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Hosoya index of unicyclic graphs with prescribed pendent vertices

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The Hosoya index $z(G)$ of a (molecular) graph G is defined as the total number of subsets of the edge set, in which any two edges are mutually independent, i.e., the total number of independent-edge sets of G. By $G(n, l, k)$ we denote the set of unicyclic graphs on n vertices with girth and pendent vertices being resp. l and k. Let S_n^l be the graph obtained by identifying the center of the star S_{n-l+1} with any vertex of C_l. By $R_n^{l,k}$ we denote the graph obtained by identifying one pendent vertex of the path $P_{n-l-k+1}$ with one pendent vertex of S_{l+k}^l. In this paper, we show that $R_n^{l,k}$ is the unique unicyclic graph with minimal Hosoya index among all graphs in $G(n, l, k)$.

KEY WORDS: Unicyclic graph, Hosoya index, permanent, pendent vertex, girth

AMS subject classification: 05C90, 05C50

1. Introduction

The *Hosoya index*, proposed by Hosoya [1] in 1971, acts as one of important topological parameters to study the relation between molecular structure and physical and chemical properties of certain amount of hydrocarbon compounds.

Hosoya index, denoted by $z(G)$, is defined to be the total number of matchings, namely,

$$z(G) = \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m(G; s),$$

where $m(G; s)$ is the number of s-matchings of G. An s-matchings of a graph G is a subset M of its edge set with the property that $|M| = s$ and M contains no two edges sharing a common vertex. For convenience, set $m(G; 0) = 1$.

It's significant to determine the graph with extremal (maximal or minimal) Hosoya index $z(G)$. Along this line, many research results have been put forward. Gutman [2] proved that the linear hexagonal chain is the unique chain with minimal Hosoya index among all hexagonal chains. Zhang [3] showed that zig-zag hexagonal chain is the unique chain with maximal Hosoya index among all hexagonal chains. Later, Zhang et al. [4] gave a new proof of the results in Refs. [2, 3]. In ref. [5], Zhang determined the unique graph with minimal and second minimal Hosoya indices among all catacondensed systems. In ref. [6], the path and star have been shown to have the maximal and minimal Hosoya indices resp. among all trees on n vertices. Hou [7] characterized the trees having minimal and second minimal Hosoya indices among all trees with a given size of matching. Yu et al. [8] investigated the graphs having minimal Hosoya index among all graphs with given edge-independence number and cyclomatic number. In ref. [9], Yu et al. investigated the trees having minimal Hosoya index among all trees with k-pendent vertices. More recently, the author [10] determined the unique unicyclic graphs with the first and second largest Hosoya indices. He also determined the unique unicyclic graphs with the first and second smallest Hosoya indices in the successive paper [11].

In this paper, we investigate the Hosoya index of unicyclic graphs with given girth and pendent vertices. Unicyclic graph possessing prescribed girth and pendent vertices with minimal Hosoya-index is uniquely determined among all graphs in $\mathrm{G}(n, l, k)$.

2. Lemmas and results

All graphs considered here are both connected and simple. By S_n, C_n, and P_n we denote, respectively, the star graph, the cycle graph, and the path graph with n vertices. By $G(n, l, k)$ we denote the set of all unicyclic graphs on n vertices with girth and pendent vertices being resp. l and k. Let S_n^l be the graph obtained by identifying the center of S_{n-l+1} with any vertex of C_l. By $R_n^{l,k}$ we denote the graph obtained by identifying one pendent vertex of the path $P_{n-l-k+1}$ with one pendent vertex of S_{l+k}^l. Let $V_1(G)$ denote the set of pendent vertices in G. We denote, by $d_G(x,\ y)$, the length of the shortest path connecting x and y, namely, the distance between x and y. Let $d_G(x, C_l) = \min\{d_G(x, y) | y \in V(C_l)$ and $x \notin\ V(C_l)\}$. Let V_d denote the subset of $V_1(G)$ with the property that for any vertex v in V_d, we have $d_G(v, C_l) = \max\{d_G(x, C_l) | x \in V_1(G)\}$. Other notations and terminology not defined here will conform to those in ref. [12].

Figures 1 and 2 illustrate S_n^l and $R_n^{l,k}$, respectively.

In order to prove our main result, we begin with the following

Definition 1. Let $\alpha_{r,\,s,\,t} = (r,\ s,\ t)$. If $r_1 \leq r_2$ or $s_1 \leq s_2$ and $t_1 \leq t_2$, then we write $(r_1,\ s_1,\ t_1) \leq (r_2,\ s_2,\ t_2)$. Moreover, $(r_1,\ s_1,\ t_1) = (r_2,\ s_2,\ t_2)$ if and only if $r_1 = r_2$, $s_1 = s_2$, and $t_1 = t_2$.

If $(r_1,\ s_1,\ t_1) \leq (r_2,\ s_2,\ t_2)$ but $(r_1,\ s_1,\ t_1) \neq (r_2,\ s_2,\ t_2)$, then we write $(r_1,\ s_1,\ t_1) < (r_2,\ s_2,\ t_2)$.

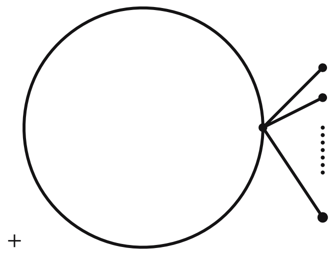

Figure 1. The graph S_n^l.

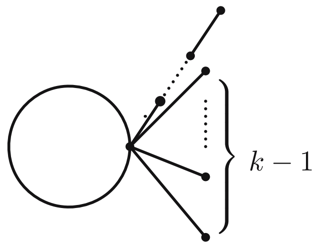

Figure 2. The graph $R_n^{l,\,k}$.

From the above definition, it's not difficult to see that if $r_1 < r_2$, $s_1 < s_2$, and $t_1 < t_2$, then $(r_1,\, s_1,\, t_1) < (r_2,\, s_2,\, t_2)$.

For $i = 1, 2$, let r_i, s_i and t_i be parameters related to graphs G_i, respectively. Set $\alpha_{r,\,s,\,t}(G_1) = (r_1,\, s_1,\, t_1)$ and $\alpha_{r,\,s,\,t}(G_2) = (r_2,\, s_2,\, t_2)$. If $(r_1,\, s_1,\, t_1) < (r_2,\, s_2,\, t_2)$, then we write $\alpha_{r,\,s,\,t}(G_1) < \alpha_{r,\,s,\,t}(G_2)$.

Let G be a n-vertex graph with adjacency matrix $A(G)$. Define the neighbor matrix $B(G)$ of G as $B(G) = A(G) + I$, where I is the unit matrix of order n. From the definition of permanent [13], we immediately have

Lemma 2. Let G be a graph with m components $G_1, G_2, \cdots G_m$. Then $\mathrm{per}B(G) = \prod_{i=1}^{m} \mathrm{per}B(G_i)$.

Lemma 3. [8] Let T be a tree on n vertices. Then $z(T) = \mathrm{per}B(T)$.

Lemma 4. [7] Let T be a n-vertex tree. Then $n = z(S_n) \leq z(T) \leq z(P_n) = F_{n+1}$, $z(S_n) < z(T)$ if and only if $T \ncong S_n$ and $z(T) < z(P_n)$ if and only if $T \ncong P_n$.

Theorem 5. Let $l \geq 3$ and $k \geq 1$. Then $z(R_n^{l,\,k}) = F_l F_{n-l-k+1} + [F_{l-1} + F_{l+1} + (k-1)F_l]F_{n-l-k+2}$.

Proof. By $T(G)$ we denote the forest obtained from G by deleting all vertices in $V(C_l)$ as well as edges incident with each vertex in $V(C_l)$.

From the definition of permanent, we obtain

$$\mathrm{per}B(R_n^{l,\,k}) = \sum_{\sigma} \prod_{i=1}^{n} b_{i,\,\sigma(i)},$$

where σ goes over all symmetric group of order n.

In the above formula, term $\prod_{i=1}^{n} b_{i,\,\sigma(i)} = 0$ if and only if either vertex i is not adjacent to vertex $\sigma(i)$ for some $i \neq \sigma(i)$ or, σ contains a cycle with length greater than 2 but not equal to l since $R_n^{l,\,k}$ contains exactly one cycle of length l. Consequently, every non-zero term of $\mathrm{per}B(R_n^{l,\,k})$ corresponds to a matching of $R_n^{l,\,k}$ with the exception of σ being one of two cycles of length l. So

$$z(R_n^{l,\,k}) = \mathrm{per}B(R_n^{l,\,k}) - 2\mathrm{per}B(T(R_n^{l,\,k})). \tag{1}$$

Note that $T(G) = (k-1)K_1 \bigcup P_{n-l-k+1}$. So by lemmas 2, 3, and 4, we obtain

$$\mathrm{per}B(T(R_n^{l,\,k})) = F_{n-l-k+2}. \tag{2}$$

Labeling vertices of $R_n^{l,\,k}$ in a way such that its neighbor matrix $B(R_n^{l,\,k})$ has the form

$$\begin{pmatrix}
1 & 1 & 0 & \cdots & 1 & 1 & 1 & \cdots & 1 & 1 & 0 & 0 & \cdots & 0 & 0 \\
1 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
1 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
1 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
1 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\
1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 1 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 1 & 1 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 1 & 1
\end{pmatrix}_{(n)}.$$

Let $N_{n-l-k+1} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 1 \end{pmatrix}_{(n-l-k+1)}$ denote the $(n-l-k+1)\times(n-l-k+1)$ matrix formed by taking the last $n-l-k+1$ rows and columns from $B(R_n^{l,\,k})$.

Let $M_{l+k-1} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 \end{pmatrix}_{(l+k-1)}$ be the $(l+k-1)\times(l+k-1)$ matrix obtained by taking the first $l+k-1$ rows and columns from $B(R_n^{l,\,k})$.

Let $Q_{n-l-k+1}$ be the matrix obtained from $N_{n-l-k+1}$ by replacing its first column by the $(n-l-k+1)$-dimension column vector $\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}^T$, that is

$$Q_{n-l-k+1} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 1 \end{pmatrix}_{(n-l-k+1)}.$$

Let $R_{l+k-1} = \begin{pmatrix} 1 & 1 & 0 & \cdots & 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 \end{pmatrix}_{(l+k-1)}$ be the matrix obtained from M_{l+k-1} by replacing its first column by the $(l+k-1)$-dimension column vector $\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}^T$.

Expanding $\text{per}B(R_n^{l,\,k})$ along its last $n-l-k+1$ rows, we obtain

$$\text{per}B(R_n^{l,\,k}) = \text{per}N_{n-l-k+1} \cdot \text{per}M_{l+k-1} + \text{per}Q_{n-l-k+1} \cdot \text{per}R_{l+k-1}. \tag{3}$$

If we expand $\text{per}M_{l+k-1}$ along its last $k-1$ rows, we obtain

$$\text{per}M_{l+k-1} = \text{per}B(C_l) \cdot \text{per}E_{k-1} + \sum_{j=1}^{k-1} \text{per}D_{l+k}^{j} \cdot \text{per}E_l,$$

where E_{k-1} is the unit matrix of order $k-1$, $E_l = \begin{pmatrix} 1 & 1 & 0 & \cdots & 1 \\ 0 & 1 & 1 & \cdots & 0 \\ 0 & 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}_{(l)}$ is obtained from $B(C_l)$ by replacing its first column by the l-dimension column vector $\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{l\times 1}$ and D_{l+k}^{j} $(j = 1, \cdots k-1)$ is obtained from E_{k-1} by replacing its jth column by the $(k-1)$-dimension column vector $\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}_{(k-1)\times 1}$.

Note that $\text{per}(E_{k-1}) = \text{Per}\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}_{(k-1)} = 1$, $\text{per}D_{l+k}^{j} = 1$ for $j = 1, 2, \ldots k-1$ and $\text{per}E_l = \text{per}B(P_{l-1})$.

So $\text{per}M_{l+k-1} = \text{per}B(C_l) + (k-1)\text{per}B(P_{l-1})$. In view of ref. [11], $\text{per}B(C_l) = F_{l+1} + F_{l-1} + 2$. So by lemma 4, we have

$$\text{per}M_{l+k-1} = F_{l+1} + F_{l-1} + 2 + (k-1)F_l. \tag{4}$$

Once again by lemma 4, one can easily obtain that

$$\text{per}N_{n-l-k+1} = \text{per}B(P_{n-l-k+1}) = F_{n-l-k+2}. \tag{5}$$

By an expansion of $\text{per}R_{l+k-1}$ along its last $(k-1)$ columns, we arrive at

$$\text{per}R_{l+k-1} = \text{per}B(P_{l-1}). \tag{6}$$

Similarly, if we expand $\mathrm{per}Q_{n-l-k+1}$ along its first column, we get that

$$\mathrm{per}Q_{n-l-k+1} = \mathrm{per}B(P_{n-l-k}) = F_{n-l-k+1}. \tag{7}$$

From the combination of equations (3)–(7), we conclude that

$$\mathrm{per}B(R_n^{l,\,k}) = F_l F_{n-l-k+1} + [F_{l-1} + F_{l+1} + (k-1)F_l + 2]F_{n-l-k+2}. \tag{8}$$

Combining equations (1), (2), and (8), the theorem follows as expected. □

The following result is obvious, so we omit its proof here.

Lemma 6. If G_1 is a subgraph of G_2, then $z(G_2) > z(G_1)$.

Lemma 7. Let $l \geq 3$, then $z(C_l) > z(P_2 \bigcup P_{l-1})$.

Proof. Since $P_2 \bigcup P_{l-1}$ contains no cycle, then each non-zero term of $\mathrm{per}B(P_2 \bigcup P_{l-1})$ corresponds to a matching of $P_2 \bigcup P_{l-1}$. Consequently, it follows that

$$\begin{aligned} z\left(P_2 \bigcup P_{l-1}\right) &= \mathrm{per}B\left(P_2 \bigcup P_{l-1}\right) \\ &= \mathrm{per}B(P_2)\mathrm{per}B(P_{l-1}) \\ &= z(P_2)z(P_{l-1}) \\ &= 2F_l \end{aligned}$$

from the combination of lemmas 2, 3, and 4.

Note that

$$m(C_l; s) = m(P_l; s) + m(P_{l-2}; s-1)$$

for any positive integer s. This gives

$$z(C_l) = z(P_l) + z(P_{l-2}).$$

Hence, we have $z(C_l) = F_{l-1} + F_{l+1}$ by lemma 4. Thus, the result follows by a direct calculation. □

Lemma 8. For $l \geq 3$ and $n \geq l+1$, $z(R_n^{l,1}) > z(P_{l-1} \bigcup P_{n-l+2})$.

Proof. We proceed by induction on $n-l$.

When $n-l=1$, we have $R_n^{l,1} = R_{l+1}^{l,1}$ and $P_{l-1} \bigcup P_{n-l+2} = P_{l-1} \bigcup P_3$.

Note that for all positive integer s, we have

$$m(R_{l+1}^{l,1}; s) = m(C_l; s) + m(P_{l-1}; s-1) \tag{9}$$

and

$$m\left(P_{l-1} \bigcup P_3; s\right) = m\left(P_{l-1} \bigcup P_2; s\right) + m(P_{l-1}; s-1). \tag{10}$$

Combining equations (9), (10), and lemma 7, the result follows in this case.

Let $t \geq 2$ and suppose the result holds for $n - l < t$. When $n - l = t$, we have $R_n^{l,1} = R_{l+t}^{l,1}$ and $P_{l-1} \bigcup P_{n-l+2} = P_{l-1} \bigcup P_{t+2}$.

Note that

$$m(R_{l+t}^{l,1}; s) = m(R_{l+t-1}^{l,1}; s) + m(R_{l+t-2}^{l,1}; s-1) \tag{11}$$

and

$$m\left(P_{l-1} \bigcup P_{t+2}; s\right) = m\left(P_{l-1} \bigcup P_{t+1}; s\right) + m\left(P_{l-1} \bigcup P_t; s-1\right) \tag{12}$$

for all positive integer s.

From inductive assumption, we have

$$z\left(R_{l+t-1}^{l,1}\right) > z\left(P_{l-1} \bigcup P_{t+1}\right) \tag{13}$$

and

$$z\left(R_{l+t-2}^{l,1}\right) > z\left(P_{l-1} \bigcup P_t\right). \tag{14}$$

Therefore, the result follows from the combination of equations (11)–(14). □

Lemma 9. [12] Let G be a connected n-vertex unicyclic graph. If $g(G) = l$, then $z(G) \geq F_{l+1} + (n-l)F_l + F_{l-1}$, with the equality holding if and only if $G \cong S_n^l$.

Theorem 10. Let $G \in G(n, l, k)$ with $l \geq 3$ and $k \geq 1$. If $G \ncong R_n^{l,\,k}$, then $z(G) > z(R_n^{l,\,k})$.

Proof. Let q denote the number of vertices in $V(G)$ other than all pendent vertices as well as all vertices in $V(C_l)$. It's evident that for any graph $G \in G(n, l, k)$, we have $q \geq 0$ and $n = l + k + q \geq l + 1$.

If $\alpha_{k,q,n}(G) = (1, q, n)$, the result holds clearly. If $\alpha_{k,q,n}(G) = (k, 0, n)$, the result follows from lemma 9. In what follows, we will show that the theorem holds for the case when $\alpha_{k,q,n}(G) = (k, 1, n)$ with $k \geq 2$.

Since $q = 1$, there're exactly $n - l - 1$ pendent vertices in G. Let $v \in V_d$, then we have $d_G(v, C_l) = 2$ and $|V_d| = 1$. Let u be the unique neighbor of v. The following two cases should be distinguished between.

• The case when $d(u) = 2$.

Let $G - uv = G_0 \bigcup K_1$, where $G_0 = G - v$. Then $G_0 \in G(n-1, l, k)$ and $G - v - u \in G(n-2, l, k-1)$. In this case, we clearly have $R_{n-1}^{l,k} (\cong S_{n-1}^l) \in$

$G(n-1,l,k)$ and $R_{n-2}^{l,k-1}(\cong S_{n-2}^{l}) \in G(n-2,l,k-1)$. From lemma 9, we arrive at

$$z(G_0) \geq z(S_{n-1}^{l}) = z(R_{n-1}^{l,k}) \tag{15}$$

and

$$z(G-v-u) \geq z(S_{n-2}^{l}) = z(R_{n-2}^{l,k-1}) \tag{16}$$

with equality holding if and only if $G_0 \cong S_{n-1}^{l}$ and $G-v-u \cong S_{n-2}^{l}$. Bearing in mind that

$$\begin{aligned} z(G) &= \sum_{s=1}^{\lfloor \frac{n}{2} \rfloor} m(G;s) + 1 \\ &= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m(G-vu;s) + \sum_{s=1}^{\lfloor \frac{n}{2} \rfloor} m(G-v-u;s-1) \\ &= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\Big(G_0 \bigcup K_1;s\Big) + z(G-v-u) \\ &= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m(G_0;s) + z(G-v-u), \end{aligned}$$

which gives

$$z(G) = z(G_0) + z(G-v-u). \tag{17}$$

Substituting equations (15) and (16) into equation (17) yields that

$$\begin{aligned} z(G) &\geq z(R_{n-1}^{l,k}) + z\Big(R_{n-2}^{l,k-1}\Big) \\ &= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\Big(R_{n-1}^{l,k} \bigcup K_1;s\Big) + \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\Big(R_{n-2}^{l,k-1} \bigcup 2K_1;s\Big) \\ &= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\Big(R_{n-1}^{l,k};s\Big) + \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\Big(R_{n-2}^{l,k-1};s\Big) \\ &= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\Big(R_{n-1}^{l,k};s\Big) + \sum_{s=1}^{\lfloor \frac{n}{2} \rfloor} m\Big(R_{n-2}^{l,k-1};s-1\Big) \end{aligned}$$

$$= \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\left(R_n^{l,k}; s\right)$$
$$= z\left(R_n^{l,k}\right).$$

The above equality holds if and only if $G_0 \cong R_{n-1}^{l,k}$ and $G - v - u \cong R_{n-2}^{l,k-1}$, that is $G \cong R_n^{l,k}$. So the result holds in this case.

• The case when $d(u) \geq 3$.

In this case, we clearly have $G \ncong R_n^{l,k}$. Let $d(u) = m + 1$. It's not difficult to see that there're exactly m pendent vertices in $N(u)$ since $v \in V_d$.

Let G_0 be defined as in the previous case. Then $G_0 \in G(n-1, l, k-1)$ in this case. From lemma 9, we have

$$z(G_0) \geq z\left(R_{n-1}^{l,k-1}\right). \tag{18}$$

Obviously, $G - v - u$ contains C_l as its subgraph. From lemmas 6 and 7, we obtain

$$z(G - v - u) > z(C_l) > z\left(P_{l-1} \bigcup P_2\right). \tag{19}$$

In view of equations (17)–(19), we have $z(G) = z(G_0) + z(G-v-u) > z(R_{n-1}^{l,k-1}) + z\left(P_{l-1} \bigcup P_2\right) = z(R_n^{l,k})$. Consequently, the result follows.

Hence, we may assume that $k, q \geq 2$ hereinafter.

Let $v \in V_d$, then we have $d_G(v, C_l) \geq 2$. We consider the following two cases.

Case 1. $d_G(v, C_l) = 2$.

It's evident that $G \ncong R_n^{l,k}$ in this case.

We proceed by induction on $\alpha_{k,q,n}(G)$.

Suppose that the theorem holds for all unicyclic graphs G' with $\alpha_{k,q,n}(G') < \alpha_{k,q,n}(G)$.

Subcase 1.1 $d(u) = 2$.

Let $G - vu = G_0 \bigcup K_1$, where $G_0 = G - v$. Then $G_0 \in G(n-1, l, k)$ and $G - v - u \in G(n-2, l, k-1)$. Obviously, $\alpha_{k,q,n}(G_0) = (k, q-1, n-1) < (p, q, n) = \alpha_{k,q,n}(G)$ and $\alpha_{k,q,n}(G - v - u) = (k-1, q-1, n-2) < (k, q, n) = \alpha_{k,q,n}(G)$. Then by induction hypothesis, we have

$$z(G_0) \geq z\left(R_{n-1}^{l,k}\right) \tag{20}$$

and

$$z(G - v - u) \geq z\left(R_{n-2}^{l,k-1}\right). \tag{21}$$

Since $q \geq 2$, then

$$z(R_n^{l,k}) = \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} m\left(R_{n-1}^{l,k}; s\right) + \sum_{s=1}^{\lfloor \frac{n}{2} \rfloor} m\left(R_{n-2}^{l,k}; s-1\right) = z\left(R_{n-1}^{l,k}\right) + z\left(R_{n-2}^{l,k}\right). \quad (22)$$

From the combination of equations (20)–(22) and (17), we know that if $z(R_{n-2}^{l,k-1}) > z(R_{n-2}^{l,k})$, then $z(G) > z(R_n^{l,k})$.

If $(n-2) - l - k = 0$, the theorem follows readily from lemma 9. So it will be assumed that $(n-2) - l - k \geq 1$, that is $(n-4) - l - (k-1) \geq 0$.

Note that

$$\begin{aligned} z\left(R_{n-2}^{l,k-1}\right) &= \sum_{s=1}^{\lfloor \frac{n-2}{2} \rfloor} m\left(R_{n-2}^{l,k-1}; s\right) + 1 \\ &= \sum_{s=0}^{\lfloor \frac{n-2}{2} \rfloor} m\left(R_{n-3}^{l,k-1}; s\right) + \sum_{s=1}^{\lfloor \frac{n-2}{2} \rfloor} m\left(R_{n-4}^{l,k-1}; s-1\right). \\ &= z\left(R_{n-3}^{l,k-1}\right) + z\left(R_{n-4}^{l,k-1}\right) \end{aligned}$$

and

$$\begin{aligned} z\left(R_{n-2}^{l,k}\right) &= \sum_{s=1}^{\lfloor \frac{n-2}{2} \rfloor} m\left(R_{n-2}^{l,k-1}; s\right) + 1 \\ &= \sum_{s=0}^{\lfloor \frac{n-2}{2} \rfloor} m\left(R_{n-3}^{l,k-1}; s\right) + \sum_{s=1}^{\lfloor \frac{n-2}{2} \rfloor} m\left(P_{l-1} \bigcup P_{n-l-k-1}; s-1\right). \\ &= z\left(R_{n-3}^{l,k-1}\right) + z\left(P_{l-1} \bigcup P_{n-l-k-1}\right). \end{aligned}$$

So what remains is to prove that

$$z\left(R_{n-4}^{l,\,k-1}\right) > z\left(P_{l-1} \bigcup P_{n-l-k-1}\right). \quad (23)$$

It's easy to see that $R_{n-4}^{l,\,k-1}$ contains $P_{l-1} \bigcup P_{n-l-k-1}$ as its proper subgraph. Hence equation (23) follows from lemma 6. Therefore the theorem holds in this case.

Subcase 1.2 $d(u) \geq 3$.

As being proved above, all vertices but one in $N(u)$ are pendent vertices. Let $G - vu = G_0 \bigcup K_1$ and $G - v - u = G_1 \bigcup (m-1)K_1$, where $G_0 = G - v$ and G_1 denote the subgraph containing C_l of $G - v - u$. Then $G_0 \in G(n-1, l,\ k-1)$ and $G_1 \in G(n-m-1, l,\ k-m)$. Obviously, $\alpha_{k,\,q,\,n}(G_0) = (k-1, q, n-1) < (k, q, n) =$

$\alpha_{k,q,n}(G)$ and $\alpha_{k,q,n}(G_1) = (k-m, q-1, n-m-1) < (k,q,n) = \alpha_{k,q,n}(G)$. Then by induction hypothesis, we have

$$z(G_0) \geq z(R_{n-1}^{l,k-1}) \tag{24}$$

and

$$z(G_1) \geq z(R_{n-m-1}^{l,k-m}). \tag{25}$$

It's easy to obtain

$$z(G) = z(G_0) + z(G_1) \tag{26}$$

and

$$z(R_n^{l,k}) = z\left(R_{n-1}^{l,k-1}\right) + z\left(P_{l-1} \bigcup P_{n-l-k+1}\right). \tag{27}$$

In view of equations (24)–(27), we know that if $z(R_{n-m-1}^{l,k-m}) > z(P_{l-1} \bigcup P_{n-l-k+1})$, then the result holds. Since $P_{l-1} \bigcup P_{n-l-k+1}$ is a proper subgraph of $R_{n-m-1}^{l,k-m}$, then we complete the proof of subcase 1.2 by lemma 6.

Case 2 $d_G(v, C_l) \geq 3$.

We proceed by induction on $\alpha_{k,q,n}(G)$.

Suppose that the theorem holds for all unicyclic graphs G' with $\alpha_{k,q,n}(G') < \alpha_{k,q,n}(G)$.

Let $d(u) = m+1$. As being shown above, there's exactly one vertex, say w, in $N(u)$ with $d(w) \geq 2$. We distinguish among the following four subcases.

Subcase 2.1 $d(u) = 2$ and $d(w) = 2$.

Let $G - uv = G_0 \bigcup K_1$, where $G_0 = G - v$.

Then $G_0 \in G(n-1, l, k)$ and $G - v - u \in G(n-2, l, k)$. Since $\alpha_{k,q,n}(G_0) = (k, q-1, n-1) < (k,q,n) = \alpha_{k,q,n}(G)$ and $\alpha_{k,q,n}(G - v - u) = (k, q-2, n-2) < (k,q,n) = \alpha_{k,q,n}(G)$. Then by induction hypothesis, we have

$$z(G_0) \geq z(R_{n-1}^{l,k}) \tag{28}$$

and

$$z(G - v - u) \geq z(R_{n-2}^{l,k}). \tag{29}$$

In view of equations (17), (18), and (29), the result follows.

Subcase 2.2 $d(u) = 2$ and $d(w) \geq 3$.

Let $G - uv = G_0 \bigcup K_1$, where $G_0 = G - v$.

Then $G_0 \in G(n-1, l, k)$ and $G - v - u \in G(n-2, l, k-1)$. Since $\alpha_{k,q,n}(G_0) = (k, q-1, n-1) < (k,q,n) = \alpha_{k,q,n}(G)$ and $\alpha_{k,q,n}(G - v - u) = (k-1, q-1, n-2) < (k,q,n) = \alpha_{k,q,n}(G)$. Then by induction hypothesis, we have

$$z(G_0) \geq z(R_{n-1}^{l,k}) \tag{30}$$

and

$$z(G - v - u) \geq z\left(R_{n-2}^{l,k-1}\right). \tag{31}$$

What remains is completely similar to that of subcase 1.1, we omit here.

Subcase 2.3 $d(u) \geq 3$ and $d(w) = 2$.

Let $G - uv = G_0 \bigcup K_1$ and $G - v - u = G_1 \bigcup (m-1)K_1$, where $G_0 = G - v$ and G_1 denotes the subgraph containing C_l of $G - v - u$.

Then $G_0 \in G(n-1, l, k-1)$ and $G_1 \in G(n-m-1, l, k-m+1)$. Note that $\alpha_{k,q,n}(G_0) < \alpha_{k,q,n}(G)$ and $\alpha_{k,q,n}(G_1) < \alpha_{k,q,n}(G)$. From induction hypothesis, we obtain

$$z(G_0) \geq z\left(R_{n-1}^{l,k-1}\right) \tag{32}$$

and

$$z(G_1) \geq z\left(R_{n-m-1}^{l,k-m+1}\right). \tag{33}$$

From the combination of equations (26)–(27) and (32)–(33), we know that if $z\left(R_{n-m-1}^{l,k-m+1}\right) > z(P_{l-1} \bigcup P_{n-l-k+1})$ then the theorem follows.

If $k = m$, then $R_{n-m-1}^{l,k-m+1} \cong R_{n-k-1}^{l,1}$. Since $n - l - k = q \geq 2$, then the desired result follows immediately from lemma 8.

Suppose that $k \geq m + 1$, that is $k - m + 1 \geq 2$. One can easily obtain that $P_{l-1} \bigcup P_{n-l-m}$ is a proper subgraph of $R_{n-m-1}^{l,k-m+1}$. Thus $R_{n-m-1}^{l,k-m+1}$ contains $P_{l-1} \bigcup P_{n-l-k+1}$ as its proper subgraph, so the theorem follows by lemma 6.

Subcase 2.4 $d(u) \geq 3$ and $d(w) \geq 3$.

Let $G - uv = G_0 \bigcup K_1$ and $G - v - u = G_1 \bigcup (m-1)K_1$, where $G_0 = G - v$ and G_1 denotes the subgraph containing C_l of $G - v - u$.

Then $G_0 \in G(n-1, l, k-1)$ and $G - v - u \in G(n-m-1, l, k-m)$. Obviously, $k \geq m+1$ since $d(w) \geq 3$. The rest thing we should do is in full analogy with that of subcase 1.2.

From the above arguments it follows the desired result. □

Theorem 11. Let $G \in G(n, l, k)$ with $l \geq 3$ and $k \geq 1$. Then $z(G) \geq F_l F_{n-l-k+1} + [F_{l-1} + F_{l+1} + (k-1)F_l]F_{n-l-k+2}$ with equality holding if and only if $G \cong R_n^{l,k}$.

Proof. From theorems 5 and 10 it follows the present theorem straightforwardly.

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