

## Research Article

# The Ordering of the Unicyclic Graphs with respect to Largest Matching Root with Given Matching Number

Luozhong Gong <sup>1</sup> and Weijun Liu<sup>2</sup>

<sup>1</sup>School of Mathematics, Changsha Normal University, Changsha, Hunan 410100, China

<sup>2</sup>School of Mathematics and Statistics, Central South University, Changsha, Hunan 410100, China

Correspondence should be addressed to Luozhong Gong; [gonglzt@126.com](mailto:gonglzt@126.com)

Received 15 December 2021; Accepted 23 April 2022; Published 28 May 2022

Academic Editor: Musavarah Sarwar

Copyright © 2022 Luozhong Gong and Weijun Liu. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The matching roots of a simple connected graph  $G$  are the roots of the matching polynomial which is defined as  $M_G(x) = \sum_{k=0}^{n/2} (-1)^k m(G, k) x^{n-2k}$ , where  $m(G, k)$  is the number of the  $k$  matchings of  $G$ . Let  $\lambda_1(G)$  denote the largest matching root of the graph  $G$ . In this paper, among the unicyclic graphs of order  $n$ , we present the ordering of the unicyclic graphs with matching number 2 according to the  $\lambda_1(G)$  values for  $n \geq 11$  and also determine the graphs with the first and second largest  $\lambda_1(G)$  values with matching number 3.

## 1. Introduction

In this paper, all of the graphs considered are connected and finite. Let  $G = (V(G), E(G))$  be a graph of order  $n$ , where  $V(G)$  and  $E(G)$  denote the vertex set and edge set of  $G$ , respectively. Let  $N(u)$  and  $d_G(u)$  be the neighbor set and the degree of the vertex  $u \in V(G)$  in  $G$ , respectively. A  $k$ -edge matching of  $G$  is a set of  $k$  mutually independent edges, and the number of all the  $k$ -edge matchings of  $G$  is denoted by  $m(G, k)$ . Obviously,  $m(G, k) = 0$  if  $k > n/2$ . For convenience, we set  $m(G, 0) = 1$ .

The original definition of the matching polynomial was introduced in [9] as  $\sum_k m(G, k) x^k$ , which is now defined in [14] as

$$M_G(x) = \sum_{k=0}^{n/2} (-1)^k m(G, k) x^{n-2k}. \quad (1)$$

Each root of the matching polynomial  $M_G(x)$  is called a matching root of  $G$ . The largest matching root of a graph  $G$  which is denoted by  $\lambda_1(G)$  is the largest root of  $M_G(x)$ . In particular,  $\lambda_1(G)$  has been proved to be positive real numbers excepting for the edgeless graphs in [3, 4].

The matching polynomial of a graph has been used in various branches of physics and chemistry. In analogy with the traditional graph energy, the matching energy of a graph has been conceived as the sum of the absolute values of the roots of the matching polynomial. This graph invariant has recently attracted much attention (see [2, 3, 5–11]). In [15], Gutman and Zhang have ordered the graphs by matching numbers. Zhang et al. [18] investigated the largest matching root  $\lambda_1(G)$  for unicyclic graphs and characterized the extremal graph. Zhang and Chen [10] studied the largest matching roots of unicyclic graphs and trees with a given number of fixed matching numbers and characterized the extremal graph with respect to the largest matching roots. In [3], Liu et al. determined the graphs with the four largest and two smallest  $\lambda_1(G)$  values.

Motivated by the previous research, in this paper, we focus on the ordering of the unicyclic graph with the fixed matching number with respect to the largest matching root  $\lambda_1(G)$ . Among the unicyclic graphs of order  $n$ , we order the unicyclic graphs with matching number 2 according to the  $\lambda_1(G)$  values for  $n \geq 11$  and also determine the graphs with the first and second largest  $\lambda_1(G)$  values with matching number 3.

## 2. Preliminaries

Let  $H$  be a subgraph of  $G$ . If  $V(H) = V(G)$ , then  $H$  is said to be a spanning subgraph of  $G$ . The following lemma about the largest matching root is well known.

**Lemma 1** (see [8]). *Let  $H$  be a spanning subgraph of  $G$  and  $\lambda_1(G)$  the largest matching root of  $G$ . If  $\kappa \geq \lambda_1(G)$ , then  $M_H(\kappa) \geq M_G(\kappa)$ ; if  $H$  is a proper subgraph of  $G$  and  $\kappa > \lambda_1(G)$ , then  $M_H(\kappa) > M_G(\kappa)$ .*

*Definition 1.* Let  $u, v$  denote two vertices of  $G$ . The Kelmans transformation of  $G$  is defined as follows (cf. Figure 1): delete all edges which are with one end  $v$  and another end in  $N(v) \setminus (N(u) \cup u)$  and add all edges between  $u$  and  $N(v) \setminus (N(u) \cup u)$ .

Let  $G'$  denote the graph obtained from  $G$  by a series of Kelmans transformation without referring to the vertices  $u, v$ . Obviously,  $G'$  and  $G$  have the same size.

The relationship between the largest matching roots of  $G'$  and  $G$  is given as follows.

**Lemma 2** (see [7]). *Let  $G'$  be the graph obtained from  $G$  by some Kelmans transformation. Then,  $\lambda_1(G') \geq \lambda_1(G)$ .*

In [3], Liu et al. characterized the unicyclic graphs with a triangle as given in Figure 2 and obtained the following lemma.

**Lemma 3** (see [3]). *ie graphs of order  $nD_k$  and  $D_{k-1}$  are shown in Figure 2. If  $2 \leq k \leq n/2 - 1$ , then  $\lambda_1(D_k) \leq \lambda_1(D_{k-1})$ , with equality holding if and only if  $k = n/2 - 1$ .*

Let  $S_n$  be the star graph of order  $n$  and  $S_n^+$  the unicyclic graph obtained by adding a new edge to  $S_n$ . Let  $C_{n-1}$  be a cycle of length  $n - 1$  and  $C_n^2$  the graph obtained from  $C_{n-1}$  by adding a new pendent edge. Let  $D_n^2$  be the graph obtained by identifying one end vertex of the path  $P_{n-2}$  and one vertex of the triangle  $C_3$ .

**Lemma 4** (see [3]). *Among all connected unicyclic graphs with  $n$  ( $n \geq 8$ ) vertices, the first four largest matching roots are  $\lambda_1(S_n^+) > \lambda_1(S_n^2) > \lambda_1(S_n^3) > \lambda_1(S_n^4)$ , and the last three largest matching roots are  $\lambda_1(C_n^2)$  or  $\lambda_1(D_n^2)$  and  $\lambda_1(C_n)$ , where  $S_n^2, S_n^3$ , and  $S_n^4$  are shown in Figure 3.*

**Lemma 5** (see [11]). *Let  $G$  be a graph of order  $n$ . Then,  $\lambda_1^2(G) \geq 4|E(G)|/n - 1$ , where  $|E(G)|$  is the number of edges of  $G$ .*

**Corollary 1.** *Let  $G$  be a connected unicyclic graph with  $n$  vertices. Then,  $\lambda_1(G) \geq \sqrt{3}$ .*

## 3. Main Results

In this section, we first investigate the largest matching root of unicyclic graphs with matching number 2.

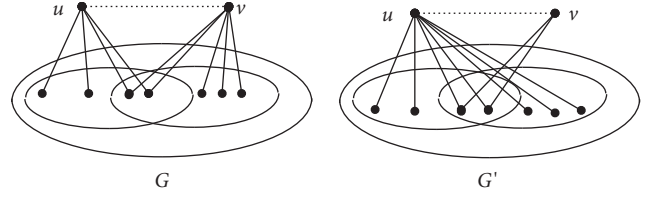


FIGURE 1: The Kelmans transformation.

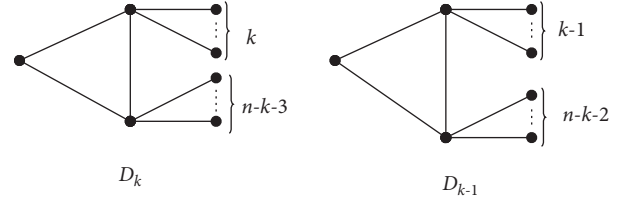


FIGURE 2: Two graphs  $D_k$  and  $D_{k-1}$ .

For  $k \geq 2$ , let  $S_k$  be a star graph with center  $u$ . Let  $v_1, v_2$  be two vertices of  $S_{n-k+1}^+$  which are of degree 1 and 2, respectively. We write  $D_{n,k}(C_{n,k})$  denote the graph obtained by identifying  $u$  with  $v_1$  ( $v_2$ ). In fact,  $C_{n,k}$  is the graph  $D_{k-1}$  in Figure 2. All the connected unicyclic graphs with matching number 2 are  $S_n^+$ ,  $C_{n,k}$ ,  $D_{n,n-3}$ ,  $S_n^4$ , and  $T_n^k$  as shown in Figure 4.

**Theorem 1.**  $\lambda_1(C_{n,k+1}) > \lambda_1(T_n^k) > \lambda_1(C_{n,k+2}) > \lambda_1(T_n^{k+1})$ ,  $k < n - 4/3$ .

*Proof.* We can easily get  $m(T_n^k, 2) = n + kn - k^2 - 2k - 3$ ,  $m(T_n^{k+1}, 2) = 2n + kn - k^2 - 4k - 6$  and  $m(C_{n,k+1}, 2) = n + kn - k^2 - 3k - 3$ ,  $m(C_{n,k+2}, 2) = 2n + kn - k^2 - 5k - 7$ , then the matching polynomial of graphs  $T_n^k$  and  $T_n^{k+1}$  is

$$\begin{aligned} M_{T_n^{k+1}}(x) &= x^n - nx^{n-2} + (2n + kn - k^2 - 4k - 6)x^{n-4}, \\ M_{T_n^k}(x) &= x^n - nx^{n-2} + (n + kn - k^2 - 2k - 3)x^{n-4}, \\ M_{C_{n,k+1}}(x) &= x^n - nx^{n-2} + (n + kn - k^2 - 3k - 3)x^{n-4}, \\ M_{C_{n,k+2}}(x) &= x^n - nx^{n-2} + (2n + kn - k^2 - 5k - 7)x^{n-4}. \end{aligned} \quad (2)$$

Therefore,

$$\begin{aligned} M_{T_n^{k+1}}(x) - M_{T_n^k}(x) &= (n - 2k - 3)x^{n-4}, \\ M_{C_{n,k+1}}(x) - M_{T_n^k}(x) &= -kx^{n-4}, \\ M_{C_{n,k+2}}(x) - M_{T_n^k}(x) &= (n - 3k - 4)x^{n-4}. \end{aligned} \quad (3)$$

Then  $M_{T_n^{k+1}}(\lambda_1(T_n^k)) > 0$ ,  $M_{C_{n,k+1}}(\lambda_1(T_n^k)) < 0$ , and  $M_{C_{n,k+2}}(\lambda_1(T_n^k)) > 0$ , so  $\lambda_1(C_{n,k+1}) > \lambda_1(T_n^k) > \lambda_1(C_{n,k+2}) > \lambda_1(T_n^{k+1})$ , since the  $M_G(x)$  is strictly monotonically increasing for  $x > 0$ .  $\square$

**Theorem 2.** *Among all connected unicyclic graphs of order  $n$  ( $n \geq 11$ ) with matching number 2,  $\lambda_1(S_n^+) > \lambda_1(C_{n,2}) > \lambda_1(S_n^4) > \lambda_1(C_{n,3}) > \lambda_1(D_{n,n-3}) = \lambda_1(T_n^2) > \lambda_1(C_{n,4}) > \dots >$*

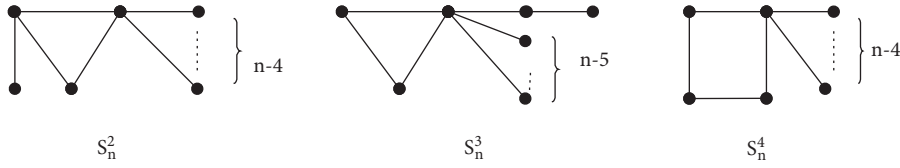


FIGURE 3: Graphs  $S_n^2$ ,  $S_n^3$ , and  $S_n^4$ .

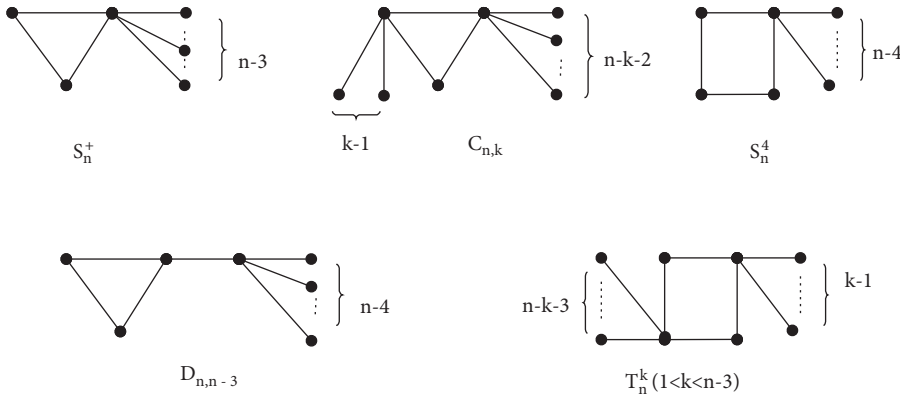


FIGURE 4: Graphs  $S_n^+$ ,  $C_{n,k}$ ,  $S_n^4$ ,  $D_{n,n-3}$ , and  $T_n^k$ .

$$\lambda_1(C_{n,k+1}) > \lambda_1(T_n^k) > \lambda_1(C_{n,k+2}) > \lambda_1(T_n^{k+1}), \quad \text{with } k < n - 4/3.$$

*Proof.* It is obvious that  $m(G, 1) = n$  for any connected unicyclic graph  $G$  of order  $n$ . By simple calculations, we have

$$\begin{aligned} m(C_{n,2}, 2) &= 2n - 7, m(S_n^4, 2) = 2n - 6, m(C_{n,3}, 2) = 3n - 13, \\ m(D_{n,n-3}, 2) &= 3n - 11, m(C_{n,4}, 2) \end{aligned} \tag{4}$$

Then,

$$\begin{aligned} M_{C_{n,2}}(x) &= x^n - nx^{n-2} + (2n - 7)x^{n-4}, \\ M_{S_n^4}(x) &= x^n - nx^{n-2} + (2n - 6)x^{n-4}, \\ M_{C_{n,3}}(x) &= x^n - nx^{n-2} + (3n - 13)x^{n-4}, \\ M_{D_{n,n-3}}(x) &= M_{T_n^2}(x) = x^n - nx^{n-2} + (3n - 11)x^{n-4}, \\ M_{C_{n,4}}(x) &= x^n - nx^{n-2} + (4n - 21)x^{n-4}. \end{aligned} \tag{5}$$

Since  $M_{S_n^4}(x) - M_{C_{n,2}}(x) = x^{n-4}$ , then  $M_{S_n^4}(\lambda_1(C_{n,2})) > 0$ . Since the matching polynomial  $M_G(x)$  is strictly monotonically increasing for  $x > 0$ ,  $\lambda_1(C_{n,2}) > \lambda_1(S_n^4)$ . Similarly, since  $M_{C_{n,3}}(x) - M_{S_n^4}(x) = (n - 7)x^{n-4}$ , then  $M_{C_{n,3}}(\lambda_1(S_n^4)) > 0$  by putting  $x = \lambda_1(S_n^4)$ , and so  $\lambda_1(S_n^4) > \lambda_1(C_{n,3})$ . Similarly, we have

$$\begin{aligned} M_{C_{n,3}}(x) - M_{D_{n,n-3}}(x) &= -2x^{n-4}, \\ M_{D_{n,n-3}}(x) - M_{C_{n,4}}(x) &= (-n + 10)x^{n-4}, \\ M_{D_{n,n-3}}(x) - M_{T_n^2}(x) &= 0. \end{aligned} \tag{6}$$

Putting  $x = \lambda_1(C_{n,3})$  and  $x = \lambda_1(D_{n,n-3})$  to the above two equations, respectively, we have

$$\lambda_1(C_{n,3}) > \lambda_1(D_{n,n-3}) = \lambda_1(T_n^2) > \lambda_1(C_{n,4}). \tag{7}$$

Since  $S_n^+$  can be obtained from  $C_{n,k}$  by Kelmans transformations, then  $\lambda_1(S_n^+) > \lambda_1(C_{n,k})$  by Lemma 3. By Lemma 3, we have  $\lambda_1(C_{n,k-1}) > \lambda_1(C_{n,k})$ . Combining the discussions above and Theorem 1, the proof is completed.  $\square$

We now investigate the largest matching root of graphs with matching number 3.

**Theorem 3.** Let the graphs  $D_{n,k+1}$  and  $D_{n,k}$  be defined above. Then,  $\lambda_1(D_{n,k+1}) < \lambda_1(D_{n,k})$  if  $2 \leq k \leq n - 1/2$  and  $\lambda_1(D_{n,k+1}) > \lambda_1(D_{n,k})$  if  $k > n - 1/2$ .

*Proof.* By simple calculations, it is obtained that

$$\begin{aligned} m(D_{n,k+1}, 1) &= n, m(D_{n,k+1}, 2) = kn - k^2 - 2k + n - 3, m(D_{n,k+1}, 3) = kn - k^2 - 4k, \\ m(D_{n,k}, 1) &= n, m(D_{n,k}, 2) = kn - k^2 - 2, m(D_{n,k}, 3) = kn - k^2 - 2k - n + 3. \end{aligned} \quad (8)$$

Then,

$$\begin{aligned} M_{D_{n,k+1}}(x) &= x^n - nx^{n-2} + (kn - k^2 - 2k + n - 3)x^{n-4} - (kn - k^2 - 4k)x^{n-6}, \\ M_{D_{n,k}}(x) &= x^n - nx^{n-2} + (kn - k^2 - 2)x^{n-4} - (kn - k^2 - 2k - n + 3)x^{n-6}. \end{aligned} \quad (9)$$

If  $k \neq n - 1/2$ , then

$$M_{D_{n,k+1}}(x) - M_{D_{n,k}}(x) = (n - 2k - 1)x^{n-6} \left( x^2 - \frac{n - 2k - 3}{n - 2k - 1} \right). \quad (10)$$

Putting  $x = \lambda_1(D_{n,k+1})$ . Since  $D_{n,k+1}$  is a connected unicyclic graph, then  $\lambda_1^2(D_{n,k+1}) \geq 3$  by Lemma 5. Thus, if  $2 \leq k < n - 1/2$ , then  $M_{D_{n,k}}(\lambda_1(D_{n,k+1})) < 0$  and so  $\lambda_1(D_{n,k+1}) < \lambda_1(D_{n,k})$ . If  $k > n - 1/2$ , then  $M_{D_{n,k}}(\lambda_1(D_{n,k+1})) > 0$  and so  $\lambda_1(D_{n,k+1}) > \lambda_1(D_{n,k})$ .

If  $k = n - 1/2$ , then  $M_{D_{n,k+1}}(x) - M_{D_{n,k}}(x) = 2x^{n-6}$  and so  $\lambda_1(D_{n,k+1}) < \lambda_1(D_{n,k})$ .  $\square$

**Theorem 4.** Let  $L_k$  and  $L_{k-1}$  be the graphs as shown in Figure 5. If  $2 \leq k \leq n - 3/2$ , then  $\lambda_1(L_k) \leq \lambda_1(L_{k-1})$ , with equality holding if and only if  $k = n - 3/2$ .

*Proof.* By simple calculations, it is obtained that

$$\begin{aligned} m(L_k, 1) &= n, m(L_k, 2) = kn - k^2 - 4k + 2n - 6, m(L_k, 3) = kn - k^2 - 4k, \\ m(L_{k-1}, 1) &= n, m(L_{k-1}, 2) = kn - k^2 - 2k + n - 3, m(L_{k-1}, 3) = kn - k^2 - 2k - n + 3. \end{aligned} \quad (11)$$

Then,

$$\begin{aligned} M_{L_k}(x) &= x^n - nx^{n-2} + (kn - k^2 - 4k + 2n - 6)x^{n-4} - (kn - k^2 - 4k)x^{n-6}, \\ M_{L_{k-1}}(x) &= x^n - nx^{n-2} + (kn - k^2 - 2k + n - 3)x^{n-4} - (kn - k^2 - 2k - n + 3)x^{n-6}. \end{aligned} \quad (12)$$

It follows that

$$M_{L_k}(x) - M_{L_{k-1}}(x) = (n - 2k - 3)x^{n-6}(x^2 - 1). \quad (13)$$

By Lemma 5,  $\lambda_1^2(L_k) \geq 3$ . Therefore, putting  $x = \lambda_1(L_k)$ , if  $k \leq n - 3/2$ , then  $M_{L_{k-1}}(\lambda_1(L_k)) \leq 0$  and so  $\lambda_1(L_k) \leq \lambda_1(L_{k-1})$ , with equality holding if and only if  $k = n - 3/2$ .  $\square$

**Theorem 5.** The graphs  $G(a, b, c)$  and  $G(a, b - 1, c + 1)$  with  $n$  vertices are shown in Figure 6, where  $a + b + c = n - 3$ . If  $a \geq n/3 - 1$  and  $b \geq c$ , then  $\lambda_1(G(a, b, c)) < \lambda_1(G(a, b + 1, c - 1))$ . If  $a = 1$  and  $b \geq c$ , then  $\lambda_1(G(a, b, c)) < \lambda_1(G(a, b + 1, c - 1))$ .

*Proof.* Let  $G_1, G_2$  denote the graphs  $G(a, b, c)$  and  $G(a, b + 1, c - 1)$ , respectively. Without loss of generality, assume that  $a \geq n/3 - 1$  and  $b \geq c$ . It is easy to get that

$$\begin{aligned} m(G_1, 1) &= n, m(G_1, 2) = ab + ac + bc + a + b + c, m(G_1, 3) = abc, \\ m(G_2, 1) &= n, m(G_2, 2) = ab + ac + bc + a + 2c - 1, m(G_2, 3) = abc + ac - ab - a. \end{aligned} \quad (14)$$

Then,

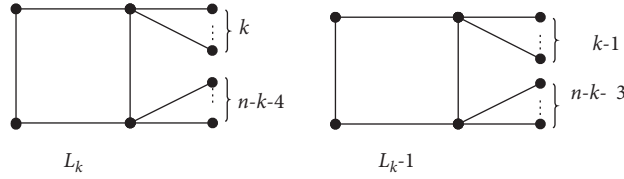


FIGURE 5: Graph transformation in Theorem 4.

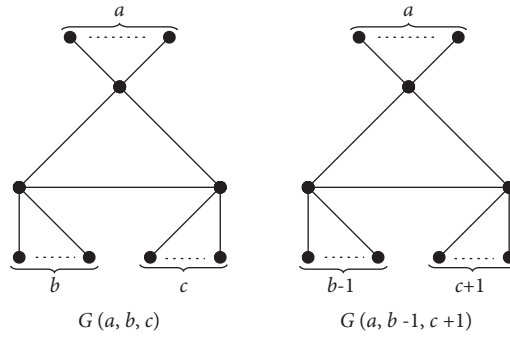


FIGURE 6: Graph in Theorem 5.

$$\begin{aligned}
 M_{G_1}(x) &= x^n - nx^{n-2} + (ab + ac + bc + a + b + c)x^{n-4} - abcx^{n-6}, \\
 M_{G_2}(x) &= x^n - nx^{n-2} + (ab + ac + bc + a + 2c - 1)x^{n-4} - (abc + ac - ab - a)x^{n-6}.
 \end{aligned}
 \tag{15}$$

Putting  $x = \sqrt{a+1}$  to  $M_{G_1}(x)$ , then

$$M_{G_1}(\sqrt{a+1}) = (a+1)^{n/2-3} [(a+1)^3 - n(a+1)^2 + (ab + ac + bc + a + b + c)(a+1) - abc].
 \tag{16}$$

Since  $a + b + c = n - 3$ , then

$$M_{G_1}(\sqrt{a+1}) = (a+1)^{n/2-3} (-a^2 - 3a - 2 + bc).
 \tag{17}$$

Since  $a \geq n/3 - 1$  and  $a + b + c = n - 3$ , then

$$bc \leq \left(\frac{b+c}{2}\right)^2 \leq \left(\frac{n-3}{3}\right)^2 < a^2 + 3a + 2.
 \tag{18}$$

Therefore,  $M_{G_1}(\sqrt{a+1}) < 0$ , and so  $\lambda_1(G_1) > \sqrt{a+1}$ . Moreover,  $M_{G_1}(x) - M_{G_2}(x) = (b - c + 1)x^{n-6}(x^2 - a)$ .

Since  $b \geq c$ , then  $M_{G_1}(x) - M_{G_2}(x) < 0$  for any  $x > \sqrt{a+1}$ . Thus, if  $a \geq n/2 - 1$  and  $b \geq c$ , then

$$M_{G_1}(\lambda_1(G_1)) - M_{G_2}(\lambda_1(G_1)) > 0,
 \tag{19}$$

that is,  $M_{G_2}(\lambda_1(G_1)) < 0$ . Therefore,  $\lambda_1(G_1) < \lambda_1(G_2)$ .

We now discuss the case for  $a = 1$ . Without loss of generality, assume that  $b \geq c$ . Obviously, we have

$$\begin{aligned}
 M_{G_1}(x) &= x^n - nx^{n-2} + (2b + 2c + bc + 1)x^{n-4} - bcx^{n-6}, \\
 M_{G_2}(x) &= x^n - nx^{n-2} + (b + 3c + bc)x^{n-4} - (bc + c - b - 1)x^{n-6}.
 \end{aligned}
 \tag{20}$$

Then,

$$M_{G_1}(x) - M_{G_2}(x) = (b - c + 1)x^{n-6}(x^2 - 1).
 \tag{21}$$

By Corollary 1,  $\lambda_1^2(G_1) \geq 3$ . Thus, if  $b \geq c$ , then  $M_{G_2}(\lambda_1(G_1)) < 0$ . Hence,  $\lambda_1(G_1) < \lambda_1(G_2)$ .  $\square$

**Theorem 6.** The graphs  $H_i (i = 1, 2, \dots, 5)$  with  $n (> 8)$  vertices are shown in Figure 7. Then,  $\lambda_1(H_1) > \lambda_1(H_2) > \lambda_1(H_3) = \lambda_1(H_4) > \lambda_1(H_5)$ .

*Proof.* Obviously,  $m(H_i, 1) = n$  (for  $i = 1, 2, 3, 4, 5$ ) and

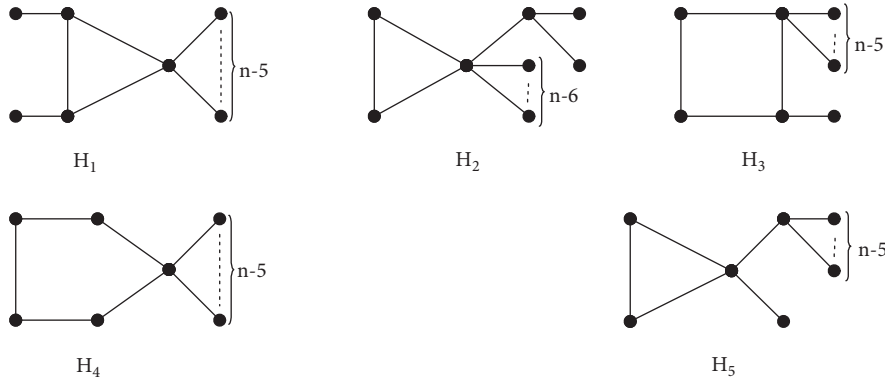


FIGURE 7: Five graphs in Theorem 6.

$$\begin{aligned}
 m(H_1, 2) &= 3n - 12, m(H_1, 3) = n - 5, \\
 m(H_2, 2) &= 3n - 11, m(H_2, 3) = 2n - 12, \\
 m(H_3, 2) &= 3n - 10, m(H_3, 3) = n - 5, \\
 m(H_4, 2) &= 3n - 10, m(H_4, 3) = n - 5, \\
 m(H_5, 2) &= 4n - 18, m(H_5, 3) = n - 5.
 \end{aligned}
 \tag{22}$$

Then,

$$\begin{aligned}
 M_{H_1}(x) &= x^n - nx^{n-2} + (3n - 12)x^{n-4} - (n - 5)x^{n-6}, \\
 M_{H_2}(x) &= x^n - nx^{n-2} + (3n - 11)x^{n-4} - (2n - 12)x^{n-6}, \\
 M_{H_3}(x) &= x^n - nx^{n-2} + (3n - 10)x^{n-4} - (n - 5)x^{n-6}, \\
 M_{H_4}(x) &= x^n - nx^{n-2} + (3n - 10)x^{n-4} - (n - 5)x^{n-6}, \\
 M_{H_5}(x) &= x^n - nx^{n-2} + (4n - 18)x^{n-4} - (n - 5)x^{n-6}.
 \end{aligned}
 \tag{23}$$

Putting  $x = \sqrt{n - 6}$  to matching polynomial of  $H_2$ , we have

$$\begin{aligned}
 M_{H_2}(\sqrt{n - 6}) &= (n - 6)^{n/2-3} [(n - 6)^3 - n(n - 6)^2 + (3n - 11)(n - 6) - 2(n - 6)], \\
 &= (n - 6)^{n/2-3} (-3n^2 + 41n - 138).
 \end{aligned}
 \tag{24}$$

Since  $n > 8$ , then  $M_{H_2}(\sqrt{n - 6}) < 0$  and so  $\lambda_1(H_2) > \sqrt{n - 6}$ . Since  $M_{H_2}(x) - M_{H_1}(x) = x^{n-6}[x^2 - (n - 7)]$ , then  $M_{H_2}(x) - M_{H_1}(x) > 0$  for any  $x > \sqrt{n - 6}$ . Therefore,  $M_{H_1}(\lambda_1(H_2)) < 0$ , and thus,  $\lambda_1(H_1) > \lambda_1(H_2)$ .

Since  $M_{H_3}(x) - M_{H_2}(x) = x^{n-6}[x^2 + (n - 7)]$ , then  $M_{H_3}(\lambda_1(H_3)) - M_{H_2}(\lambda_1(H_3)) > 0$ , and thus,  $\lambda_1(H_2) > \lambda_1(H_3)$ . It is obvious that  $\lambda_1(H_3) = \lambda_1(H_4)$ . Since  $M_{H_4}(x) - M_{H_5}(x) = (-n + 8)x^{n-4}$  and  $n > 8$ , then  $M_{H_4}(\lambda_1(H_4)) - M_{H_5}(\lambda_1(H_4)) < 0$  and so  $\lambda_1(H_4) > \lambda_1(H_5)$ . Therefore,  $\lambda_1(H_1) > \lambda_1(H_2) > \lambda_1(H_3) = \lambda_1(H_4) > \lambda_1(H_5)$ .  $\square$

**Theorem 7.** Among all unicyclic graphs of order  $n (> 8)$  with matching number 3, the graphs with the first second largest matching root are  $D_{n,2}$  and  $H_1$ .

*Proof.* Since  $D_{n,2} \cong S_n^3$ , then the graph with the largest matching root among all unicyclic graphs with matching number 3 is  $D_{n,2}$  by Lemma 4.

Let  $G$  be the unicyclic graph of order  $n (\geq 8)$  with the second largest matching root among all graphs with matching number 3. Since  $G$  is a unicyclic graph of order  $n$  with matching number 3, then the girth  $g$  of  $G$  is possibly 3, 4, or 5.  $\square$

**3.1. Case 1:  $g = 3$ .** Under the Kelmans transformation,  $G$  is  $D_{n,k}$  or  $G(a, b, c)$  in Figure 6. By Theorem 3,  $\lambda_1(D_{n,k+1}) < \lambda_1(D_{n,k})$  if  $2 \leq k < n - 1/2$  and  $\lambda_1(D_{n,k+1}) > \lambda_1(D_{n,k})$  if  $k > n - 1/2$ . Therefore, among all the graphs of type  $D_{n,k}$ ,  $G$  is  $D_{n,3}$  or  $D_{n,n-4}$ . Since  $D_{n,3} \cong H_2$  and  $D_{n,n-4} \cong H_5$ , then  $\lambda_1(D_{n,3}) > \lambda_1(D_{n,n-4})$  by Theorem 6.

By Theorem 5,  $G(1, n - 5, 1)$  is the graph with the first largest matching root among the graphs of type  $G(a, b, c)$ . Moreover,  $G(1, n - 5, 1) \cong H_1$ . Thus, by Theorem 6, the graph with the second largest matching root and girth 3 is  $H_1$ .  $\square$

**3.2. Case 2:  $g = 4$ .** In this case,  $G$  possibly is the graph  $T_i (i = 1, 2, 3, 4, 5)$  in Figure 8. Obviously,  $T_1$  can be obtained by a series of Kelmans transformations from the graph  $T_i (i = 2, 3, 4, 5)$ . Moreover,  $T_1$  is the graph  $L_k$  in Theorem 4. By Theorem 4, the graph with the largest matching roots among graphs of type  $L_k$  is  $L_1$  which is isomorphic to  $H_3$ . Therefore, the graph with the largest matching root among the graphs with matching number 3 and girth 4 is  $H_3$ .

**3.3. Case 3:  $g = 5$ .** In this case, the unicyclic graphs with matching number 3 isomorphism to the following four families graphs denoted by  $C(n - 5, 0, 0, 0, 0)$

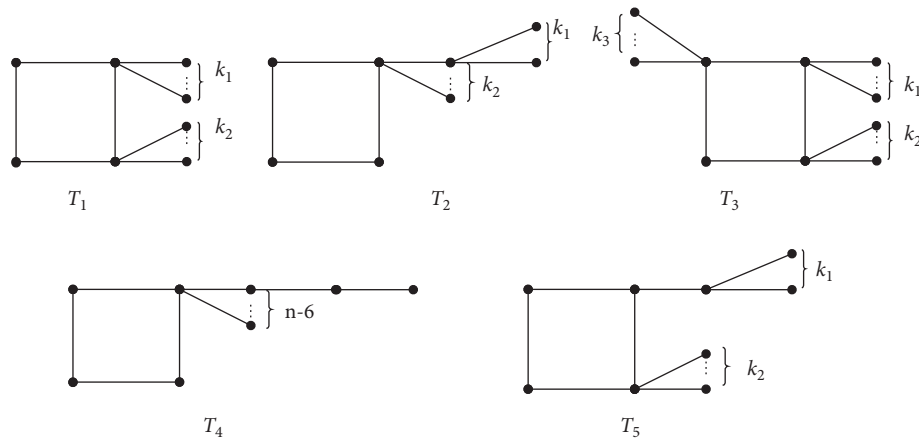


FIGURE 8: Five graphs in Case 2.

,  $C(n - 5 - k, k, 0, 0, 0)$ ,  $C(n - 5 - k, 0, k, 0, 0)$ , and  $C(n - 5 - k_1 - k_2, 0, k_1, 0, k_2)$ , where  $C(m_1, m_2, m_3, m_4, m_5)$  denote the unicyclic graphs with girth 5, such that there are  $m_i$  pendent edges attached to the vertex  $v_i$  of the cycle. Obviously,  $C(n - 5, 0, 0, 0, 0)$  is isomorphic to  $H_4$  in Theorem 5, and the rest three families can arrive at graphs of Case 1 or 2 by a series of Kelmans transformations. Thus,  $G$  is  $H_4$  in this case.

Therefore, by Theorem 6, the graph with the second largest matching root is  $H_1$ .

#### 4. Further Remarks

In the introduction, we already talk about that the matching energies have been getting a lot of attention recently. The graphs with maximum and minimum values of matching roots are the graphs with minimum and maximum matching energy. Therefore, any result for the largest matching roots can reveal the structural dependence of the matching energy or at least provide guidance for its research. Recently, References [2,5,6] showed some new findings on the matching energy of unicyclic graphs. Therefore, the results of this paper have a direct application value [4, 16].

#### Data Availability

The data used to support the findings of this study are included within the article.

#### Conflicts of Interest

The authors declare that they have no conflicts of interest.

#### Acknowledgments

This work was supported by the National Natural Science Foundation of China (no. 12071484 and 11701046) and the Natural Science Foundation of Hunan Province, China (nos. 2020JJ4675, 2017JJ2280 and 2018JJ2450).

#### References

- [1] E. J. Farrell, "An introduction to matching polynomials," *Journal of Combinatorial Theory - Series B*, vol. 27, no. 1, pp. 75–86, 1979.
- [2] C. D. Godsil and I. Gutman, "On the theory of the matching polynomial," *Journal of Graph Theory*, vol. 5, no. 2, pp. 137–144, 1981.
- [3] D. C. Fisher and J. Ryan, "Bounds on the largest root of the matching polynomial," *Discrete Mathematics*, vol. 110, no. 1-3, pp. 275–278, 1992.
- [4] O. J. Heilmann and E. H. Lieb, "Monomers and dimers," *Physical Review Letters*, vol. 24, no. 25, pp. 1412–1414, 1970.
- [5] J. Zhu, "Ordering of unicyclic graphs with perfect matchings by minimal matching energies," *Open Journal of Discrete Mathematics*, vol. 09, no. 01, pp. 17–32, 2019.
- [6] H. Zhang and G. T. Chen, "The largest matching roots of unicyclic graphs with a fixed matching number," *Cogent Mathematics*, vol. 4, no. 1, Article ID 1280912, 2017.
- [7] D. Cvetković, M. Doob, I. Gutman, and A. Torgašev, *Recent Results in the Theory of Graph Spectra*, North-Holland, Amsterdam, 1988.
- [8] E. Ghorbani, "Graphs with few matching roots," *Graphs and Combinatorics*, vol. 29, no. 5, pp. 1377–1389, 2013.
- [9] C. D. Godsil, *Algebraic Combinatorics*, Chapman & Hall, London, 1993.
- [10] C. Y. Ku and W. Chen, "An analogue of the Gallai–Edmonds structure theorem for non-zero roots of the matching polynomial," *Journal of Combinatorial Theory - Series B*, vol. 100, no. 2, pp. 119–127, 2010.
- [11] H. Zhang, G. Yu, and S. Li, "Graphs with six distinct matching roots," *Information Processing Letters*, vol. 115, no. 5, pp. 521–526, 2015.
- [12] I. Gutman and F. Zhang, "On the ordering of graphs with respect to their matching numbers," *Discrete Applied Mathematics*, vol. 15, no. 1, pp. 25–33, 1986.
- [13] H. Zhang, R. Lin, and G. Yu, "The largest matching root of unicyclic graphs," *Information Processing Letters*, vol. 113, no. 19-21, pp. 804–806, 2013.
- [14] H. L. Zhang and G. T. Chen, "The largest matching roots of unicyclic graphs with a fixed matching number," *Cogent Mathematics*, vol. 4, no. 1, Article ID 1280912, 2017.

- [15] W. Liu, Q. Guo, Y. Zhang, L. Feng, and I. Gutman, "Further results on the largest matching root of unicyclic graphs," *Discrete Applied Mathematics*, vol. 221, pp. 82–88, 2017.
- [16] P. Csikvári, "Applications of the Kelmans transformation: extremality of the threshold graphs," *Electronic Journal of Combinatorics*, vol. 18, no. 1, Article ID P182, 2011.
- [17] H. M. Chen and Y. Liu, "Extremal graphs with respect to matching energy for random six-membered ring spiro chains," *Acta Mathematicae Applicatae Sinica, English Series*, vol. 35, no. 2, pp. 319–326, 2019.
- [18] L. Chen and Y. T. Shi, "The maximal matching energy of tricyclic graphs," *MATCH Commun. Math. Comput. Chem.* vol. 73, pp. 105–120, 2015.
- [19] X. Chen, X. Li, and H. Lian, "The matching energy of random graphs," *Discrete Applied Mathematics*, vol. 193, pp. 102–109, 2015.