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# On the spectral radius of unicyclic graphs with perfect matchings

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#### Abstract

Let  $\mathcal{U}^+(2k)$  be the set of all unicyclic graphs on 2k ( $k \ge 2$ ) vertices with perfect matchings. Let  $U_{2k}^1$  be the graph on 2k vertices obtained from  $C_3$  by attaching a pendant edge and k-2 paths of length 2 at one vertex of  $C_3$ ; Let  $U_{2k}^2$  be the graph on 2k vertices obtained from  $C_3$  by adding a pendant edge at each vertex together with k-3 paths of length 2 at one of three vertices. In this paper, we prove that  $U_{2k}^1$  and  $U_{2k}^2$  have the largest and the second largest spectral radius among the graphs in  $\mathcal{U}^+(2k)$  when  $k \ne 3$ . © 2003 Elsevier Inc. All rights reserved.

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#### 1. Introduction

We discuss only finite undirected graphs without loops or multiple edges. Let G be a graph with n vertices, and let A(G) be a (0, 1)-adjacency matrix of G. Since

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A(G) is symmetric, its eigenvalues are real. These eigenvalues of A(G) are independent of the ordering of the vertices of G, and consequently, without loss of generality, we can write them in decreasing order as  $\lambda_1(G) \ge \lambda_2(G) \ge \lambda_3(G) \ge \cdots \ge \lambda_n(G)$  and call them the eigenvalues of G. The characteristic polynomial of G is just **Det**( $\lambda I - A(G)$ ), denoted by  $P(G; \lambda)$ . The largest eigenvalue  $\lambda_1(G)$  is called the spectral radius of G. If G is connected, then A(G) is irreducible and so by the Perron–Frobenius theory of non-negative matrices  $\lambda_1(G)$  has multiplicity one and there exists a unique positive unit eigenvector corresponding to  $\lambda_1(G)$ .

Unicyclic graphs are connected graphs in which the number of edges equals the number of vertices. A unicyclic graph is either a cycle or a cycle with trees attached. Let  $\mathcal{U}(n)$  and  $\mathcal{U}^+(2k)$  denote the set of all unicyclic graphs on *n* vertices and the set of all unicyclic graphs with perfect matchings on 2k vertices, respectively. The eigenvalues of graphs in  $\mathcal{U}(n)$  have been studied by several authors (see [1–6]). In particular, the following result on the spectral radius of a graph in  $\mathcal{U}(n)$  may be found in several papers (see [1–3]).

**Theorem 1.1.** Let  $S_n^*$  denote the graph obtained from the star  $S_n$  on n vertices by joining any two vertices of degree 1 in  $S_n$ . Among the graphs in  $\mathcal{U}(n)$ , the graph  $S_n^*$  alone has the largest spectral radius and the cycle  $C_n$  alone has the smallest spectral radius.

One may formulate Theorem 1.1 in the following way.

**Corollary 1.1** [3]. *Let* G *be a graph in*  $\mathcal{U}(n)$ *. Then* 

 $2 \leq \lambda_1(G) \leq \sqrt{n}$  when  $n \geq 9$ 

and the second equality is attained if and only if n = 9.

The second statement in Theorem 1.1 also holds for the graphs in  $\mathcal{U}^+(2k)$ . Accordingly we have an immediate consequence: the cycle  $C_{2k}$  alone has the smallest spectral radius among the graphs in  $\mathcal{U}^+(2k)$ . But the graph  $S_{2k}^*$  does not belong to  $\mathcal{U}^+(2k)$  except for  $S_4^*$  (in the case k = 2,  $S_4^*$  is the unique graph with the largest spectral radius in  $\mathcal{U}^+(4)$ ). In fact, very little is known about the eigenvalues of graphs in  $\mathcal{U}^+(2k)$  for the present. The purpose of this paper is to find the upper bound for the spectral radius of graphs in  $\mathcal{U}^+(2k)$  by searching for the graphs with the largest spectral radius in  $\mathcal{U}^+(2k)$ .

# 2. Preliminaries

We denote by  $K_n$ ,  $S_n$ ,  $C_n$  and  $P_n$  the complete graph, the star, the cycle, and the path, respectively, each on *n* vertices, and denote by rG the disjoint union of *r* copies of the graph *G*. If a graph *G* has components  $G_1, G_2, \ldots, G_t$ , then *G* is denoted by  $\bigcup_{i=1}^{t} G_i$ .

**Lemma 2.1** [13]. If  $G_1, G_2, \ldots, G_t$  are the components of a graph G, then we have

$$P(G,\lambda) = P(G_1,\lambda)P(G_2,\lambda)\cdots P(G_t,\lambda) = \prod_{i=1}^t P(G_i,\lambda).$$

Recall that the spectral radius of *G* is just the largest root of  $P(G; \lambda)$ . Hence,  $P(G; \lambda) > 0$  for all  $\lambda > \lambda_1(G)$ . Accordingly, we have as an immediate consequence the following.

**Lemma 2.2** [12]. Let  $G_1$  and  $G_2$  be two graphs. If  $P(G_1, \lambda) < P(G_2, \lambda)$  for  $\lambda \ge \lambda_1(G_2)$ , then  $\lambda_1(G_1) > \lambda_1(G_2)$ .

Since the roots of the characteristic polynomial of a graph are real, we consider only polynomials with real roots in this paper. If f(x) is a polynomial in the variable x, the degree of f(x) is denoted by  $\partial(f)$ , and the largest root of f(x) by  $\lambda_1(f)$ . Many of the discussions in the following often involve comparing the largest root of a polynomial with that of another polynomial. The next result provides an effective method of doing this.

**Lemma 2.3** [11]. Let f(x), g(x) be two monic polynomials with real roots, and  $\partial(f) \ge \partial(g)$ . If f(x) = q(x)g(x) + r(x), where q(x) is also a monic polynomial, and  $\partial(r) \le \partial(g)$ ,  $\lambda_1(g) > \lambda_1(q)$ , then

(i) when r(x) = 0, then  $\lambda_1(f) = \lambda_1(g)$ ; (ii) when r(x) > 0 for any x satisfying  $x \ge \lambda_1(g)$ , then  $\lambda_1(f) < \lambda_1(g)$ ; (iii) when  $r(\lambda_1(g)) < 0$ , then  $\lambda_1(f) > \lambda_1(g)$ .

The following result is often used to calculate the characteristic polynomials of unicyclic graphs.

**Lemma 2.4** [8,10,13]. Let e = uv be an edge of G, and let  $\mathscr{C}(e)$  be the set of all cycles containing e. The characteristic polynomial of G satisfies

$$P(G,\lambda) = P(G-e,\lambda) - P(G-u-v,\lambda) - 2\sum_{Z \in \mathscr{C}(e)} P(G \setminus V(Z),\lambda),$$

where the summation extends over all  $Z \in \mathscr{C}(e)$ .

**Lemma 2.5** [13]. Let G be the graph obtained by joining the vertex u of the graph  $G_1$  to the vertex v of the graph  $G_2$  by an edge. Then

$$P(G,\lambda) = P(G_1,\lambda)P(G_2,\lambda) - P(G_1 \setminus u,\lambda)P(G_2 \setminus v,\lambda).$$

**Lemma 2.6** [13]. *Let* v *be a vertex of degree* 1 *in the graph* G *and* u *be the vertex adjacent to* v. *Then* 

 $P(G,\lambda) = \lambda P(G \setminus v, \lambda) - P(G \setminus \{u, v\}, \lambda).$ 

It is well-known that if G' is a proper spanning subgraph of a connected graph G, then  $\lambda_1(G) > \lambda_1(G')$ . Furthermore, we have the following result.

Lemma 2.7 [6,12,14].

- (i) Let G be a connected graph, and let G' be a proper spanning subgraph of G. Then P(G', λ) > P(G, λ) for all λ ≥ λ<sub>1</sub>(G).
- (ii) Let G', H' be spanning subgraphs of the connected graphs G and H, respectively. If  $\lambda_1(G) \ge \lambda_1(H)$  and G' is a proper subgraph of G, then

 $P(G' \cup H', \lambda) > P(G \cup H, \lambda)$  for all  $\lambda \ge \lambda_1(G)$ .

Two edges of a graph *G* are said to be independent if they are not adjacent in *G*. A matching of *G* is a set of mutually independent edges of *G*, and a perfect matching of *G* is a matching that includes every vertex of *G*. For any  $G \in \mathcal{U}^+(2k)$ , *G* consists of a unique cycle, denoted by  $C_G$ , and some trees attached to some vertices on the cycle. Those vertices attached to trees, for convenience, are called the roots of the trees attached to them. A root may have more than one tree attached to it.

**Lemma 2.8.** Let G be a graph in  $\mathcal{U}^+(2k)$ ,  $k \ge 3$ , and let T be a tree in G attached to a root r. If  $v \in V(T)$  is a vertex furthest from the root r, then v is a pendant vertex and adjacent to a vertex u of degree 2.

**Proof.** The first statement is obvious. Since uv is a pendant edge, uv must belong to each perfect matching of G. Moreover, the other edges incident with u are not in any perfect matching of G. If the degree of u is not 2, there would be a pendant vertex  $v' \neq v$  joined to u, and G cannot have perfect matchings. This contradiction completes the proof.  $\Box$ 

**Lemma 2.9** [9]. Let u and v be two vertices in a non-trivial connected graph G and suppose that s paths of length 2 are attached to G at u, and t paths of length 2 are attached to G at v to form  $G_{s,t}$ . Then

either  $\lambda_1(G_{s+i,t-i}) > \lambda_1(G_{s,t})$   $(1 \le i \le t)$ or  $\lambda_1(G_{s-i,t+i}) > \lambda_1(G_{s,t})$   $(1 \le i \le s)$ .

**Lemma 2.10** [13]. Let *H* be the graph obtained from the graph *G* with vertex set  $V(G) = \{v_1, v_2, ..., v_k\}$  in the following way:

(i) for each vertex  $v_i$  of G a set  $V_i$  of p new isolated vertices is added; and (ii)  $v_i$  is joined by an edge to each of the p vertices of  $V_i$  (i = 1, 2, ..., k).

Then  $P(H, \lambda) = \lambda^{kp} P(G, \lambda - (p/\lambda)).$ 

## 3. Main results

First, we turn to a slightly more general situation. Let G be a connected graph with perfect matchings which, as shown in Fig. 1, consists of a connected subgraph H and a tree T such that T is attached to a vertex r of H.

The vertex *r* is called the root of the tree *T*, or the root-vertex of *G*. The distance between the root *r* and the vertex of *T* furthest from *r* is defined as the height of the tree *T*. Throughout the paper, |V(T)| is the number of vertices of an attached tree *T* not including the root *r* of *T*. Suppose that |V(T)| is greater than 2. If *v* is the vertex of *T* furthest from the root *r*, since *G* has perfect matchings, as in Lemma 2.8, we can prove that *v* is a pendant vertex and adjacent with a vertex *u* of degree 2. Now we carry out a transformation on *G* in the following way: first, take off the edge uv to obtain the graph G - u - v; then attach a path of length 2, say ru'v', to the root *r*. This procedure results a graph  $G_1$  which still has perfect matchings and is displayed in Fig. 1. If |V(T - u - v)| is greater than 2, we can repeat above transformation on  $G_1$ . And finally we get a graph  $G_0$  when |V(T)| is odd or a graph  $H_0$  when |V(T)| is even. Both  $G_0$  and  $H_0$  are shown in Fig. 2.

**Lemma 3.1.** Let G,  $G_0$  and  $H_0$  be the above three graphs shown in Figs. 1 and 2. Then

$$P(G,\lambda) > P(G_0,\lambda) \quad \text{for all } \lambda \ge \lambda_1(G)$$
 (1)

or

$$P(G,\lambda) > P(H_0,\lambda) \quad \text{for all } \lambda \ge \lambda_1(G).$$
 (2)

In particular, we have  $\lambda_1(G_0) > \lambda_1(G)$  and  $\lambda_1(H_0) > \lambda_1(G)$ , respectively.



Fig. 1. The graph G in Lemma 3.1 and the resulting graph  $G_1$ .



Fig. 2. Two graphs  $G_0$  and  $H_0$  in Lemma 3.1.

**Proof.** By Lemma 2.2, it is sufficient to prove (1) and (2). The proof is by induction on |V(T)|. Let |V(T)| = p. For p = 1, 2, the result holds obviously since  $G \cong G_0$  when p = 1 and  $G \cong H_0$  when p = 2. Now suppose further that the result holds for the positive integers smaller than p. We have to distinguish the following two cases.

Case i: p is odd. By Lemma 2.6, we have

$$P(G,\lambda) = (\lambda^2 - 1)P(G - u - v, \lambda) - \lambda P(G \setminus \{u, v, w\}, \lambda),$$
(\*)

$$P(G_0, \lambda) = (\lambda^2 - 1)P(G_0 - u' - v', \lambda) - \lambda P(G_0 \setminus \{u', v', r\}, \lambda).$$
(\*\*)

By the induction hypothesis, we have

$$P(G - u - v, \lambda) > P(G_0 - u' - v', \lambda)$$
 for all  $\lambda \ge \lambda_1(G - u - v)$ .

Since

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$$G_0 \setminus \{u', v', r\} = (H - r) \bigcup \left(\frac{p - 1}{2}\right) K_2 \bigcup K_1$$

is a proper spanning subgraph of  $G \setminus \{u, v, w\}$ , by Lemma 2.7, we have

 $P(G_0 \setminus \{u', v', r\}, \lambda) > P(G \setminus \{u, v, w\}, \lambda) \quad \text{for all } \lambda \ge \lambda_1(G \setminus \{u, v, w\}).$ 

Since  $G \setminus \{u, v, w\}$  is a proper subgraph of G - u - v, we have  $\lambda_1(G - u - v) > \lambda_1(G \setminus \{u, v, w\})$ . Hence, when  $\lambda \ge \lambda_1(G - u - v)$ , we have by (\*) and (\*\*) that

 $P(G,\lambda) > P(G_0,\lambda).$ 

Again, since G - u - v is a proper subgraphs of G, we have  $\lambda_1(G) > \lambda_1(G - u - v)$ and  $\lambda_1(G) > (G \setminus \{u, v, w\})$ .

Thus, for  $\lambda \ge \lambda_1(G)$ , we have  $P(G, \lambda) > P(G_0, \lambda)$ .

Therefore the result is established by induction in this case.

**Case ii:** *p is even*. The proof is similar to (i). This completes the proof.  $\Box$ 

Now we consider the set  $\mathcal{U}^+(2k)$ . From the two tables of the spectra of connected graphs on *n* vertices,  $2 \le n \le 5$  in [13] and n = 6 in [7], respectively, we know that there exist two graphs in  $\mathcal{U}^+(4)$  when k = 2 and eight graphs in  $\mathcal{U}^+(6)$  when k = 3. We already know by Theorem 1.1 that the graph  $S_4^*$  alone has the largest spectral radius in  $\mathcal{U}^+(4)$ . Among the eight graphs in  $\mathcal{U}^+(6)$ , the graph obtained by attaching a pendant edge to each vertex of  $C_3$  alone has the largest spectral radius. Accordingly we assume that  $k \ge 4$ .

We first focus on the set  $\mathscr{U}_3^+(2k)$  of all graphs in  $\mathscr{U}^+(2k)$  whose unique cycle is  $C_3$ . Let  $U_{2k}^1$  be the graph on 2k vertices obtained from  $C_3$  by attaching a pendant edge together with k - 2 paths of length 2 at one vertex. Let  $U_{2k}^2$  be the graph on 2k



vertices obtained from  $C_3$  by attaching a pendant edge and k-3 paths of length 2 at one vertex, and single pendant edges at the other vertices, respectively; Let  $U_{2k}^3$  be the graph on 2k vertices obtained from  $C_3$  by attaching a pendant edge at one vertex and k-2 paths of length 2 at another vertex. The three graphs  $U_{2k}^1, U_{2k}^2$  and  $U_{2k}^3$  are displayed in Fig. 3. Obviously,  $U_{2k}^1, U_{2k}^2$  and  $U_{2k}^3$  all belong to the set  $\mathcal{U}_3^+(2k)$ , and each has a unique perfect matching. Note that  $U_{2k}^1 = U_{2k}^3$  when k = 2.

# Lemma 3.2

$$\begin{split} P(U_{2k}^{1},\lambda) &= (\lambda^{2}-1)^{k-2} [\lambda^{4}-(k+2)\lambda^{2}-2\lambda+1], \\ P(U_{2k}^{2},\lambda) &= (\lambda^{2}-1)^{k-4} (\lambda^{2}+\lambda-1) \\ &\times [\lambda^{6}-\lambda^{5}-(k+2)\lambda^{4}+(k-1)\lambda^{3}+(k+2)\lambda^{2}-\lambda-1], \\ P(U_{2k}^{3},\lambda) &= (\lambda^{2}-1)^{k-3} [\lambda^{6}-(k+3)\lambda^{4}-2\lambda^{3}+(2k+1)\lambda^{2}+2\lambda-1]. \end{split}$$

**Proof.** In  $U_{2k}^1$ , we choose one edge  $e_1 = uv$  of  $C_3$  which is not in the unique perfect matching of  $U_{2k}^1$ . By Lemma 2.4, we have

$$P(U_{2k}^{1},\lambda) = P(U_{2k}^{1}-e_{1},\lambda) - P(U_{2k}^{1}-u-v,\lambda) - 2P(U_{2k}^{1} \setminus V(C_{3}),\lambda).$$

Taking  $G = S_k$ , p = 1 in Lemma 2.10, we have

$$P(U_{2k}^{1} - e_{1}, \lambda) = \lambda^{k} P\left(S_{k}, \lambda - \frac{1}{\lambda}\right)$$
$$= \lambda^{k} \left(\lambda - \frac{1}{\lambda}\right)^{k-2} \left[\left(\lambda - \frac{1}{\lambda}\right)^{2} - (k-1)\right]$$
$$= (\lambda^{2} - 1)^{k-2} [\lambda^{4} - (k+1)\lambda^{2} + 1].$$

Since  $U_{2k}^1 - u - v \cong (k-2)K_2 \cup 2K_1$ , and  $U_{2k}^1 \setminus V(C_3) \cong (k-2)K_2 \cup K_1$ , thus

$$P(U_{2k}^{1}, \lambda) = (\lambda^{2} - 1)^{k-2} [\lambda^{4} - (k+1)\lambda^{2} + 1] -\lambda^{2} (\lambda^{2} - 1)^{k-2} - 2\lambda (\lambda^{2} - 1)^{k-2} = (\lambda^{2} - 1)^{k-2} [\lambda^{4} - (k+2)\lambda^{2} - 2\lambda + 1].$$

By Lemmas 2.4 and 2.5, it is not difficult to show that  $P(S_k^*) = \lambda^{k-4}(\lambda^4 - k\lambda^2 - 2\lambda + k - 3)$ . Taking  $G = S_k^*$ , p = 1 in Lemma 2.10, we have

$$\begin{split} P(U_{2k}^2,\lambda) &= \lambda^k P\left(S_k^*,\lambda-\frac{1}{\lambda}\right) \\ &= \lambda^k \left(\lambda-\frac{1}{\lambda}\right)^{k-4} \\ &\times \left[\left(\lambda-\frac{1}{\lambda}\right)^4 - k\left(\lambda-\frac{1}{\lambda}\right)^2 - 2\left(\lambda-\frac{1}{\lambda}\right) + k - 3\right] \\ &= (\lambda^2-1)^{k-4}(\lambda^2+\lambda-1) \\ &\times [\lambda^6-\lambda^5 - (k+2)\lambda^4 + (k-1)\lambda^3 + (k+2)\lambda^2 - \lambda - 1]. \end{split}$$

For  $U_{2k}^3$  consider the edge e' = u'v' of  $C_3$ , where a pendant edge is attached at u' and paths of length 2 are attached at v'. By Lemma 2.4, we have

$$P(U_{2k}^{3}, \lambda) = P(U_{2k}^{3} - e', \lambda) - P(U_{2k}^{3} - u' - v', \lambda) - 2P(U_{2k}^{3} \setminus V(C_{3}), \lambda)$$
  
=  $P(U_{2k}^{3} - e', \lambda) - P((k-2)K_{2} \cup 2K_{1}, \lambda)$   
 $- 2P((k-2)K_{2} \cup K_{1}, \lambda).$ 

And by Lemmas 2.5 and 2.6, it is not difficult but somewhat tedious to show that

$$P(U_{2k}^3 - e', \lambda) = (\lambda^2 - 1)^{k-3} [\lambda^6 - (k+2)\lambda^4 + 2k\lambda^2 - 1].$$

Hence,

$$\begin{split} P(U_{2k}^3,\lambda) &= (\lambda^2 - 1)^{k-3} [\lambda^6 - (k+2)\lambda^4 + 2k\lambda^2 - 1] \\ &- \lambda^2 (\lambda^2 - 1)^{k-2} - 2\lambda (\lambda^2 - 1)^{k-2} \\ &= (\lambda^2 - 1)^{k-3} [\lambda^6 - (k+3)\lambda^4 - 2\lambda^3 + (2k+1)\lambda^2 + 2\lambda - 1]. \end{split}$$

The proof is completed.  $\Box$ 

**Theorem 3.3.** Among the all graphs in  $\mathcal{U}_3^+(2k)$ ,  $k \ge 4$ ,  $U_{2k}^1$  and  $U_{2k}^2$  are the graphs with the largest and the second largest spectral radius, respectively.

**Proof.** Let G be a graph in  $\mathscr{U}_3^+(2k)$ , and M a perfect matching of G. We distinguish the following two cases.

**Case 1.** One of three edges of  $C_3$  in G is in M.

Suppose that e = uv is an edge of  $C_3$ , and  $e \in M$ . Then all trees attached to u or v have even order, and among the trees attached at the third vertex of  $C_3$ , exactly one has odd order. By Lemmas 3.1 and 2.9, G can be transformed into one of the two graphs  $U_{2k}^1$  and  $U_{2k}^3$ , and  $\lambda_1(G)$  is strictly less than both  $\lambda_1(U_{2k}^1)$  and  $\lambda_1(U_{2k}^3)$  if  $G \ncong U_{2k}^1$  and  $G \ncong U_{2k}^3$ .

## **Case 2.** No edge of $C_3$ in G lies in M.

Then each vertex of  $C_3$  is attached to some trees, and exactly one of these trees has odd order. Also, by Lemmas 3.1 and 2.9, *G* can be transformed into the graph  $U_{2k}^2$  and  $\lambda_1(G) < \lambda_1(U_{2k}^2)$  if  $G \not\cong U_{2k}^2$ .

Now it suffices to show that  $\lambda_1(U_{2k}^1) > \lambda_1(U_{2k}^2) > \lambda_1(U_{2k}^3)$ . For the first inequality, we know from Lemma 3.2 that  $\lambda_1(U_{2k}^1)$  and  $\lambda_1(U_{2k}^2)$  are the largest roots of the polynomials  $\lambda^4 - (k+2)\lambda^2 - 2\lambda + 1$  and  $\lambda^6 - \lambda^5 - (k+2)\lambda^4 + (k-1)\lambda^3 + (k+2)\lambda^2 - \lambda - 1$ , respectively. Let  $f(\lambda) = \lambda^4 - (k+2)\lambda^2 - 2\lambda + 1$  and  $g(\lambda) = \lambda^6 - \lambda^5 - (k+2)\lambda^4 + (k-1)\lambda^3 + (k+2)\lambda^2 - \lambda - 1$ . Then we have

$$g(\lambda) = \lambda(\lambda - 1)f(\lambda) + (k - 1)\lambda^2 - \lambda^3 - 1.$$

Let  $r_1(\lambda) = (k-1)\lambda^2 - \lambda^3 - 1$ , so that we have  $r'_1(\lambda) = 2(k-1)\lambda - 3\lambda^2$ . Thus  $r'_1(\lambda) > 0$  when  $\lambda < \frac{2}{3}(k-1)$ .

By Corollary 1.1, here  $\lambda$  also satisfies  $\lambda < \sqrt{2k}$ . It is easy to see from the condition  $\sqrt{2k} < \frac{2}{3}(k-1)$  that

$$r'_1(\lambda) > 0$$
 when  $k \ge 7$ .

That is,  $r_1(\lambda)$  is an increasing function of  $\lambda$  when  $k \ge 7$ . Since  $S_{k+2}$  is a proper subgraph of  $U_{2k}^1$ , we have  $\lambda_1(U_{2k}^1) > \lambda_1(S_{k+2}) = \sqrt{k+1}$ . Moreover, it is easy to verify that

$$r_1\left(\sqrt{k+1}\right) > 0 \quad \text{when } k \ge 5.$$

So we have  $r_1(\lambda) > 0$  for  $\lambda \ge \lambda_1(U_{2k}^1)$ . Then, by Lemma 2.3, an immediate consequence is that  $\lambda_1(U_{2k}^1) > \lambda_1(U_{2k}^2)$  when  $k \ge 7$ .

When k = 4, 5, 6, by direct calculation we obtain that  $\lambda_1(U_8^1) \approx 2.5741$ ,  $\lambda_1(U_8^2) \approx 2.5606$ ;  $\lambda_1(U_{10}^1) \approx 2.7557$ ,  $\lambda_1(U_{10}^2) \approx 2.7117$ ;  $\lambda_1(U_{12}^1) \approx 2.9269$ ,  $\lambda_1(U_{12}^2) \approx 2.8634$ . Thus the first inequality holds for all  $k \ge 4$ .

For the second inequality, we consider the edge  $e_2 = xy$  of  $U_{2k}^2$ , where a pendant edge is attached at x and y, respectively, and the edge e'' = u'w' of  $U_{2k}^3$ , where a pendant edge is attached at u' and w' is the vertex of degree 2 of  $U_{2k}^3$ . Then by Lemma 2.4, we have

$$P(U_{2k}^{2}, \lambda) = P(U_{2k}^{2} - e_{2}, \lambda) - P(U_{2k}^{2} - x - y, \lambda) - 2P(3K_{1} \cup (k - 3)K_{2}, \lambda),$$
(i)  
$$P(U_{2k}^{3}, \lambda) = P(U_{2k}^{3} - e'', \lambda) - P(U_{2k}^{3} - u' - w', \lambda)$$

$$-2P(K_1 \cup (k-2)K_2, \lambda).$$
 (ii)

Obviously, we have  $U_{2k}^2 - e_2 \cong U_{2k}^3 - e''$ , thus,

$$P(U_{2k}^2 - e_2, \lambda) = P(U_{2k}^3 - e''\lambda).$$

Since  $U_{2k}^2 - x - y$  is a proper spanning subgraph of  $U_{2k}^3 - u' - w'$ , and by Lemma 2.7, we have

$$P(U_{2k}^2 - x - y, \lambda) > P(U_{2k}^3 - u' - w', \lambda)$$
 for all  $\lambda \ge \lambda_1(U_{2k}^3 - u' - w')$ .

It is easy to verify that

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$$P(3K_1 \cup (k-3)K_2, \lambda) > P(K_1 \cup (k-2)K_2, \lambda)$$
 when  $\lambda > 1$ .

Since  $U_{2k}^3 - u' - w'$  is a proper subgraph of  $U_{2k}^3$ , we have  $\lambda_1(U_{2k}^3) > \lambda_1(U_{2k}^3 - u' - w')$ . Hence by Eqs. (i) and (ii), we get

$$P(U_{2k}^2, \lambda) < P(U_{2k}^3, \lambda) \text{ for all } \lambda \ge \lambda_1(U_{2k}^3).$$

Thus we have the result. The proof is completed.  $\Box$ 

Let *G* be a graph in  $\mathscr{U}_{2k}^+$ ,  $k \ge 4$ , and let  $C_G$  be the cycle of *G*,  $C_G \not\cong C_3$ . If there exists a vertex *r* on  $C_G$  such that

- (i) if *r* is a root of *G*, the orders of all trees attached to *r* are even;
- (ii) a neighbour v of r on  $C_G$  is not root of G and the edge rv is in a perfect matching of G.

Let G' be the graph obtained from G by contracting the edge e = rv (i.e., coalescencing the root r with v), and then attaching a pendant edge rv' to r. This procedure is shown in Fig. 4.

**Lemma 3.4.** Let G and G' be the two graphs in Fig. 4. Then

 $P(G, \lambda) > P(G', \lambda)$  for all  $\lambda \ge \lambda_1(G)$ .

In particular,  $\lambda_1(G') \ge \lambda_1(G)$ .

**Proof.** Consider the edge  $e_1 = vu$  ( $u \neq r$ ) of  $C_G$  and the edge and the edge  $e'_1 = ru$  of  $C_{G'}$ . Note that  $|V(C_{G'})| = |V(C_G)| - 1$ . By Lemma 2.4, we have

$$P(G,\lambda) = P(G - e_1,\lambda) - P(G - v - u,\lambda) - 2P(G \setminus V(C_G),\lambda),$$

$$P(G',\lambda) = P(G'-e_1',\lambda) - P(G'-r-u,\lambda) - 2P(G' \setminus V(C_{G'}),\lambda).$$



Fig. 4. The graph G and the resulting graph G' in Lemma 3.4.

Moreover, it is easy to see that we have

$$G - e_1 \cong G' - e'_1,$$
  

$$G' - r - u \subset G - v - u,$$
  

$$G' \setminus V(C_{G'}) = G \setminus V(C_G) \cup \{v'\}$$

Hence,

$$P(G - e_1, \lambda) = P(G' - e'_1, \lambda),$$
  

$$P(G' \setminus V(C_{G'}), \lambda) = \lambda P(G \setminus V(C_G), \lambda) > P(G \setminus V(C_G), \lambda) \quad \text{when } \lambda > 1,$$

and by Lemma 2.7, we have

$$P(G' - r - u, \lambda) > P(G - v - u, \lambda)$$
 for all  $\lambda \ge \lambda_1(G - v - u)$ .

Since G - v - u is a proper subgraph of *G*, we have  $\lambda_1(G) > \lambda_1(G - v - u)$ . Therefore, it follows immediately from the above that  $P(G, \lambda) > P(G', \lambda)$  for all  $\lambda \ge \lambda_1(G)$ .

The proof is completed.  $\Box$ 

**Theorem 3.5.** Let G be a graph in  $\mathscr{U}_{2k}^+$ ,  $k \ge 4$ . Then

 $\lambda_1(G) \leq \lambda_1(U_{2k}^1)$ 

and the equality holds if and only if  $G \cong U_{2k}^1$ , where  $\lambda_1(U_{2k}^1)$  is the largest root of the polynomial  $\lambda^4 - (k+2)\lambda^2 - 2\lambda + 1$ .

**Proof.** Suppose that *G* is a graph in  $\mathscr{U}_{2k}^+$ ,  $k \ge 4$ . If  $G \cong C_{2k}$ , the result is obvious. If the cycle  $C_G$  is  $C_3$ , by Theorem 3.3, the result also holds. So now we assume  $G \cong C_{2k}$ , and  $|V(C_G)| \ge 4$ . Consequently, there exist trees attached to roots on the cycle  $C_G$  of G. If the heights of all trees attached on the cycle  $C_G$  are not greater than 2, then these trees are either pendant edges or paths of length 2. Note that it is evident that two pendant edges cannot be attached to a common root since G has perfect matchings. If there exist some trees with height more than 2 in G, we can transform G, using Lemma 3.1 repeatedly, into a graph  $G_0$  such that the heights of all attached trees of  $G_0$  are not greater than 2, and  $\lambda_1(G) < \lambda_1(G_0)$ . Therefore, it is sufficient to focus our attention on those unicyclic graphs in  $\mathscr{U}_{2k}^+$  whose attached trees all have heights not greater than 2. We can transform such a  $G_0$ , using Lemma 2.9 repeatedly, into a graph  $G_1$  such that all trees of height 2 are attached to a root r on the cycle  $C_{G_1}$  of  $G_1$ , and  $\lambda_1(G_0) < \lambda_1(G_1)$ . If there is no a pendant edge attached to r, then there must exist an edge incident with r on  $C_{G_1}$  which belongs to a perfect matching of  $G_1$ . By Lemma 3.4,  $G_1$  can be transformed into a graph  $U_0$  with the root r attached to a pendant edge and all paths of length 2. Assume that the number of these paths is i, and the other roots of  $U_0$  are attached to only one pendant edge. And



Fig. 5. The procedure in the transformation on  $U_0$  in Theorem 3.5.

we also have  $\lambda_1(G_1) < \lambda_1(U_0)$ . Note that the number of vertices between two roots with only one pendant edge attached in  $U_0$  must be even since all pendant edges belong to perfect matchings of  $U_0$ .

For the graph  $U_0$ , we distinguish the following two cases:

- (i) The cycle  $C_{U_0}$  of  $U_0$  is  $C_3$ . Then  $U_0$  must be one of two graphs  $U_{2k}^1$  and  $U_{2k}^2$ . By Theorem 3.3, the result holds immediately.
- (ii) The cycle  $C_{U_0}$  of  $U_0$  is not  $C_3$ . Then we have  $|V(C_{U_0})| \ge 4$ . Assume that u is the vertex adjacent to the root r on  $C_{U_0}$  clockwise. If u is not a root-vertex, then u is a vertex of degree 2, and so is its other adjacent vertex, say  $v_0$ , on  $C_{U_0}$ , and the edge  $uv_0$  belongs to perfect matchings of  $U_0$ .

By Lemma 3.4, one can transform  $U_0$  into a graph  $U_1$  such that u is a rootvertex of  $U_1$  to which a pendant edge, say uv, is attached, and  $\lambda_1(U_0) < \lambda_1(U_1)$ . If  $U_1 \cong U_{2k}^2$ , then we have the result by Theorem 3.3; If  $|V(C_{U_1})| \ge 4$ , we continue to carry out the following transformation on  $U_1$ : first, take off the vertex v from  $U_1$ to obtain the graph  $U_1 - v$ ; then contract the edge ru, and attach a path of length 2, say ru'v', to the root r. The resulting graph is denoted by  $U_2$ . This procedure is shown in Fig. 5. Now we have to prove the following Claim.

**Claim.**  $\lambda_1(U_1) < \lambda_1(U_2)$ .

Let  $u_1$  be the vertex on  $C_{U_1}$  adjacent to u clockwise. Then  $u_1$  is adjacent to the root r in  $U_2$ . Consider the edge  $e_1 = uu_1$  of  $U_1$  and the edge  $e_2 = ru_1$  of  $U_2$ . By Lemma 2.4, we have

$$P(U_1, \lambda) = P(U_1 - e_1, \lambda) - P(U_1 - u - u_1, \lambda) - 2P(U_1 \setminus V(C_{U_1}), \lambda),$$
  

$$P(U_2, \lambda) = P(U_2 - e_2, \lambda) - P(U_2 - r - u_1, \lambda) - 2P(U_2 \setminus V(C_{U_2}), \lambda).$$

It is obvious that  $U_1 - e_1 \cong U_2 - e_2$  and  $U_2 - r - u_1 \subset U_1 - u - u_1$ .

Thus,  $P(U_1 - e_1, \lambda) = P(U_2 - e_2, \lambda)$ .

And, by Lemma 2.7, we have  $P(U_2 - r - u_1, \lambda) > P(U_1 - u - u_1, \lambda)$  when  $\lambda \ge \lambda_1(U_1 - u - u_1)$ .

Moreover,

$$P(U_1 \setminus V(C_{U_1}), \lambda) = \lambda^s (\lambda^2 - 1)^i,$$
  

$$P(U_2 \setminus V(C_{U_2}), \lambda) = \lambda^{s-1} (\lambda^2 - 1)^{i+1}$$

where s is the number of pendant edges attached to roots of  $U_1$ . Then

$$P(U_2 \setminus V(C_{U_2}), \lambda) - P(U_1 \setminus V(C_{U_1}), \lambda) = \lambda^{s-1} (\lambda^2 - 1)^i (\lambda^2 - \lambda - 1).$$

Therefore,  $P(U_2 \setminus V(C_{U_2}), \lambda) > P(U_1 \setminus V(C_{U_1}), \lambda)$  when  $\lambda > (1 + \sqrt{5})/2$ .

Since  $U_1 - u - u_1$  is a proper subgraph of  $U_1$ , we know that  $\lambda_1(U_1) > \lambda_1(U_1 - u - u_1)$ . Thus, when  $\lambda \ge \lambda_1(U_1)$  (>  $(1 + \sqrt{5})/2$ ), we have  $P(U_1, \lambda) > P(U_2, \lambda)$ . So the Claim is established.

By the above Claim, if  $U_2 \cong U_{2k}^1$  or  $U_2 \cong U_{2k}^2$ , then we have the result by Theorem 3.3. Otherwise, the graph  $U_2$  satisfies  $|V(C_{U_2})| \ge 4$ , and then the transformations above can be carry out on  $U_2$  similarly. This procedure continues until the resulting graph is one of  $U_{2k}^1$  and  $U_{2k}^2$ . So the result follows by Theorem 3.3.

The proof is completed.  $\Box$ 

The next result follows immediately by Theorem 3.3 and the proof of Theorem 3.5.

**Theorem 3.6.** Let G be a graph in  $\mathcal{U}_{2k}^+$ ,  $k \ge 4$ , and  $G \ncong U_{2k}^1$ . Then

 $\lambda_1(G) \leqslant \lambda_1(U_{2k}^2)$ 

and the equality holds if and only if  $G \cong U_{2k}^2$ , where  $\lambda_1(U_{2k}^2)$  is the largest root of the polynomial  $\lambda^6 - \lambda^5 - (k+2)\lambda^4 + (k-1)\lambda^3 + (k+2)\lambda^2 - \lambda - 1$ .

**Remark.** From the table of spectra of the connected graphs on six vertices (see [7]) we know that  $U_6^2$  and  $U_6^1$  are the graphs with the largest and second largest spectral radius in  $\mathcal{U}_6^+$ , respectively. Also notice that we have  $U_4^1 = S_4^*$ . Accordingly Theorems 3.5 and 3.6 may be restated as follows.

**Theorem 3.7.** Among the graphs in  $\mathscr{U}_{2k}^+$  ( $k \neq 3$ ), two graphs  $U_{2k}^1$  and  $U_{2k}^2$  have the largest and the second largest spectral radius, respectively.

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