9. Let $0 < \alpha < 1$ and G be a graph in $\mathcal{U}_k(2m, m)$ such that $R_\alpha^0(G)$ is as large as possible, then $T(v_i) \cong P_{n_i}$ for each $v_i \in S$ where $n_i = n(T(v_i))$. Moreover, v_i is one pendent vertex of P_{n_i}.

Lemma 3.10. Let $0 < \alpha < 1$ and G be a graph in $\mathcal{U}_k(2m, m)$ such that $R_\alpha^0(G)$ is as small as possible, then for each $v_i \in S$, we have $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$ or $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$. Moreover, if $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$, then $d(v_i) - 2 = \triangle(T^0(n_i, \frac{n_i}{2}))$; if $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$, then v_i is one pendent vertex of $T^0(n_i, \frac{n_i-1}{2})$ which is adjacent to the maximum-degree vertex of $T^0(n_i, \frac{n_i-1}{2})$.

The following theorem will give a sharp lower bound for $R_\alpha^0(G)$ among all conjugated unicyclic graphs in $\mathcal{U}_k(2m, m)$.

Theorem 3.11. Let G be a graph in $\mathcal{U}_k(2m, m)$ and $\alpha > 1$ or $\alpha < 0$, then $R_\alpha^0(G) \geqslant 1+3^\alpha+(2m-2)2^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (P_{2m-k+1}, v_i)$, where v_i is any vertex of C_k and one pendent vertex of P_{2m-k+1}, respectively.

Proof. Let G be a graph in $\mathcal{U}_k(2m, m)$ with $R_\alpha^0(G)$ taking the smallest value. Then by lemma 3.7, $T(v_{ij}) \cong P_{n_{ij}}$ for each $v_{ij} \in S$, where $n_{ij} = n(T(v_{ij}))$.

If $|S| = 1$, then the result holds. Now assume that $|S| \geqslant 2$.

Since $T(v_{ij}) \cong P_{n_{ij}}$ $(j = 1, \dots |S|)$, we denote $T(v_{ij}) = x_0^{(j)} x_1^{(j)} \dots x_{t_j}^{(j)}$ $(t_j \geqslant 1)$, where $x_0^{(j)} = v_{ij} (j = 1, \dots |S|)$.

Set $G' = G - x_0^{(2)} x_1^{(2)} - x_0^{(3)} x_1^{(3)} - \dots - x_0^{(|S|)} x_1^{(|S|)} + x_{t_1}^{(1)} x_1^{(2)} + x_{t_2}^{(2)} x_1^{(3)} + \dots + x_{t_{(|S|-1)}}^{(|S|-1)} x_1^{(|S|)}$.

Obviously, $G' \in \mathcal{U}_k(2m, m)$ and

$$R_\alpha^0(G') - R_\alpha^0(G) = (|S| - 1)(2^\alpha - 3^\alpha) + (|S| - 1)(2^\alpha - 1).$$

For $\alpha > 1$ or $\alpha < 0$, we have $R_\alpha^0(G') < R_\alpha^0(G)$, which contradicting the minimality of $R_\alpha^0(G)$. So $|S| = 1$ and the proof is completed. □

The next theorem follows readily from the proof theorem 3.11 and lemma 3.9.

Theorem 3.12. Let G be a graph in $\mathcal{U}_k(2m, m)$ and $0 < \alpha < 1$, then $R_\alpha^0(G) \leqslant 1+3^\alpha+(2m-2)2^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (P_{2m-k+1}, v_i)$, where v_i is any vertex of C_k and one pendent vertex of P_{2m-k+1}, respectively.

Lemma 3.13. Let $f(x) = (x + 2)^\alpha + x^\alpha - 2(x + 1)^\alpha$ be defined in the interval $[1, +\infty)$, then $f(x)$ is a monotonically increasing function in $[1, +\infty)$ where α is a constant greater than 2.

Proof. Note that $f(x) = [(x + 2)^\alpha - (x + 1)^\alpha] - [(x + 1)^\alpha - x^\alpha]$, then

$$\begin{aligned}\frac{\mathrm{d}f(x)}{\mathrm{d}x} &= \alpha[(x + 2)^{\alpha-1} - (x + 1)^{\alpha-1}] - \alpha[(x + 1)^{\alpha-1} - x^{\alpha-1}] \\ &= \alpha(\alpha - 1)(\xi^{\alpha-2} - \eta^{\alpha-2}),\end{aligned}$$

where $1 \leqslant x < \eta < x + 1 < \xi < x + 2$.

When $\alpha > 2$, we have $\frac{\mathrm{d}f(x)}{\mathrm{d}x} > 0$. This implies the desired result. □

In the following, we will give a sharp upper bound for $R_\alpha^0(G)$ among all conjugated unicyclic in $\mathcal{U}_k(2m, m)$.

Theorem 3.14. Suppose G is a graph in $\mathcal{U}_k(2m, m)$ and $\alpha > 2$, we have the following

(i) If $2m = k + 2$, then $R^0_\alpha(G) \leqslant 2 + (k-2)2^\alpha + 3^\alpha$ with equality holding if and only if $G \ncong (C_k, P_3)$.

(ii) If $2m \geqslant k + 3$ and k is odd, then $R^0_\alpha(G) \leqslant (m - \frac{k-1}{2}) + (m + \frac{k-3}{2})2^\alpha + (m - \frac{k-5}{2})^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (T^0(2m - k + 1, \frac{2m-k+1}{2}), v_i)$. Moreover, $d_{v_i} - 2 = \triangle((T^0(2m - k + 1, \frac{2m-k+1}{2}), v_i))$.

(iii) If $2m \geqslant k+3$ and k is even, then $R^0_\alpha(G) \leqslant (m - \frac{k}{2}) + (m + \frac{k}{2} - 2)2^\alpha + 3^\alpha + (m + 1 - \frac{k}{2})^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (T^0(2m - k + 1, \frac{2m-k}{2}), v_i)$. Moreover , $d(v_i) = 3$ and u is the maximum-degree vertex of $(T^0(2m - k + 1, \frac{2m-k}{2}), v_i)$ where $u = N(v_i) - \{v_{i-1}, v_{i-1}\}$.

Proof. Let G be a graph in $\mathcal{U}_k(2m, m)$ with $R^0_\alpha(G)$ taking the maximum cardinality. It follows from lemma 3.8 that $T(v_i) \cong T^0(n_i, \frac{n_i-1}{2})$ or $T(v_i) \cong T^0(n_i, \frac{n_i}{2})$ for each $v_i \in S$.

If $|S| = 1$, then we must have $2m \neq k+2$. If $2m = k+2$, then $G \cong (C_k, P_3)$ since $G \in \mathcal{U}_k(2m, m)$. By theorem 3.11, we have $R^0_\alpha(G) = R^0_\alpha((C_k, P_3)) < R^0_\alpha(G')$ for any $G' \ncong (C_k, P_3)$, contradicting the choice of G. So, $2m \geqslant k+3$. By lemma 3.8, (ii) or (iii) holds.

Suppose $|S| \geqslant 2$, we consider the following several cases:

Case 1. $2m = k + 2$.

In this case, we can easily see that for any two graphs G_1 and G_2 in $\mathcal{U}_k(2m, m)$, $G_1 \ncong (C_k, P_3)$ and $G_2 \ncong (C_k, P_3)$. Moreover, $R^0_\alpha(G_1) = R^0_\alpha(G_2)$. Furthermore, by theorem 3.11, we have $R^0_\alpha(G) > R^0_\alpha((C_k, P_3))$ if $G \ncong (C_k, P_3)$, so (i) holds.

Case 2. $2m \geqslant k + 3$.

We distinguish the following subcases:

For any vertex $v_{i_j} \in S$, $j = 1, \ldots |S|$,we will denote $n(T(v_{i_j}))$ by n_j hereinafter.

Subcase 2.1. $n_j = 2$ for each $v_{i_j} \in S$.

Let $V(G) - V(C_k) = \{x_1, \ldots x_{|S|}\}$ and $N(x_j) = v_{i_j}$, $j = 1, \ldots |S|$. Let $N(v_{i_j}) - \{x_j\} = \{v_{i_j-1}, v_{i_j+1}\}$, $j = 1, \ldots |S|$.

In this case, $|S| \geqslant 3$.

If $|S| = 3$, let $G' = G - v_{i_2}x_2 - v_{i_3}x_3 + v_{i_1}x_2 + x_2x_3$; If $|S| \geqslant 4$, let $G' = G - v_{i_2}x_2 - v_{i_3}x_3 - v_{i_2-1}v_{i_2} - v_{i_2}v_{i_2+1} - v_{i_3}v_{i_3+1} + v_{i_2-1}v_{i_2+1} + v_{i_2}v_{i_3} + v_{i_2}v_{i_3+1} + v_{i_1}x_2 + x_2x_3$. In either cases, we have $G' \in \mathcal{U}_k(2m, m)$ and

$$\begin{aligned} R^0_\alpha(G') - R^0_\alpha(G) &= (4^\alpha - 3^\alpha) + (2^\alpha - 1) - 2(3^\alpha - 2^\alpha) \\ &= (4^\alpha + 2^\alpha - 2.3^\alpha) - (3^\alpha + 1 - 2.2^\alpha). \end{aligned}$$

Since $\alpha > 2$, then $R_\alpha^0(G') > R_\alpha^0(G)$ by lemma 3.13, a contradiction to the choice of G.

Subcase 2.2. There exists some $v_{i_l} \in S$ such that $n_l = 3$.

Since $|S| \geqslant 2$, there exists at least one vertex v_{i_t} in $S - \{v_{i_l}\}$.

Set $G' = G - v_{i_l}x_l + v_{i_t}x_l$, then $G' \in \mathfrak{U}_k(2m, m)$ and

$$R_\alpha^0(G') - R_\alpha^0(G) = [(d_{v_{i_t}} + 1)^\alpha - d_{v_{i_t}}^\alpha] - (3^\alpha - 2^\alpha).$$

Since $d_{v_{i_t}} \geqslant 3$ and $\alpha > 2$, then $R_\alpha^0(G') > R_\alpha^0(G)$, a contradiction once again.

Subcase 2.3. For any vertex v_{i_j} in S, $n_j \geqslant 4$.

The following two subcases should be considered:

Subcase 2.3.1. There exists some $v_{i_l} \in S$ such that $d(v_{i_l}) = \triangle(G)$.

Since $|S| \geqslant 2$, there exists some vertex v_{i_t} in $S - \{v_{i_l}\}$. By lemmas 3.6, 2.1, and 3.1, there exists a pair of adjacent vertices x_t and y_t in $T(v_{i_t})$ such that $d(x_t) = 2$ and $d(y_t) = 1$. Let $N(x_t) - \{y_t\} = \{z_t\}$.

Set $G' = G - z_t x_t + v_{i_l} x_t$, then $G' \in \mathfrak{U}_k(2m, m)$ and

$$R_\alpha^0(G') - R_\alpha^0(G) = [(d_{v_{i_l}} + 1)^\alpha - d_{v_{i_l}}^\alpha] - [d_{z_t}^\alpha - (d_{z_t} - 1)^\alpha] = \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}) > 0.$$

Since $d_{z_t} - 1 < \eta < d_{z_t} < d(v_{i_t}) \leqslant d(v_{i_l}) < \xi < d(v_{i_l}) + 1$ and $\alpha > 2$. This contradicts the maximality of $R_\alpha^0(G)$.

Subcase 2.3.2. For any vertex $v_{i_j} \in S$, $d(v_{i_j}) < \triangle(G)$. Let u be a vertex in G such that $d(u) = \triangle(G)$, then $u \in T(v_{i_l})$ for some positive integer l.

Since $|S| \geqslant 2$, there exists some vertex v_{i_t} in $S - \{v_{i_l}\}$. By lemmas 3.6, 2.1, and 3.1, there exists a pair of adjacent vertices x_t and y_t in $T(v_{i_t})$ such that $d(x_t) = 2$ and $d(y_t) = 1$. Let $N(x_t) - \{y_t\} = \{z_t\}$.

The left thing we have to do is completely similar to that has been done in subcase 2.3.1, and then an analogous contradiction occurs once again.

From the above argument, the desired result follows. □

For each $v_i \in S$, if $n(T(v_i)) \geqslant 3$, we have the following theorems.

Theorem 3.15. Suppose G is a graph in $\mathfrak{U}_k(2m, m)$ and $\alpha > 1$ or $\alpha < 0$. If $n(T(v_i)) \geqslant 3$ for each $v_i \in S$, then

(i)If k is odd, then $R_\alpha^0(G) \leqslant (m - \frac{k-1}{2}) + (m + \frac{k-3}{2})2^\alpha + (m - \frac{k-5}{2})^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (T^0(2m - k + 1, \frac{2m-k+1}{2}), v_i)$. Moreover, $d(v_i) - 2 = \triangle((T^0(2m - k + 1, \frac{2m-k+1}{2}), v_i))$.

(ii) If k is even, then $R_\alpha^0(G) \leqslant (m - \frac{k}{2}) + (m + \frac{k}{2} - 2)2^\alpha + 3^\alpha + (m + 1 - \frac{k}{2})^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (T^0(2m - k + 1, \frac{2m-k}{2}), v_i)$. Moreover, $d(v_i) = 3$ and u is the maximum-degree vertex of $(T^0(2m - k + 1, \frac{2m-k}{2}), v_i)$ where $u = N(v_i) - \{v_{i-1}, v_{i+1}\}$.

From the proof of theorem 3.14, theorem 3.15 is then obvious.

Similarly, we have the following:

Theorem 3.16. Suppose G is a graph in $\mathcal{U}_k(2m, m)$ and $0 < \alpha < 1$. If $n(T(v_i)) \geqslant 3$ for each $v_i \in S$, then

(i) If k is odd, then $R_\alpha^0(G) \geqslant (m - \frac{k-1}{2}) + (m + \frac{k-3}{2})2^\alpha + (m - \frac{k-5}{2})^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (T^0(2m-k+1, \frac{2m-k+1}{2}), v_i)$. Moreover, $d(v_i) - 2 = \triangle((T^0(2m-k+1, \frac{2m-k+1}{2}), v_i))$.

(ii)If k is even, then $R_\alpha^0(G) \geqslant (m - \frac{k}{2}) + (m + \frac{k}{2} - 2)2^\alpha + 3^\alpha + (m + 1 - \frac{k}{2})^\alpha$ with equality holds if and only if $G \cong (C_k, v_i) \bowtie (T^0(2m-k+1, \frac{2m-k}{2}), v_i)$. Moreover, $d(v_i) = 3$ and u is the maximum-degree vertex of $(T^0(2m-k+1, \frac{2m-k}{2}), v_i)$ where $u = N(v_i) - \{v_{i-1}, v_{i+1}\}$.

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