Available online at www.sciencedirect.com
ScienceDirect
Discrete Applied Mathematics 156 (2008) 2679–2697
DISCRETE APPLIED MATHEMATICS
www.elsevier.com/locate/dam

Some results on the ordering of the Laplacian spectral radii of unicyclic graphs☆

Ying Liu*, Jia-Yu Shao, Xi-Ying Yuan

Department of Mathematics, Tongji University, Shanghai, 200092, China

Received 17 June 2006; received in revised form 29 October 2007; accepted 2 November 2007
Available online 21 February 2008

Abstract

A unicyclic graph is a graph whose number of edges is equal to the number of vertices. Guo Shu-Guang [S.G. Guo, The largest Laplacian spectral radius of unicyclic graph, Appl. Math. J. Chinese Univ. Ser. A. 16 (2) (2001) 131–135] determined the first four largest Laplacian spectral radii together with the corresponding graphs among all unicyclic graphs on n vertices. In this paper, we extend this ordering by determining the fifth to the ninth largest Laplacian spectral radii together with the corresponding graphs among all unicyclic graphs on n vertices.

Keywords: Unicyclic graph; Laplacian spectral radius; Characteristic polynomial

1. Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set E. Denote by d_i the degree of the vertex v_i of the graph G. Let $A(G)$ be the adjacency matrix of G and $L(G) = D(G) - A(G)$ the Laplacian matrix of the graph G where $D(G) =\mathrm{diag}(d_1, d_2, \ldots, d_n)$ denotes the diagonal matrix of vertex degrees of G. Without loss of generality, we assume $d_1 \geq d_2 \geq \cdots \geq d_n$, and $\pi(G) = (d_1, d_2, \ldots, d_n)$ is the degree sequence of G. It is easy to see that $L(G)$ is a positive semidefinite symmetric matrix and its rows sum to 0, so $L(G)$ is singular. Denote its eigenvalues by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$, which are always enumerated in non-increasing order and repeated according to their multiplicity. We call the largest eigenvalue of $L(G)$ the Laplacian spectral radius of the graph G, denoted by $\mu(G)$. Let X be an eigenvector of G corresponding to $\mu(G)$. It will be convenient to associate with X a labelling of G in which vertex v is labelled x_v.

A unicyclic graph is a graph whose number of edges is equal to the number of vertices. Let U_n be the set of all unicyclic graphs of order n. Let G_1–G_{10} be the following unicyclic graphs of order n as shown in Fig. 1:

It is easy to see that each unicyclic graph can be obtained by attaching rooted trees to the vertices of a cycle C_k of length k. Thus if $R_1, \ldots, R_k$ are k rooted trees (of orders $n_1, \ldots, n_k$, say), then we adopt the notation $U_k(R_1, \ldots, R_k)$ (or simply $U(R_1, \ldots, R_k)$ sometimes for convenience) to denote the unicyclic graph G (of order $n = n_1 + \cdots + n_k$)

☆ Research supported by the National Natural Science Foundation of China 10331020 and 10731040.
* Corresponding author.
E-mail addresses: lymaths@126.com (Y. Liu), jyshao@sh163.net (J.-Y. Shao).

0166-218X/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.dam.2007.11.006

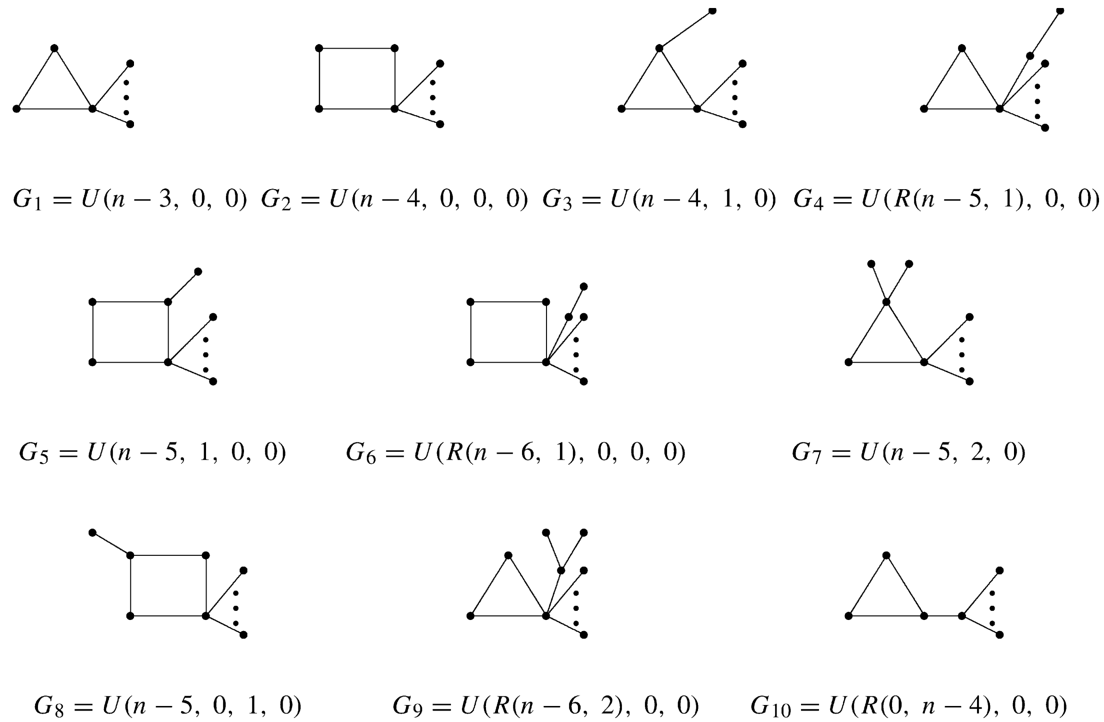


Fig. 1. The graphs G_1–G_{10} of order n.

obtained by attaching the rooted tree R_i to the vertex v_i of a cycle $C_k = v_1 v_2 \cdots v_k v_1$ (i.e., by identifying the root of R_i with the vertex v_i) for $i = 1, \ldots, k$.

In the special case when R_i is a rooted star K_{1,a_i} with the center of the star as its root, we will simplify the notation by replacing R_i by the number a_i.

Let $S(a, b)$ be the tree of order $a + b + 2$ obtained from $K_{1,a}$ and $K_{1,b}$ by adding a edge $e = uv$, where u, v are the star centers of $K_{1,a}$ and $K_{1,b}$, respectively.

Let $R(a, b)$ be the rooted tree with $S(a, b)$ as its underlying tree and with the vertex of degree $a + 1$ as its root.

Using the above defined notations, we can write the above graphs G_1–G_{10} (in Fig. 1) in the following way:

$$G_1 = U(n-3, 0, 0), \qquad G_2 = U(n-4, 0, 0, 0), \qquad G_3 = U(n-4, 1, 0),$$
$$G_4 = U(R(n-5, 1), 0, 0),$$
$$G_5 = U(n-5, 1, 0, 0), \qquad G_6 = U(R(n-6, 1), 0, 0, 0), \qquad G_7 = U(n-5, 2, 0),$$
$$G_8 = U(n-5, 0, 1, 0), \qquad G_9 = U(R(n-6, 2), 0, 0), \qquad G_{10} = U(R(0, n-4), 0, 0).$$

Throughout this paper, we shall denote by $\Phi(B; x) = \det(xI - B)$ the characteristic polynomial of the square matrix B. Let $f(x) = x^n + a_1 x_{n-1} + \cdots + a_{n-1} x + a_n$ be a polynomial with $a_i \in R$. If the equation $f(x) = 0$ has only real roots, then we use $\mu(f)$ to denote the largest root of $f(x) = 0$.

In [1], Guo Shu-Guang determined the first four largest Laplacian spectral radii together with the corresponding graphs among all unicyclic graphs of order n (see graphs G_1–G_4 in Fig. 1). In this paper, we extend this ordering by determining the fifth to the ninth largest Laplacian spectral radii together with the corresponding graphs among all unicyclic graphs of order n (see graphs G_5–G_{10} in Fig. 1).

2. The effect of a graph perturbation on the Laplacian spectral radii

There is a graph perturbation (which can be called "moving the pendant paths") whose effects on the Laplacian spectral radii are very useful in the comparison of the Laplacian spectral radii. Guo Ji-Ming studied this graph perturbation in [2]. In this section, we will introduce Guo's result on this perturbation and give some examples to show the effect of this perturbation on the comparison of the Laplacian spectral radii of the unicyclic graphs.

A pendant path of a graph is a path with one of its end vertices having degree one and all the internal vertices having degree two. Obviously, a pendant path of length one is just a pendant edge.

Definition 2.1. *Let v be a non-pendant vertex of a connected graph G and u be a vertex different from v. Suppose that $P_1, \ldots, P_t$ are t pendant paths of G with v as one of its end vertices. Let v_i be the vertex on the path P_i which is adjacent to $v (i = 1, \ldots, t)$. Let*

$$M_G^t(v, u) = G - vv_1 - vv_2 - \cdots - vv_t + uv_1 + uv_2 + \cdots + uv_t.$$

Then we call the graph $M_G^t(v, u)$, the graph obtained from G by moving t pendant paths from v to u.

Lemma 2.1 ([2]). *Let G and $M_G^t(v, u)$ be the graphs as defined in Definition 2.1. Suppose $\Delta(G) \geq 3$, where $\Delta(G)$ is the maximum degree of the graph G. Let X be a unit eigenvector of G corresponding to $\mu(G)$. If $|x_u| \geq |x_v|$, then*

$$\mu(G) \leq \mu(M_G^t(v, u)).$$

Furthermore, if $|x_u| > |x_v|$, then $\mu(G) < \mu(M_G^t(v, u))$.

Since at least one of the two conditions $|x_u| \geq |x_v|$ and $|x_v| \geq |x_u|$ holds, we have the following corollary.

Corollary 2.1. *Let u and v be two distinct non-pendant vertices of a connected graph G. Suppose that $P_1, \ldots, P_t$ are t pendant paths of G with v as one of its end vertices, and $Q_1, \ldots, Q_s$ are s pendant paths of G with u as one of its end vertices.*

Let $M_G^t(v, u)$ (and $M_G^s(u, v)$) be the graph obtained from G by moving t pendant paths from v to u (and by moving s pendant paths from u to v, respectively) as in Definition 2.1. Suppose $\Delta(G) \geq 3$, where $\Delta(G)$ is the maximum degree of the graph G. Then we have

$$\mu(G) \leq \max\{\mu(M_G^t(v, u)), \mu(M_G^s(u, v))\}. \tag{2.1}$$

Furthermore, if X is a unit eigenvector of G corresponding to $\mu(G)$ with $|x_u| \neq |x_v|$, then this inequality is strict.

Proof. If $|x_u| \geq |x_v|$, then from Lemma 2.1 we have

$$\mu(G) \leq \mu(M_G^t(v, u)).$$

While if $|x_v| \geq |x_u|$, then from Lemma 2.1 we also have

$$\mu(G) \leq \mu(M_G^s(u, v)).$$

Combining these two cases, we get the desired inequality.

Furthermore, if $|x_u| \neq |x_v|$, then either $|x_u| > |x_v|$ or $|x_v| > |x_u|$, so by Lemma 2.1 the strict inequality holds. □

The following two examples show how Lemma 2.1 and Corollary 2.1 can be used in the comparison of the Laplacian spectral radii of graphs.

Example 2.1. *If $0 \leq a \leq \min\{c, d\}$ and $a + b = c + d$, R is any rooted tree, then*

$$\mu(U(c, d, R)) \leq \mu(U(a, b, R)).$$

Proof. Let $G = U(c, d, R)$. Let v be the vertex on the cycle of G with $d(v) = c + 2$ and u be the vertex on the cycle of G with $d(u) = d + 2$. Let $M_G^{c-a}(v, u)$ (and $M_G^{d-a}(u, v)$) be the graph obtained from G by moving $c - a$ pendant edges from v to u (and by moving $d - a$ pendant edges from u to v, respectively), then it is easy to see that both of the two graphs $M_G^{c-a}(v, u)$ and $M_G^{d-a}(u, v)$ are isomorphic to $U(a, b, R)$. Thus from Corollary 2.1 we have

$$\mu(G) \leq \max\{\mu(M_G^{c-a}(v, u)), \mu(M_G^{d-a}(u, v))\} = \mu(U(a, b, R)). \quad \square$$

Similarly we have,

$$\mu(U(c, d, R_1, R_2)) \leq \mu(U(a, b, R_1, R_2)),$$
$$\mu(U(c, R_1, d, R_2)) \leq \mu(U(a, R_1, b, R_2)).$$

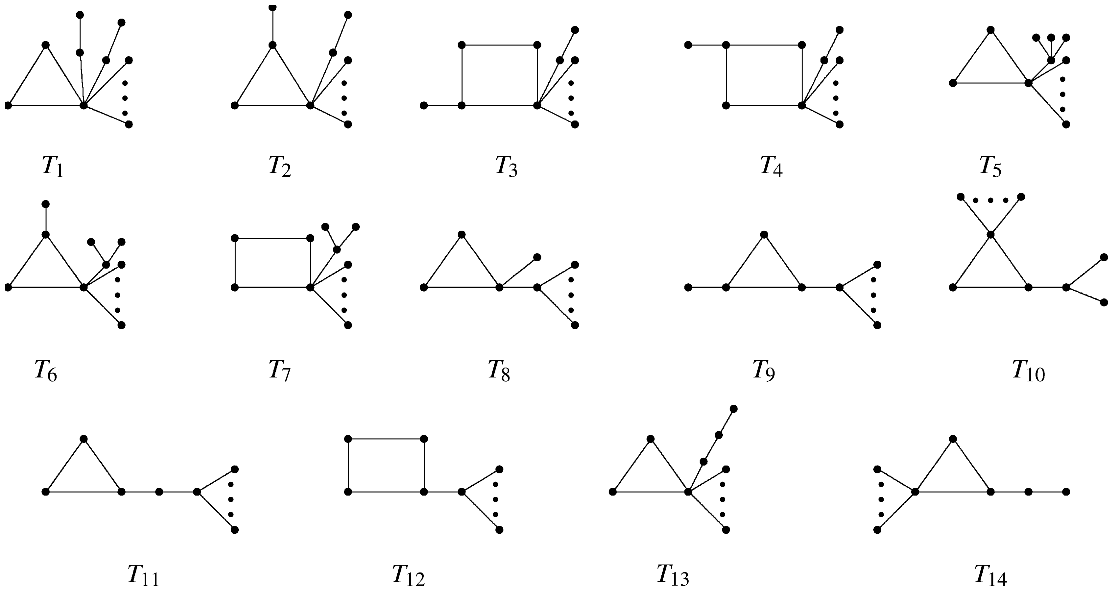


Fig. 2. The graphs T_1–T_{14} of order n.

Example 2.2. *If* $0 \le b \le \min\{c-3, d\}$ *and* $a+b=c+d$, *R is any rooted tree, then*

$$\mu(U(R(c-3,1),d,R)) \le \mu(U(R(a-3,1),b,R)).$$

Proof. Let $G = U(R(c-3,1),d,R)$. Let u be the vertex on the cycle of G with $d(u)=c$ (and with $c-3$ pendant edges and one pendant path of length 2 attached to u), and v be the vertex on the cycle of G with $d(v)=d+2$ and d pendant edges attached to v.

Let $M_G^{d-b}(v,u)$ be the graph obtained from G by moving $d-b$ pendant edges from v to u, and $M_G^{c-2-b}(u,v)$ be the graph obtained from G by moving $c-3-b$ pendant edges and one pendant path of length 2 from u to v, respectively. Then it is easy to see that both of the two graphs $M_G^{d-b}(v,u)$ and $M_G^{c-2-b}(u,v)$ are isomorphic to $U(R(a-3,1),b,R)$. Thus from Corollary 2.1 we have

$$\mu(G) \le \max\{\mu(M_G^{d-b}(v,u)), \mu(M_G^{c-2-b}(u,v))\} = \mu(U(R(a-3,1),b,R)). \quad \square$$

3. The auxiliary graphs T_1–T_{14}

The basic strategy of proving our main results consists of the following steps:

Step 1: To prove that for each graph $G \in U_n \setminus \{G_1,\ldots,G_{10}\}$, we have $\mu(G) < \mu(G_{10})$.

For this purpose, we need to do the following two substeps.

Substep 1.1: We define the 14 auxiliary graphs T_1–T_{14} in U_n (see Fig. 2) and then show that

$$\mu(T_i) < \mu(G_{10}) \quad (i=1,\ldots,14).$$

Substep 1.2: We show that for each graph $G \in U_n \setminus \{G_1,\ldots,G_{10}\}$, we have either $\mu(G) < \mu(G_{10})$ or $\mu(G) \le \mu(T_i)$ for some $i \in \{1,\ldots,14\}$.

Step 2: To prove that

$$\mu(G_{10}) = \mu(G_9) < \mu(G_8) < \mu(G_7) < \mu(G_6) < \mu(G_5) < \mu(G_4) < \mu(G_3) < \mu(G_2) < \mu(G_1).$$

(Notice that $\mu(G_5) < \mu(G_4) < \mu(G_3) < \mu(G_2) < \mu(G_1)$ has already been proved by Guo in [1].)

We will settle Substep 1.1 in Section 3, settle Substep 1.2 in Section 4 and settle Step 2 in Section 5.

First we need to introduce the following lemmas from [1,3–7] before introducing the auxiliary graphs T_1–T_{14}.

Lemma 3.1 *([1]). Let G be a unicyclic graph on n vertices, $v_1, v_2 \in V(G)$, then*

(1) *If v_1, v_2 are adjacent, then $d(v_1) + d(v_2) \leq n + 1$;*
(2) *If v_1, v_2 are not adjacent, then $d(v_1) + d(v_2) \leq n$.*

Lemma 3.2 *([3]). Let G be a graph on n vertices. Then*

$$\mu(G) \leq \max\{d_i + m_i \mid v_i \in V(G)\},$$

where $m_i = \frac{\sum_{v_i v_j \in E} d(v_j)}{d(v_i)}$ is the average of the degrees of the vertices of G adjacent to v_i, which is called the average 2-degree of the vertex v_i.

Lemma 3.3 *([4]). Let G be a connected graph on n vertices with the degree sequence $\pi(G) = (d_1, d_2, \ldots, d_n)$ $(d_1 \geq d_2 \geq \cdots \geq d_n)$. Then $\mu(G) \leq d_1 + d_2$.*

Lemma 3.4 *([5]). (The operation of "grafting pendant edges") Let G be a connected graph on $n \geq 2$ vertices and v be a vertex of G. Let $G_{k,l}$ be the graph obtained from G by attaching two new paths $P : v(= v_0)v_1v_2 \cdots v_k$ and $Q : v(= v_0)u_1u_2 \cdots u_l$ of lengths k and l at v, respectively, where $u_1, u_2, \ldots, u_l$ and $v_1, v_2, \ldots, v_k$ are distinct new vertices. Let*

$$G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_l v_k.$$

If $l \geq k \geq 1$, then

$$\mu(G_{k-1,l+1}) \leq \mu(G_{k,l})$$

with equality if and only if there exists a unit eigenvector of $G_{k,l}$ corresponding to $\mu(G_{k,l})$ taking the value 0 on vertex v.

Lemma 3.5 *([6,7]). Let G be a connected graph on n vertices with at least one edge, then $\mu(G) \geq \Delta(G) + 1$, where $\Delta(G)$ is the maximum degree of the graph G, with equality if and only if $\Delta(G) = n - 1$.*

Now we introduce the following auxiliary graphs T_1–T_{14} of order n in Fig. 2.

By employing the notations in Section 1, we can write these graphs (except $\{T_1, T_{11}, T_{13}\}$) in the following way:

$$T_2 = U(R(n-6,1),1,0), \quad T_3 = U(R(n-7,1),1,0,0), \quad T_4 = U(R(n-7,1),0,1,0),$$
$$T_5 = U(R(n-7,3),0,0), \quad T_6 = U(R(n-7,2),1,0), \quad T_7 = U(R(n-7,2),0,0,0),$$
$$T_8 = U(R(1,n-5),0,0), \quad T_9 = U(R(0,n-5),1,0), \quad T_{10} = U(R(0,2),n-6,0),$$
$$T_{12} = U(R(0,n-5),0,0,0), \quad T_{14} = U(R(0,1),n-5,0).$$

First we prove the following bounds for $\mu(G_9)$ and $\mu(G_{10})$.

Proposition 3.1. *Let G_9, G_{10} be the unicyclic graphs on n $(n \geq 6)$ vertices as in Fig. 1. Then*

$$n - 2 < \mu(G_9) = \mu(G_{10}) < n - 1.$$

Proof. By Lemma 3.5, we have

$$\mu(G_9) > \Delta(G_9) + 1 = n - 2,$$
$$\mu(G_{10}) > \Delta(G_{10}) + 1 = n - 2.$$

It is not difficult to calculate (recursively) that

$$\Phi(G_9; \lambda) = \Phi(G_{10}; \lambda) = \lambda(\lambda - 3)(\lambda - 1)^{n-5} h(\lambda), \tag{3.1}$$

where

$$h(\lambda) = \lambda^3 - (n+2)\lambda^2 + (4n-7)\lambda - n.$$

For $n \geq 6$, we have

$$h(0) = -n < 0, \qquad h(1) = 2(n-4) > 0,$$
$$h(n-2) = -2 < 0, \qquad h(n-1) = n^2 - 6n + 4 > 0.$$

But $h(\lambda)$ is a cubic polynomial, so $h(\lambda) > 0$ if $\lambda \geq n-1$. So

$$\Phi(G_9; \lambda) = \Phi(G_{10}; \lambda) = \lambda(\lambda - 3)(\lambda - 1)^{n-5} h(\lambda) > 0 \quad (\text{for } \lambda \geq n-1).$$

Thus we have

$$n - 2 < \mu(G_9) = \mu(G_{10}) = \mu(h) < n - 1. \quad \square$$

Now we begin to show that $\mu(T_i) < \mu(G_{10})$ $(i = 1, \ldots, 14)$.

Proposition 3.2. *Let $U(n-5, 1, 1)$, $U(n-5, 0, 0, 0, 0)$ and T_1 (Fig. 2) be the unicyclic graphs on n $(n \geq 7)$ vertices. Then*

$$\mu(U(n-5, 1, 1)) = \mu(U(n-5, 0, 0, 0, 0)) = \mu(T_1) < \mu(G_{10}).$$

Proof. It is not difficult to calculate recursively that

$$\Phi(U(n-5, 1, 1); \lambda) = \lambda(\lambda - 1)^{n-6}(\lambda^2 - 5\lambda + 3)h_1(\lambda), \tag{3.2}$$

$$\Phi(T_1; \lambda) = \lambda(\lambda - 3)(\lambda - 1)^{n-7}(\lambda^2 - 3\lambda + 1)h_1(\lambda), \tag{3.3}$$

$$\Phi(U(n-5, 0, 0, 0, 0); \lambda) = \lambda(\lambda - 1)^{n-6}(\lambda^2 - 5\lambda + 5)h_1(\lambda), \tag{3.4}$$

where

$$h_1(\lambda) = \lambda^3 - (n+1)\lambda^2 + (3n-5)\lambda - n.$$

By Lemma 3.5, we have

$$\mu(U(n-5, 1, 1)) > \Delta(U(n-5, 1, 1)) + 1 = n - 2,$$
$$\mu(T_1) > \Delta(T_1) + 1 = n - 2,$$
$$\mu(U(n-5, 0, 0, 0, 0)) > \Delta(U(n-5, 0, 0, 0, 0)) + 1 = n - 2,$$

so $\mu(U(n-5, 1, 1))$, $\mu(T_1)$, $\mu(U(n-5, 0, 0, 0, 0))$ are the largest roots of $h_1(\lambda)$. Thus

$$\mu(U(n-5, 1, 1)) = \mu(T_1) = \mu(U(n-5, 0, 0, 0, 0)).$$

Next by (3.1) and (3.3), we have

$$\Phi(T_1; \lambda) - \Phi(G_{10}; \lambda) = \lambda^2(\lambda - 3)(\lambda - 1)^{n-7} g_1(\lambda),$$

where

$$g_1(\lambda) = \lambda^2 - (n-2)\lambda + 2.$$

It is easy to check that for $\lambda \geq n-2$, we have $g_1(\lambda) > 0$. So if $\lambda \geq \mu(G_{10}) > n-2$, then

$$\Phi(T_1; \lambda) - \Phi(G_{10}; \lambda) = \lambda^2(\lambda - 3)(\lambda - 1)^{n-7} g_1(\lambda) > 0.$$

Thus we have

$$\mu(U_3(n-5, 1, 1)) = \mu(U(n-5, 0, 0, 0, 0)) = \mu(T_1) < \mu(G_{10}). \quad \square$$

By the similar method as in Proposition 3.2, we can obtain the following propositions.

Proposition 3.3. *Let T_2 (Fig. 2) be a unicyclic graph on n $(n \geq 6)$ vertices. Then*

$$\mu(T_2) < \mu(G_{10}).$$

Proof. It is not difficult to calculate recursively that

$$\Phi(T_2;\lambda) = \lambda(\lambda-1)^{n-7}h_2(\lambda), \tag{3.5}$$

where

$$h_2(\lambda) = \lambda^6 - (n+7)\lambda^5 + (9n+10)\lambda^4 - (28n-18)\lambda^3 + (36n-42)\lambda^2 - (18n-14)\lambda + 3n.$$

Then by (3.1), we have

$$\Phi(T_2;\lambda) - \Phi(G_{10};\lambda) = \lambda^2(\lambda-1)^{n-7}(\lambda+n-7).$$

So if $\lambda \geq \mu(G_{10}) > n-2$, we have

$$\Phi(T_2;\lambda) - \Phi(G_{10};\lambda) = \lambda^2(\lambda-1)^{n-7}(\lambda+n-7) > 0$$

since $n \geq 6$. Thus we have

$$\mu(T_2) < \mu(G_{10}). \quad \square$$

Proposition 3.4. *Let T_{14} (Fig. 2) be a unicyclic graph on n $(n \geq 6)$ vertices. Then*

$$\mu(T_{14}) < \mu(G_{10}).$$

Proof. It is not difficult to calculate recursively that

$$\Phi(T_{14};\lambda) = \lambda(\lambda-1)^{n-6}h_3(\lambda), \tag{3.6}$$

where

$$h_3(\lambda) = \lambda^5 - (n+6)\lambda^4 + (8n+4)\lambda^3 - (20n-22)\lambda^2 + (17n-26)\lambda - 3n.$$

Next by (3.1) and (3.6), we have

$$\Phi(T_{14};\lambda) - \Phi(G_{10};\lambda) = \lambda^2(\lambda-1)^{n-6}(n-5).$$

So if $\lambda \geq \mu(G_{10}) > n-2$, then

$$\Phi(T_{14};\lambda) - \Phi(G_{10};\lambda) = \lambda^2(\lambda-1)^{n-6}(n-5) > 0.$$

Thus

$$\mu(T_{14}) < \mu(G_{10}). \quad \square$$

Proposition 3.5. *Let $T \in \{T_3, \ldots, T_{12}\}$ (Fig. 2) be a unicyclic graph on n $(n \geq 10)$ vertices. Then*

$$\mu(T) < n-2.$$

Proof. We use $\mu(T) \leq \max\{d_i + m_i \mid v_i \in V(T)\}$ from Lemma 3.2. Assume $d_1 \geq d_2 \geq \cdots \geq d_n$. Then for $T \in \{T_3, \ldots, T_{12}\}$ we can check that

$$d_1 = n-4, \qquad d_2 \leq 4, \qquad d_3 \leq 3, \qquad d_4 \leq 2. \tag{3.7}$$

Thus if $d_i \neq d_1$, then $1 \leq d_i \leq 4$. Now for each $i \in \{1, \ldots, n\}$, we estimate the quantity $d_i + m_i$ according to the following cases:

Case 1: $d_i = d_1$.

Then

$$d_1 + m_1 = d_1 + \frac{\sum\limits_{v_1 v_j \in E} d_j}{d_1} > d_1 + 1 = n-3.$$

Case 2: $d_i = 1$.

Then

$$d_i + m_i = 1 + \frac{d_j}{1} = 1 + d_j \le d_1 + 1.$$

Case 3: $d_i = 2$.

Then from (3.7) we have

$$d_i + m_i \le 2 + \frac{d_1 + d_2}{2} \le 2 + \frac{n}{2} \le n - 3 = d_1 + 1.$$

Case 4: $d_i = 3$.

Then from (3.7) we have

$$d_i + m_i \le 3 + \frac{d_1 + d_2 + d_3}{3} \le 3 + \frac{n+3}{3} \le n - 3 = d_1 + 1.$$

Case 5: $d_i = 4$.

Then from (3.7) we have

$$d_i + m_i \le 4 + \frac{d_1 + d_2 + d_3 + d_4}{4} \le 4 + \frac{n+5}{4} \le n - 3 = d_1 + 1.$$

Combining Cases 1–5, we have

$$\begin{aligned} \mu(T) &\le \max\{d_i + m_i \mid v_i \in V(T)\} = d_1 + m_1 \\ &\le n - 4 + \frac{\sum_{j=1}^{n} d_j - (d_1 + d_s + d_t + d_k)}{n-4} \\ &\le n - 4 + \frac{2n - (n - 4 + 1 + 1 + 1)}{n-4} \\ &= n - 3 + \frac{5}{n-4} < n - 2. \quad \square \end{aligned}$$

Now from the above Propositions 3.2–3.5 and Lemma 3.2, we can obtain the following theorem which settles Substep 1.1.

Theorem 3.1. *Let T_i $(i = 1, \ldots, 14)$ (Fig. 2) be a unicyclic graph on n $(n \ge 10)$ vertices. Then*

$$\mu(T_i) < \mu(G_{10}) \quad (i = 1, \ldots, 14).$$

Proof. By using the operation of "grafting pendant edges" in Lemma 3.4 (for the case $l = k = 2$), we can see that T_1 can be transformed to T_{13}. So by Lemma 3.4 we have

$$\mu(T_{13}) \le \mu(T_1).$$

Also from Proposition 3.5, we have

$$\mu(T_i) < n - 2 < \mu(G_{10}) \quad (i = 3, \ldots, 12).$$

So by combining these two relations with Propositions 3.2–3.4, we have

$$\mu(T_i) < \mu(G_{10}) \quad (i = 1, \ldots, 14). \quad \square$$

4. The exclusions of the unicyclic graphs not in $\{G_1, \ldots, G_{10}\}$

For any connected graph G, let $C(G)$ be the graph obtained from G by contracting all pendant edges of G. It is easy to see that $C(G)$ is also a unicyclic graph if G is. Sometimes $C(G)$ is called the condensed graph of G.

In this section we will settle Substep 1.2. For this purpose, we will consider different cases according to the value of $d_1 + d_2$, and according to the degree sequence $\pi(G)$ and the condensed graph $C(G)$.

Let $\pi(G) = (d_1, d_2, \ldots, d_n)$ be the degree sequence of a unicyclic graph G on n vertices where $d_1 \geq d_2 \geq \cdots \geq d_n$. Then we have $d_1 + \cdots + d_n = 2n$, since G is unicyclic. Also by Lemma 3.1, we have

$$d_1 + d_2 \leq n + 1.$$

Now if $d_1 + d_2 \leq n - 2$, then by Lemma 3.3 and Proposition 3.1, we have

$$\mu(G) \leq d_1 + d_2 \leq n - 2 < \mu(G_{10})$$

as desired. So in what follows we may assume that $n - 1 \leq d_1 + d_2 \leq n + 1$, namely,

$$d_1 + d_2 = \{n - 1, n, n + 1\}. \tag{4.1}$$

We first consider the case $d_1 + d_2 = n + 1$.

Theorem 4.1. *If G is a unicyclic graph on n $(n \geq 10)$ vertices with $d_1 + d_2 = n + 1$ and $G \notin \{G_1, \cdots, G_{10}\}$. Then*

$$\mu(G) < \mu(G_{10}).$$

Proof. Since $d_1 + d_2 = n + 1$, we have $d_3 + \cdots + d_n = n - 1$. Thus

$$\pi(G) = (d_1, d_2, 2, 1, \ldots, 1).$$

So $C(G) = C_3$ and

$$G = U(d_1 - 2, d_2 - 2, 0).$$

But $G \notin \{G_1, G_3, G_7\}$, so $d_2 - 2 \geq 3$.

Observe that the graph obtained from G by moving all but three pendant edges at v to u and the graph obtained from G by moving all but three pendant edges at u to v are both isomorphic to $U(n-6, 3, 0)$, where $d(u) = d_1$, $d(v) = d_2$. So by Corollary 2.1 and Lemma 3.2, we have

$$\mu(G) \leq \mu(U(n - 6, 3, 0)) \leq n - 3 + \frac{5}{n - 4} < n - 2 < \mu(G_{10}). \quad \square$$

Secondly, we consider the case $d_1 + d_2 = n$.

Theorem 4.2. *If G is a unicyclic graph on n $(n \geq 10)$ vertices with $d_1 + d_2 = n$ and $G \notin \{G_1, \ldots, G_{10}\}$. Then*

$$\mu(G) < \mu(G_{10}).$$

Proof. Since $d_1 + d_2 = n$, we have $d_3 + \cdots + d_n = n$ and so

$$\pi(G) = (d_1, d_2, 3, 1, \ldots, 1) \quad \text{or} \quad (d_1, d_2, 2, 2, 1, \ldots, 1).$$

We consider the following two cases.

Case 1: $\pi(G) = (d_1, d_2, 3, 1, \ldots, 1)$.

Then we must have $d_2 \geq 3$ and

$$G = U(d_1 - 2, d_2 - 2, 1).$$

Observe that the graph obtained from G by moving all but one pendant edges at v to u and the graph obtained from G by moving all but one pendant edges at u to v are both isomorphic to $U(n-5, 1, 1)$, where $d(u) = d_1$ and $d(v) = d_2$. So by Corollary 2.1 and Proposition 3.2, we have

$$\mu(G) \leq \mu(U(n - 5, 1, 1)) < \mu(G_{10}).$$

Fig. 3. The graphs $A1$ and $A2$.

Case 2: $\pi(G) = (d_1, d_2, 2, 2, 1, \dots, 1)$.

Then the condensed graph $C(G)$ of G is a unicyclic graph of order 4. So

$$C(G) = U(1, 0, 0) \quad \text{or} \quad C_4.$$

Subcase 2.1: $C(G) = U(1, 0, 0)$.

Then $d_2 \geq 3$ since $G \neq G_4$.

Subcase 2.1.1: There is only one vertex on the cycle having degree 2.

Then G is of the type A1 (Fig. 3).

If $d(u) \geq 4$, then $G = U(R(d(u) - 3, 1), d(v) - 2, 0)$.

Now the graph obtained from G by moving all but one pendant edges at v to u and the graph obtained from G by moving all but one pendant edge among all the pendant paths at u to v are both isomorphic to $U(R(n-6, 1), 1, 0) = T_2$. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_2) < \mu(G_{10}).$$

If $d(u) = 3$, then we have $G = U(R(0, 1), n - 5, 0) = T_{14}$, so by Theorem 3.1, we have

$$\mu(G) = \mu(T_{14}) < \mu(G_{10}).$$

Subcase 2.1.2: There are two vertices on the cycle having degree 2.

Then G is of the type A2 (Fig. 3). Also $d_2 \geq 4$ since $G \notin \{G_4, G_9, G_{10}\}$.

If $|x_u| \geq |x_v|$, then the graph obtained from G by moving all but three pendant edges at v to u is isomorphic to $U(R(n-7, 3), 0, 0) = T_5$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_5) < \mu(G_{10}).$$

If $|x_u| \leq |x_v|$, then the graph obtained from G by moving all but one pendant edges at u to v is isomorphic to $U(R(1, n-5), 0, 0) = T_8$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_8) < \mu(G_{10}).$$

Subcase 2.2: $C(G) = C_4$.

Then G is either $U(d_1 - 2, d_2 - 2, 0, 0)$ or $U(d_1 - 2, 0, d_2 - 2, 0)$.

Since $G \notin \{G_2, G_5, G_8\}$, we have $d_2 \geq 4$.

Subcase 2.2.1: If $G = U(d_1 - 2, d_2 - 2, 0, 0)$, then the graph obtained from G by moving all but two pendant edges at v to u and the graph obtained from G by moving all but two pendant edges at u to v are both isomorphic to $U(n-6, 2, 0, 0)$, where $d(u) = d_1, d(v) = d_2$. So by Corollary 2.1 and Lemma 3.2, we have

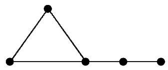
$$\mu(G) \leq \mu(U(n-6, 2, 0, 0)) \leq n - 3 + \frac{4}{n-4} < n - 2 < \mu(G_{10}).$$

Subcase 2.2.2: If $G = U(d_1 - 2, 0, d_2 - 2, 0)$, then the graph obtained from G by moving all but two pendant edges at v to u and the graph obtained from G by moving all but two pendant edges at u to v are both isomorphic to $U(n-6, 0, 2, 0)$, where $d(u) = d_1, d(v) = d_2$. So by Corollary 2.1 and Lemma 3.2, we have

$$\mu(G) \leq \mu(U(n-6, 0, 2, 0)) \leq n - 3 + \frac{2}{n-4} < n - 2 < \mu(G_{10}).$$

So combining Cases 1, 2, we have

$$\mu(G) < \mu(G_{10}). \quad \square$$



$U(R(0,\ 1),\ 0,\ 0)$

Fig. 4. The graph $U(R(0, 1), 0, 0)$.

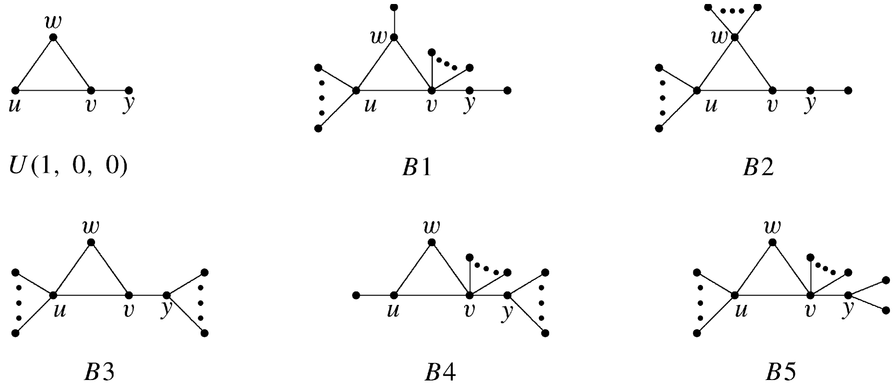


Fig. 5. The graphs $U(1, 0, 0)$ and $B1$–$B5$.

Thirdly, we consider the case $d_1 + d_2 = n - 1$.

Let $G \in U_n$ with $d_1 + d_2 = n - 1$, then we have $d_3 + \cdots + d_n = n + 1$ and so

$$\pi(G) = (d_1, d_2, 4, 1, \ldots, 1) \quad \text{or} \quad (d_1, d_2, 3, 2, 1, \ldots, 1) \quad \text{or} \quad (d_1,\ d_2, 2, 2, 2, 1, \ldots, 1).$$

(a) If $\pi(G) = (d_1, d_2, 4, 1, \ldots, 1)$, then the condensed graph $C(G) = C_3$ and so $G = U(d_1 - 2, d_2 - 2, 2)$;

(b) If $\pi(G) = (d_1, d_2, 3, 2, 1, \ldots, 1)$, then the condensed graph $C(G)$ is a unicyclic graph of order 4, so $C(G) = U(1, 0, 0)$ or C_4;

(c) If $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$, then the condensed graph $C(G)$ is a unicyclic graph of order 5, and so

$$C(G) \in \{U(2, 0, 0), U(1, 1, 0), U(R(0, 1), 0, 0), U(1, 0, 0, 0), C_5\}, \tag{4.2}$$

where $U(R(0, 1), 0, 0)$ is the graph of order 5 obtained by identifying one vertex of C_3 with one end vertex of P_3 (see Fig. 4).

These cases will be considered in Lemmas 4.1–4.4 and Theorem 4.3, respectively.

In what follows, $d_G(v)$ will denote the degree of the vertex v in the graph G.

Lemma 4.1. *If G is a unicyclic graph of order n ($n \geq 10$) with $\pi(G) = (d_1, d_2, 3, 2, 1, \ldots, 1)$ and $C(G) = U(1, 0, 0)$, then*

(1) *G is of one of the types $B1$–$B5$ as shown in Fig. 5.*

(2) $\mu(G) < \mu(G_{10})$.

Proof. Suppose $C(G) = U(1, 0, 0)$ as shown in Fig. 5.

(1) If $d_G(y) = 2$ and $d_G(v) \geq 4$ (then $d_G(u) = 3$ or $d_G(w) = 3$), then G is of the type $B1$;
If $d_G(y) = 2$ and $d_G(v) = 3$, then G is of the type $B2$;
If $d_G(w) = 2$ (or $d_G(u) = 2$) and $d_G(v) = 3$, then G is of the type $B3$;
If $d_G(w) = 2$ and $d_G(u) = 3$ (or $d_G(u) = 2$ and $d_G(w) = 3$), then G is of the type $B4$;
If $d_G(w) = 2$ (or $d_G(u) = 2$) and $d_G(y) = 3$, then G is of the type $B5$.

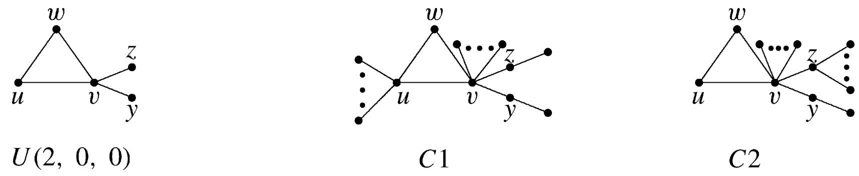


Fig. 6. The graphs $U(2, 0, 0)$, $C1$ and $C2$.

(2) Since $\pi(G) = (d_1, d_2, 3, 2, 1, \ldots, 1)$, then we have $d_2 \geq 3$.

Case 1: If G is of the type $B1$, then the graph obtained from G by moving all the pendant edges at u to v and the graph obtained from G by moving all the pendant paths at v to u are both isomorphic to $U(R(n-6, 1), 1, 0) = T_2$. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_2) < \mu(G_{10}).$$

Case 2: If G is of the type $B2$, then the graph obtained from G by moving all the pendant edges at u to w and the graph obtained from G by moving all the pendant edges at w to u are both isomorphic to $U(R(0, 1), n-5, 0) = T_{14}$. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_{14}) < \mu(G_{10}).$$

Case 3: Suppose that G is of the type $B3$.

If $|x_u| \geq |x_y|$, then the graph obtained from G by moving all but one pendant edges at y to u is isomorphic to $U(R(0, 1), n-5, 0) = T_{14}$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_{14}) < \mu(G_{10}).$$

If $|x_u| \leq |x_y|$, then the graph obtained from G by moving all but one pendant edges at u to y is isomorphic to $U(R(0, n-5), 1, 0) = T_9$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_9) < \mu(G_{10}).$$

Case 4: Suppose that G is of the type $B4$.

If $|x_v| \geq |x_y|$, then the graph obtained from G by moving all but one pendant edges at y to v is isomorphic to $U(R(n-6, 1), 1, 0) = T_2$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_2) < \mu(G_{10}).$$

If $|x_v| \leq |x_y|$, then the graph obtained from G by moving all the pendant edges at v to y is isomorphic to $U(R(0, n-5), 1, 0) = T_9$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_9) < \mu(G_{10}).$$

Case 5: Suppose that G is of the type $B5$.

If $|x_u| \geq |x_v|$, then the graph obtained from G by moving all the pendant edges at v to u is isomorphic to $U(R(0, 2), n-6, 0) = T_{10}$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_{10}) < \mu(G_{10}).$$

If $|x_u| \leq |x_v|$, then the graph obtained from G by moving all but one pendant edges at u to v is isomorphic to $U(R(n-7, 2), 1, 0) = T_6$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_6) < \mu(G_{10}).$$

So combining Cases 1–5, we have

$$\mu(G) < \mu(G_{10}). \quad \square$$

Lemma 4.2. *If G is a unicyclic graph of order n ($n \geq 10$) with $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U(2, 0, 0)$, then*

(1) *G is of one of the types $C1$, $C2$ as shown in Fig. 6.*

(2) $\mu(G) < \mu(G_{10})$.

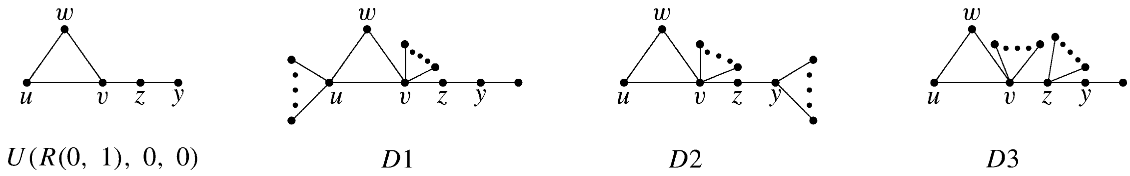


Fig. 7. The graphs $U(R(0,1),0,0)$ and $D1$–$D3$.

Proof. Suppose $C(G) = U(2,0,0)$ as shown in Fig. 6.

(1) If $d_G(y) = d_G(z) = 2$ and $d_G(w) = 2$ (or $d_G(u) = 2$), then G is of the type $C1$;
If $d_G(u) = d_G(w) = 2$ and $d_G(y) = 2$ (or $d_G(z) = 2$), then G is of the type $C2$.
(2) Since $d_3 = 2$, we have $d_2 \geq 2$.

Case 1: G is of the type $C1$.

Observe that the graph obtained from G by moving all the pendant edges at u to v and the graph obtained from G by moving all the pendant paths at v to u are both isomorphic to T_1. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_1) < \mu(G_{10}).$$

Case 2: G is of the type $C2$.

From Figs. 6 and 3 it is not difficult to see that for any graph G of the type $C2$, there exists some graph G' of the type $A2$ such that G' can be transformed to G by using the operation of "grafting pendant edges". So by Lemma 3.4 and the Subcase 2.1.2 of Theorem 4.2, we have

$$\mu(G) \leq \mu(G') < \mu(G_{10}).$$

So combining Cases 1, 2, we have

$$\mu(G) < \mu(G_{10}). \quad \square$$

Lemma 4.3. *If G is a unicyclic graph of order n ($n \geq 10$) with $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U(R(0,1),0,0)$, then*

(1) *G is of one of the types $D1$–$D3$ as shown in Fig. 7.*
(2) $\mu(G) < \mu(G_{10})$.

Proof. Suppose $C(G) = U_3(R(0,1),0,0)$ as shown in Fig. 7.

(1) If $d_G(y) = d_G(z) = d_G(w) = 2$ (or $d_G(y) = d_G(z) = d_G(u) = 2$), then G is of the type $D1$;
If $d_G(u) = d_G(w) = d_G(z) = 2$, then G is of the type $D2$;
If $d_G(u) = d_G(w) = d_G(y) = 2$, then G is of the type $D3$.
(2) We consider the following cases.

Case 1: G is of the type $D1$.

Observe that the graph obtained from G by moving all the pendant edges at u to v and the graph obtained from G by moving all the pendant paths at v to u are both isomorphic to T_{13}. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_{13}) < \mu(G_{10}).$$

Case 2: G is of the type $D2$.

If $|x_v| \geq |x_y|$, then the graph obtained from G by moving all but one pendant edges at y to v is isomorphic to T_{13}. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_{13}) < \mu(G_{10}).$$

If $|x_v| \leq |x_y|$, then the graph obtained from G by moving all the pendant edges at v to y is isomorphic to T_{11}. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_{11}) < \mu(G_{10}).$$

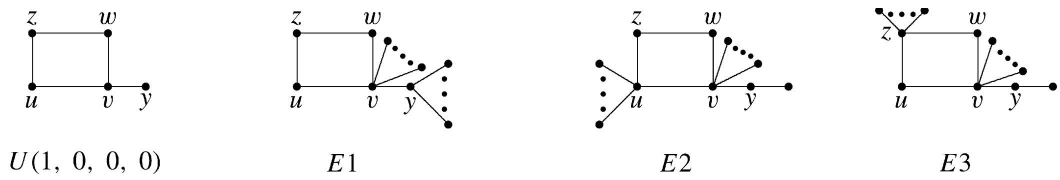


Fig. 8. The graphs $U(1,0,0,0)$ and $E1$–$E3$.

Case 3: G is of the type $D3$.

From Figs. 7 and 3 it is not difficult to see that for any graph G of the type $D3$, there exists some graph G' of the type $A2$ such that G' can be transformed to G by using the operation of "grafting pendant edges". So by Lemma 3.4 and the Subcase 2.1.2 of Theorem 4.2, we have

$$\mu(G) \le \mu(G') < \mu(G_{10}).$$

Combining Cases 1–3, we have

$$\mu(G) < \mu(G_{10}). \quad \square$$

Lemma 4.4. *Let G be a unicyclic graph of order n ($n \ge 10$) with $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U(1,0,0,0)$, then*

(1) *G is of one of the types $E1$–$E3$ as shown in Fig. 8.*
(2) *If $G \ne G_6$, then $\mu(G) < \mu(G_{10})$.*

Proof. Suppose $C(G) = U(1,0,0,0)$ as shown in Fig. 8.

(1) If $d_G(z) = d_G(u) = d_G(w) = 2$, then G is of the type $E1$;
If $d_G(y) = d_G(w) = d_G(z) = 2$ (or $d_G(y) = d_G(u) = d_G(z) = 2$), then G is of the type $E2$;
If $d_G(u) = d_G(w) = d_G(y) = 2$, then G is of the type $E3$.
(2) Since $G \ne G_6$, then we have $d_2 \ge 3$.

Case 1: G is of the type $E1$.

If $|x_v| \ge |x_y|$, then the graph obtained from G by moving all but two pendant edges at y to v is isomorphic to $U(R(n-7,2),0,0,0) = T_7$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \le \mu(T_7) < \mu(G_{10}).$$

If $|x_v| \le |x_y|$, then the graph obtained from G by moving all the pendant edges at v to y is isomorphic to $U(R(0,n-5),0,0,0) = T_{12}$. So by Lemma 2.1 and Theorem 3.1, we have

$$\mu(G) \le \mu(T_{12}) < \mu(G_{10}).$$

Case 2: G is of the type $E2$.

If $d(v) \ge 4$, then the graph obtained from G by moving all but one pendant edges at u to v and the graph obtained from G by moving all but one pendant edge among all the pendant paths at v to u are both isomorphic to $U(R(n-7,1),1,0,0) = T_3$. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \le \mu(T_3) < \mu(G_{10}).$$

If $d(v) = 3$, then $G = U(R(0,1), n-6, 0, 0)$. So by Lemma 3.2, we have

$$\mu(G) \le n - 3 + \frac{3}{n-4} < n - 2 < \mu(G_{10}).$$

Case 3: G is of the type $E3$.

If $d(v) \ge 4$, then the graph obtained from G by moving all but one pendant edges at z to v and the graph obtained from G by moving all but one pendant edge among all the pendant paths at v to z are both isomorphic to $U(R(n-7,1),0,1,0) = T_4$. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \le \mu(T_4) < \mu(G_{10}).$$

If $d(v) = 3$, then $G = U(R(0, 1), 0, n - 6, 0)$. So by Lemma 3.2, we have

$$\mu(G) \le n - 3 + \frac{2}{n-4} < n - 2 < \mu(G_{10}).$$

So combining Cases 1–3, we have

$$\mu(G) < \mu(G_{10}). \quad \square$$

Theorem 4.3. *If G is a unicyclic graph on n $(n \ge 10)$ vertices with $d_1 + d_2 = n - 1$ and $G \notin \{G_1, \ldots, G_{10}\}$, then*

$$\mu(G) < \mu(G_{10}).$$

Proof. We will divide the proof into eight cases according to the degree sequence $\pi(G)$ and the condensed graph $C(G)$.

Case 1: $\pi(G) = (d_1, d_2, 4, 1, \ldots, 1)$.

Then we have $d_2 \ge 4$ and $G = U(d_1 - 2, d_2 - 2, 2)$.

Observe that the graph obtained from G by moving all but one pendant edges at v to u and the graph obtained from G by moving all but one pendant edges at u to v are both isomorphic to $U(n - 6, 2, 1)$, where $d(u) = d_1, d(v) = d_2$. So by Corollary 2.1 and Lemma 3.2, we have

$$\mu(G) \le \mu(U(n - 6, 2, 1)) \le n - 3 + \frac{5}{n-4} < n - 2 < \mu(G_{10}).$$

Case 2: $\pi(G) = (d_1, d_2, 3, 2, 1, \ldots, 1)$ and $C(G) = U(1, 0, 0)$.

By Lemma 4.1, we have $\mu(G) < \mu(G_{10})$.

Case 3: $\pi(G) = (d_1, d_2, 3, 2, 1, \ldots, 1)$ and $C(G) = C_4$.

Then we have $d_2 \ge 3$ and

$$G = U(d_1 - 2, d_2 - 2, 0, 1) \quad \text{or} \quad U(d_1 - 2, 1, d_2 - 2, 0).$$

Subcase 3.1: $G = U(d_1 - 2, d_2 - 2, 0, 1)$.

Suppose that $d(u) = d_1, d(v) = d_2$.

If $|x_u| \ge |x_v|$, then the graph obtained from G by moving all but one pendant edges at v to u is isomorphic to $U(n - 6, 1, 0, 1)$. So by Corollary 2.1 and Lemma 3.2, we have

$$\mu(G) \le \mu(U(n - 6, 1, 0, 1)) \le n - 3 + \frac{4}{n-4} < n - 2 < \mu(G_{10}).$$

If $|x_u| \le |x_v|$, then the graph obtained from G by moving all but one pendant edges at u to v is isomorphic to $U(n - 6, 0, 1, 1)$. So by Corollary 2.1 and Lemma 3.2, we have

$$\mu(G) \le \mu(U(n - 6, 0, 1, 1)) \le n - 3 + \frac{3}{n-4} < n - 2 < \mu(G_{10}).$$

Subcase 3.2: $G = U(d_1 - 2, 1, d_2 - 2, 0)$.

Observe that the graph obtained from G by moving all but one pendant edges at v to u and the graph obtained from G by moving all but one pendant edges at u to v are both isomorphic to $U(n-6, 0, 1, 1)$, where $d(u) = d_1, d(v) = d_2$. So by Corollary 2.1 and Lemma 3.2, we have

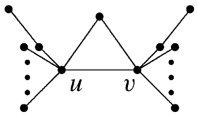
$$\mu(G) \le \mu(U(n - 6, 0, 1, 1)) \le n - 3 + \frac{3}{n-4} < n - 2 < \mu(G_{10}).$$

Case 4: $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U(2, 0, 0)$.

By Lemma 4.2, we have $\mu(G) < \mu(G_{10})$.

Case 5: $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U(1, 1, 0)$.

Then G is of the type $F = U(R(d(u) - 3, 1), R(d(v) - 3, 1), 0)$ as shown in Fig. 9, so $d_2 \ge 3$.



$F = U(R(d(u) - 3,\ 1),\ R(d(v) - 3,\ 1),\ 0)$

Fig. 9. The graph F.

Observe that the graph obtained from G by moving all the pendant paths at u to v and the graph obtained from G by moving all the pendant paths at v to u are both isomorphic to T_1. So by Corollary 2.1 and Theorem 3.1, we have

$$\mu(G) \leq \mu(T_1) < \mu(G_{10}).$$

Case 6: $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U_3(R(0, 1), 0, 0)$.
By Lemma 4.3, we have $\mu(G) < \mu(G_{10})$.

Case 7: $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = U(1, 0, 0, 0)$.
By Lemma 4.4, we have $\mu(G) < \mu(G_{10})$.

Case 8: $\pi(G) = (d_1, d_2, 2, 2, 2, 1, \ldots, 1)$ and $C(G) = C_5$.
Then we have

$$G = U(d_1 - 2, d_2 - 2, 0, 0, 0) \quad \text{or} \quad U(d_1 - 2, 0, d_2 - 2, 0, 0).$$

Observe that the graph obtained from G by moving all the pendant edges at u to v and the graph obtained from G by moving all the pendant edges at v to u are both isomorphic to $U(n-5, 0, 0, 0, 0)$, where $d(u) = d_1,\ d(v) = d_2$. So by Corollary 2.1 and Proposition 3.2, we have

$$\mu(G) \leq \mu(U(n-5, 0, 0, 0, 0)) < \mu(G_{10}).$$

So combining Cases 1–8, we obtain the desired result. □

Combining Theorems 4.1–4.3, we immediately obtain the following main result of this section.

Theorem 4.4. *If G is a unicyclic graph on n ($n \geq 10$) vertices and $G \notin \{G_1, \ldots, G_{10}\}$, then*

$$\mu(G) < \mu(G_{10}).$$

5. The ordering of the graphs in G_5–G_{10}

In this section, we will settle Step 2. Namely we will show that

$$\mu(G_{10}) = \mu(G_9) < \mu(G_8) < \mu(G_7) < \mu(G_6) < \mu(G_5).$$

Theorem 5.1. *For $n \geq 4$, we have*

$$\mu(G_{10}) = \mu(G_9) < \mu(G_8).$$

Proof. By Lemma 3.5, we can see that

$$\mu(G_8) > \Delta(G_8) + 1 = n - 2.$$

It is not difficult to calculate recursively that

$$\Phi(G_8; \lambda) = \lambda(\lambda - 2)(\lambda - 1)^{n-6} h_8(\lambda), \tag{5.1}$$

where

$$h_8(\lambda) = \lambda^4 - (n+4)\lambda^3 + (6n-4)\lambda^2 - (8n-12)\lambda + 2n.$$

By Proposition 3.1, we have

$$\mu(G_9) = \mu(G_{10}).$$

By (3.1) we have

$$\Phi(G_{10}; \lambda) - \Phi(G_8; \lambda) = \lambda(\lambda - 1)^{n-6} g_2(\lambda),$$

where

$$g_2(\lambda) = 2\lambda^2 - (2n - 3)\lambda + n = (2\lambda - 1)[\lambda - (n - 2)] + 2.$$

Thus we have $g_2(\lambda) > 0$ if $\lambda \geq n - 2$. So for $\lambda \geq n - 2$, we have

$$\Phi(G_{10}; \lambda) - \Phi(G_8; \lambda) = \lambda(\lambda - 1)^{n-6} g_2(\lambda) > 0.$$

So we have

$$\mu(G_{10}) = \mu(G_9) < \mu(G_8). \quad \square$$

By using a similar method as in Theorem 5.1, we can prove the following theorems.

Theorem 5.2. *For $n \geq 6$, we have*

$$\mu(G_8) < \mu(G_7).$$

Proof. It is not difficult to calculate recursively that

$$\Phi(G_7; \lambda) = \lambda(\lambda - 1)^{n-5} h_7(\lambda),$$

where

$$h_7(\lambda) = \lambda^4 - (n + 5)\lambda^3 + (7n - 3)\lambda^2 - (11n - 17)\lambda + 3n.$$

Then by (5.1), we have

$$\Phi(G_8; \lambda) - \Phi(G_7; \lambda) = \lambda(\lambda - 1)^{n-6} g_3(\lambda), \tag{5.2}$$

where

$$g_3(\lambda) = 2\lambda^3 - 2n\lambda^2 + (4n - 7)\lambda - n.$$

Now we have

$$\begin{aligned} 2h_8(\lambda) &= 2\lambda^4 - 2(n + 4)\lambda^3 + 2(6n - 4)\lambda^2 - 2(8n - 12)\lambda + 4n \\ &= (\lambda - 4)[2\lambda^3 - 2n\lambda^2 + (4n - 7)\lambda - n] - \lambda^2 + (n - 4)\lambda \\ &= (\lambda - 4)g_3(\lambda) - \lambda[\lambda - (n - 4)] \end{aligned}$$

and $\mu(G_8) > \mu(G_{10}) > n - 2$ by Theorem 5.1 and Proposition 3.1, so for $n \geq 6$,

$$g_3(\mu(G_8)) > 0.$$

Thus from (5.2), we have

$$\Phi(G_7; \mu(G_8)) < 0.$$

So we have $\mu(G_8) < \mu(G_7)$ as desired. $\square$

Theorem 5.3. *For $n \geq 10$, we have*

$$\mu(G_7) < \mu(G_6).$$

Proof. By Lemma 3.5, we can see that

$$\mu(G_7) > \Delta(G_7) + 1 = n - 2,$$

and also that $\mu(G_7)$ is the largest root of $h_7(\lambda) = 0$. Since for $n \geq 10$,

$$h_7(0) = 3n > 0, \qquad h_7(1) = -2(n-5) < 0,$$
$$h_7(2) = n - 2 > 0, \qquad h_7(n-2) = -2(n-5) < 0,$$
$$h_7\left(n - \frac{7}{4}\right) = \frac{1}{256}(64n^3 - 784n^2 + 2348n - 707) > 0,$$

we have $\mu(G_7) < n - \frac{7}{4}$.

It is not difficult to calculate recursively that

$$\Phi(G_6; \lambda) = \lambda(\lambda - 2)(\lambda - 1)^{n-7} h_6(\lambda), \tag{5.3}$$

where

$$h_6(\lambda) = \lambda^5 - (n+5)\lambda^4 + (7n+1)\lambda^3 - (15n-17)\lambda^2 + (10n-8)\lambda - 2n.$$

Now we have

$$\Phi(G_6; \lambda) - \Phi(G_7; \lambda) = \lambda(\lambda - 1)^{n-7} g_4(\lambda),$$

where

$$g_4(\lambda) = 3\lambda^4 - (3n+3)\lambda^3 + (8n-5)\lambda^2 - (5n+1)\lambda + n.$$

Then

$$g_4'(\lambda) = 12\lambda^3 - 9(n+1)\lambda^2 + 2(8n-5)\lambda - (5n+1).$$

It is easy to calculate that for $n \geq 10$

$$g_4'(0) = -(5n+1) < 0, \qquad g_4'(1) = 2(n-4) > 0, \qquad g_4'(3) = -3(3n-13) < 0,$$
$$g_4'(n-2) = 3n^3 - 29n^2 + 97n - 113 > 0.$$

It follows that $g_4'(\lambda) > 0$ for all $\lambda \geq n-2$ (for otherwise $g_4'(\lambda)$ would have at least 4 different roots, a contradiction). So $g_4(\lambda)$ is an increasing function in $[n-2, \infty)$. But $\mu(G_7) < n - \frac{7}{4}$ and

$$g_4\left(n - \frac{7}{4}\right) = -\frac{1}{256}(64n^3 - 1360n^2 + 6412n - 7847) < 0,$$

so $g_4(\mu(G_7)) < 0$. Thus

$$\Phi(G_6; \mu(G_7)) = \mu(G_7)[\mu(G_7) - 1]^{n-7} g_4(\mu(G_7)) < 0.$$

So we have

$$\mu(G_7) < \mu(G_6). \quad \square$$

Theorem 5.4. *For $n \geq 5$, we have*

$$\mu(G_6) < \mu(G_5).$$

Proof. By Lemmas 3.2 and 3.5, we have

$$n - 2 = \Delta(G_5) + 1 < \mu(G_5) < n - 1,$$
$$n - 2 = \Delta(G_6) + 1 < \mu(G_6) < n - 1.$$

It is not difficult to calculate recursively that

$$\Phi(G_5; \lambda) = \lambda(\lambda - 1)^{n-5} h_5(\lambda), \tag{5.4}$$

where

$$h_5(\lambda) = \lambda^4 - (n+5)\lambda^3 + (7n-1)\lambda^2 - (13n-19)\lambda + 4n.$$

By (5.3), we have

$$\Phi(G_6;\lambda) - \Phi(G_5;\lambda) = \lambda^2(\lambda-1)^{n-7} g_5(\lambda),$$

where

$$g_5(\lambda) = \lambda^3 - (n+1)\lambda^2 + (3n-3)\lambda - n - 3 = [\lambda - (n-2)](\lambda^2 - 3\lambda + 3) + 2n - 9. \tag{5.5}$$

So $g_5(\lambda) > 0$ if $\lambda \geq n-2$. Thus from (5.5) if $\lambda \geq n-2$, we have

$$\Phi(G_6;\lambda) - \Phi(G_5;\lambda) = \lambda^2(\lambda-1)^{n-7} g_5(\lambda) > 0.$$

So we have

$$\mu(G_6) < \mu(G_5).$$

Combining Theorem 4.4, Theorems 5.1–5.4 and [1], we can obtain our main result of this paper.

Theorem 5.5. *If G is a unicyclic graph of order $n \geq 10$, G_1–G_{10} are graphs as shown in Fig. 1, then*

(1) $\mu(G) < \mu(G_{10})$, *for any* $G \notin \{G_1, \ldots, G_{10}\}$.
(2) $\mu(G_{10}) = \mu(G_9) < \mu(G_8) < \mu(G_7) < \mu(G_6) < \mu(G_5) < \mu(G_4) < \mu(G_3) < \mu(G_2) < \mu(G_1)$.
(3) $\mu(G_9) = \mu(G_{10})$ *is the largest real root of the equation* $h(\lambda) = 0$, *where*

$$h(\lambda) = \lambda^3 - (n+2)\lambda^2 + (4n-7)\lambda - n$$

and $\mu(G_i)$ *is the largest real root of the equation* $h_i(\lambda) = 0$ $(i = 5, \ldots, 8)$ *respectively, where*

$$h_5(\lambda) = \lambda^4 - (n+5)\lambda^3 + (7n-1)\lambda^2 - (13n-19)\lambda + 4n,$$
$$h_6(\lambda) = \lambda^5 - (n+5)\lambda^4 + (7n+1)\lambda^3 - (15n-17)\lambda^2 + (10n-8)\lambda - 2n,$$
$$h_7(\lambda) = \lambda^4 - (n+5)\lambda^3 + (7n-3)\lambda^2 - (11n-17)\lambda + 3n,$$
$$h_8(\lambda) = \lambda^4 - (n+4)\lambda^3 + (6n-4)\lambda^2 - (8n-12)\lambda + 2n.$$

Acknowledgement

The authors would like to thank the referee for many helpful comments and suggestions on an earlier version of this paper.

References

[1] S.G. Guo, The largest Laplacian spectral radius of unicyclic graph, Appl. Math. J. Chinese Univ. Ser. A. 16 (2) (2001) 131–135.
[2] J.M. Guo, The Laplacian spectral radius of a graph under perturbation, Comput. Math. Appl. 54 (5) (2007) 709–720.
[3] R. Merris, A note on Laplacian graph eigenvalues, Linear Algebra Appl. 285 (1998) 33–35.
[4] J.S. Li, X.D. Zhang, A new upper bound for eigenvalues of Laplacian matrix of a graph, Linear Algebra Appl. 265 (1997) 93–100.
[5] J.M. Guo, The effect on the Laplacian spectral radius of a graph by adding or grafting edges, Linear Algebra Appl. 413 (2006) 59–71.
[6] R. Grone, R. Merris, The Laplacian spectrum of graph II, SIAM J. Discrete Math. 7 (1994) 221–229.
[7] R. Merris, Laplacian matrices of graphs: A survey, Linear Algebra Appl. 197–198 (1994) 143–176.