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# On the spectral radius of unicyclic graphs with perfect matchings 

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#### Abstract

Let $\mathscr{U}^{+}(2 k)$ be the set of all unicyclic graphs on $2 k(k \geqslant 2)$ vertices with perfect matchings. Let $U_{2 k}^{1}$ be the graph on $2 k$ vertices obtained from $C_{3}$ by attaching a pendant edge and $k-2$ paths of length 2 at one vertex of $C_{3}$; Let $U_{2 k}^{2}$ be the graph on $2 k$ 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 $U_{2 k}^{1}$ and $U_{2 k}^{2}$ have the largest and the second largest spectral radius among the graphs in $\mathscr{U}^{+}(2 k)$ when $k \neq 3$. © 2003 Elsevier Inc. All rights reserved. AMS classification: 05C50 Keywords: Unicyclic graphs; Spectral radius; Perfect matching


## 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

[^0]$A(G)$ 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 $\lambda_{1}(G) \geqslant \lambda_{2}(G) \geqslant \lambda_{3}(G) \geqslant \cdots \geqslant$ $\lambda_{n}(G)$ and call them the eigenvalues of $G$. The characteristic polynomial of $G$ is just $\operatorname{Det}(\lambda I-A(G))$, 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 $\mathscr{U}(n)$ and $\mathscr{U}^{+}(2 k)$ denote the set of all unicyclic graphs on $n$ vertices and the set of all unicyclic graphs with perfect matchings on $2 k$ vertices, respectively. The eigenvalues of graphs in $\mathscr{U}(n)$ have been studied by several authors (see [1-6]). In particular, the following result on the spectral radius of a graph in $\mathscr{U}(n)$ 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 $\mathscr{U}(n)$, 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 $\mathscr{U}(n)$. Then

$$
2 \leqslant \lambda_{1}(G) \leqslant \sqrt{n} \quad \text { when } n \geqslant 9
$$

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

## 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 $r G$ 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

$$
P(G, \lambda)=P\left(G_{1}, \lambda\right) P\left(G_{2}, \lambda\right) \cdots P\left(G_{t}, \lambda\right)=\prod_{i=1}^{t} P\left(G_{i}, \lambda\right) .
$$

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 $P\left(G_{1}, \lambda\right)<P\left(G_{2}, \lambda\right)$ for $\lambda \geqslant$ $\lambda_{1}\left(G_{2}\right)$, then $\lambda_{1}\left(G_{1}\right)>\lambda_{1}\left(G_{2}\right)$.

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 $\partial(f) \geqslant \partial(g)$. If $f(x)=q(x) g(x)+r(x)$, where $q(x)$ is also a monic polynomial, and $\partial(r) \leqslant \partial(g), \lambda_{1}(g)>\lambda_{1}(q)$, then
(i) when $r(x)=0$, then $\lambda_{1}(f)=\lambda_{1}(g)$;
(ii) when $r(x)>0$ for any $x$ satisfying $x \geqslant \lambda_{1}(g)$, then $\lambda_{1}(f)<\lambda_{1}(g)$;
(iii) when $r\left(\lambda_{1}(g)\right)<0$, 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 $e=u v$ be an edge of $G$, and let $\mathscr{C}(e)$ be the set of all cycles containing $e$. The characteristic polynomial of $G$ satisfies

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

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

$$
P(G, \lambda)=P\left(G_{1}, \lambda\right) P\left(G_{2}, \lambda\right)-P\left(G_{1} \backslash u, \lambda\right) P\left(G_{2} \backslash v, \lambda\right) .
$$

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

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

It is well-known that if $G^{\prime}$ is a proper spanning subgraph of a connected graph $G$, then $\lambda_{1}(G)>\lambda_{1}\left(G^{\prime}\right)$. Furthermore, we have the following result.

Lemma 2.7 [6, 12, 14].
(i) Let $G$ be a connected graph, and let $G^{\prime}$ be a proper spanning subgraph of $G$. Then $P\left(G^{\prime}, \lambda\right)>P(G, \lambda)$ for all $\lambda \geqslant \lambda_{1}(G)$.
(ii) Let $G^{\prime}, H^{\prime}$ be spanning subgraphs of the connected graphs $G$ and $H$, respectively. If $\lambda_{1}(G) \geqslant \lambda_{1}(H)$ and $G^{\prime}$ is a proper subgraph of $G$, then

$$
P\left(G^{\prime} \cup H^{\prime}, \lambda\right)>P(G \cup H, \lambda) \quad \text { for all } \lambda \geqslant \lambda_{1}(G)
$$

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 $G \in \mathscr{U}^{+}(2 k), G$ 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 $\mathscr{U}^{+}(2 k), k \geqslant 3$, 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 $u v$ is a pendant edge, $u v$ 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 $v^{\prime} \neq v$ joined to $u$, and $G$ cannot have perfect matchings. This contradiction completes the proof.

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

$$
\begin{aligned}
& \text { either } \lambda_{1}\left(G_{s+i, t-i}\right)>\lambda_{1}\left(G_{s, t}\right) \quad(1 \leqslant i \leqslant t) \\
& \text { or } \lambda_{1}\left(G_{s-i, t+i}\right)>\lambda_{1}\left(G_{s, t}\right) \quad(1 \leqslant i \leqslant s)
\end{aligned}
$$

Lemma 2.10 [13]. Let $H$ be the graph obtained from the graph $G$ with vertex set $V(G)=\left\{v_{1}, v_{2}, \ldots, v_{k}\right\}$ 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 $V_{i}(i=1,2, \ldots, k)$.

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

## 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 $u v$ to obtain the graph $G-u-v$; then attach a path of length 2 , say $r u^{\prime} v^{\prime}$, 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

$$
\begin{equation*}
P(G, \lambda)>P\left(G_{0}, \lambda\right) \quad \text { for all } \lambda \geqslant \lambda_{1}(G) \tag{1}
\end{equation*}
$$

or

$$
\begin{equation*}
P(G, \lambda)>P\left(H_{0}, \lambda\right) \text { for all } \lambda \geqslant \lambda_{1}(G) . \tag{2}
\end{equation*}
$$

In particular, we have $\lambda_{1}\left(G_{0}\right)>\lambda_{1}(G)$ and $\lambda_{1}\left(H_{0}\right)>\lambda_{1}(G)$, 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

$$
\begin{align*}
& P(G, \lambda)=\left(\lambda^{2}-1\right) P(G-u-v, \lambda)-\lambda P(G \backslash\{u, v, w\}, \lambda),  \tag{*}\\
& P\left(G_{0}, \lambda\right)=\left(\lambda^{2}-1\right) P\left(G_{0}-u^{\prime}-v^{\prime}, \lambda\right)-\lambda P\left(G_{0} \backslash\left\{u^{\prime}, v^{\prime}, r\right\}, \lambda\right) . \tag{**}
\end{align*}
$$

By the induction hypothesis, we have

$$
P(G-u-v, \lambda)>P\left(G_{0}-u^{\prime}-v^{\prime}, \lambda\right) \quad \text { for all } \lambda \geqslant \lambda_{1}(G-u-v) .
$$

Since

$$
G_{0} \backslash\left\{u^{\prime}, v^{\prime}, r\right\}=(H-r) \bigcup\left(\frac{p-1}{2}\right) K_{2} \bigcup K_{1}
$$

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

$$
P\left(G_{0} \backslash\left\{u^{\prime}, v^{\prime}, r\right\}, \lambda\right)>P(G \backslash\{u, v, w\}, \lambda) \quad \text { for all } \lambda \geqslant \lambda_{1}(G \backslash\{u, v, w\})
$$

Since $G \backslash\{u, v, w\}$ is a proper subgraph of $G-u-v$, we have $\lambda_{1}(G-u-v)>$ $\lambda_{1}(G \backslash\{u, v, w\})$. Hence, when $\lambda \geqslant \lambda_{1}(G-u-v)$, we have by $(*)$ and ( $\left.* *\right)$ that

$$
P(G, \lambda)>P\left(G_{0}, \lambda\right)
$$

Again, since $G-u-v$ is a proper subgraphs of $G$, we have $\lambda_{1}(G)>\lambda_{1}(G-u-v)$ and $\lambda_{1}(G)>(G \backslash\{u, v, w\})$.

Thus, for $\lambda \geqslant \lambda_{1}(G)$, we have $P(G, \lambda)>P\left(G_{0}, \lambda\right)$.
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.
Now we consider the set $\mathscr{U}^{+}(2 k)$. From the two tables of the spectra of connected graphs on $n$ vertices, $2 \leqslant n \leqslant 5$ in [13] and $n=6$ in [7], respectively, we know that there exist two graphs in $\mathscr{U}^{+}(4)$ when $k=2$ and eight graphs in $\mathscr{U}^{+}(6)$ when $k=3$. We already know by Theorem 1.1 that the graph $S_{4}^{*}$ alone has the largest spectral radius in $\mathscr{U}^{+}(4)$. Among the eight graphs in $\mathscr{U}^{+}(6)$, the graph obtained by attaching a pendant edge to each vertex of $C_{3}$ alone has the largest spectral radius. Accordingly we assume that $k \geqslant 4$.

We first focus on the set $\mathscr{U}_{3}^{+}(2 k)$ of all graphs in $\mathscr{U}^{+}(2 k)$ whose unique cycle is $C_{3}$. Let $U_{2 k}^{1}$ be the graph on $2 k$ vertices obtained from $C_{3}$ by attaching a pendant edge together with $k-2$ paths of length 2 at one vertex. Let $U_{2 k}^{2}$ be the graph on $2 k$


Fig. 3. Three graphs $U_{2 k}^{1}, U_{2 k}^{2}$ and $U_{2 k}^{3}$.
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 $U_{2 k}^{3}$ be the graph on $2 k$ 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 $U_{2 k}^{1}, U_{2 k}^{2}$ and $U_{2 k}^{3}$ are displayed in Fig. 3. Obviously, $U_{2 k}^{1}, U_{2 k}^{2}$ and $U_{2 k}^{3}$ all belong to the set $\mathscr{U}_{3}^{+}(2 k)$, and each has a unique perfect matching. Note that $U_{2 k}^{1}=U_{2 k}^{3}$ when $k=2$.

## Lemma 3.2

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

Proof. In $U_{2 k}^{1}$, we choose one edge $e_{1}=u v$ of $C_{3}$ which is not in the unique perfect matching of $U_{2 k}^{1}$. By Lemma 2.4, we have

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

Taking $G=S_{k}, p=1$ in Lemma 2.10, we have

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

Since $U_{2 k}^{1}-u-v \cong(k-2) K_{2} \cup 2 K_{1}$, and $U_{2 k}^{1} \backslash V\left(C_{3}\right) \cong(k-2) K_{2} \cup K_{1}$, thus

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

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

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

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

$$
\begin{aligned}
P\left(U_{2 k}^{3}, \lambda\right)= & P\left(U_{2 k}^{3}-e^{\prime}, \lambda\right)-P\left(U_{2 k}^{3}-u^{\prime}-v^{\prime}, \lambda\right)-2 P\left(U_{2 k}^{3} \backslash V\left(C_{3}\right), \lambda\right) \\
= & P\left(U_{2 k}^{3}-e^{\prime}, \lambda\right)-P\left((k-2) K_{2} \cup 2 K_{1}, \lambda\right) \\
& -2 P\left((k-2) K_{2} \cup K_{1}, \lambda\right) .
\end{aligned}
$$

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

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

Hence,

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

The proof is completed.
Theorem 3.3. Among the all graphs in $\mathscr{U}_{3}^{+}(2 k), k \geqslant 4, U_{2 k}^{1}$ and $U_{2 k}^{2}$ are the graphs with the largest and the second largest spectral radius, respectively.

Proof. Let $G$ be a graph in $\mathscr{U}_{3}^{+}(2 k)$, 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 $e=u v$ 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 $U_{2 k}^{1}$ and $U_{2 k}^{3}$, and $\lambda_{1}(G)$ is strictly less than both $\lambda_{1}\left(U_{2 k}^{1}\right)$ and $\lambda_{1}\left(U_{2 k}^{3}\right)$ if $G \not \not U_{2 k}^{1}$ and $G \not \not U_{2 k}^{3}$.

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 $U_{2 k}^{2}$ and $\lambda_{1}(G)<\lambda_{1}\left(U_{2 k}^{2}\right)$ if $G \not \not \neq U_{2 k}^{2}$.

Now it suffices to show that $\lambda_{1}\left(U_{2 k}^{1}\right)>\lambda_{1}\left(U_{2 k}^{2}\right)>\lambda_{1}\left(U_{2 k}^{3}\right)$. For the first inequality, we know from Lemma 3.2 that $\lambda_{1}\left(U_{2 k}^{1}\right)$ and $\lambda_{1}\left(U_{2 k}^{2}\right)$ 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 $r_{1}^{\prime}(\lambda)=2(k-1) \lambda-3 \lambda^{2}$.
Thus $r_{1}^{\prime}(\lambda)>0$ when $\lambda<\frac{2}{3}(k-1)$.
By Corollary 1.1, here $\lambda$ also satisfies $\lambda<\sqrt{2 k}$. It is easy to see from the condition $\sqrt{2 k}<\frac{2}{3}(k-1)$ that

$$
r_{1}^{\prime}(\lambda)>0 \quad \text { when } k \geqslant 7 .
$$

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

$$
r_{1}(\sqrt{k+1})>0 \quad \text { when } k \geqslant 5 .
$$

So we have $r_{1}(\lambda)>0$ for $\lambda \geqslant \lambda_{1}\left(U_{2 k}^{1}\right)$. Then, by Lemma 2.3, an immediate consequence is that $\lambda_{1}\left(U_{2 k}^{1}\right)>\lambda_{1}\left(U_{2 k}^{2}\right)$ when $k \geqslant 7$.

When $k=4,5,6$, by direct calculation we obtain that $\lambda_{1}\left(U_{8}^{1}\right) \approx 2.5741$, $\lambda_{1}\left(U_{8}^{2}\right) \approx 2.5606 ; \lambda_{1}\left(U_{10}^{1}\right) \approx 2.7557, \lambda_{1}\left(U_{10}^{2}\right) \approx 2.7117 ; \lambda_{1}\left(U_{12}^{1}\right) \approx 2.9269$, $\lambda_{1}\left(U_{12}^{2}\right) \approx 2.8634$. Thus the first inequality holds for all $k \geqslant 4$.

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

$$
\begin{align*}
P\left(U_{2 k}^{2}, \lambda\right)= & P\left(U_{2 k}^{2}-e_{2}, \lambda\right)-P\left(U_{2 k}^{2}-x-y, \lambda\right) \\
& -2 P\left(3 K_{1} \cup(k-3) K_{2}, \lambda\right)  \tag{i}\\
P\left(U_{2 k}^{3}, \lambda\right)= & P\left(U_{2 k}^{3}-e^{\prime \prime}, \lambda\right)-P\left(U_{2 k}^{3}-u^{\prime}-w^{\prime}, \lambda\right) \\
& -2 P\left(K_{1} \cup(k-2) K_{2}, \lambda\right) \tag{ii}
\end{align*}
$$

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

$$
P\left(U_{2 k}^{2}-e_{2}, \lambda\right)=P\left(U_{2 k}^{3}-e^{\prime \prime} \lambda\right) .
$$

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

$$
P\left(U_{2 k}^{2}-x-y, \lambda\right)>P\left(U_{2 k}^{3}-u^{\prime}-w^{\prime}, \lambda\right) \quad \text { for all } \lambda \geqslant \lambda_{1}\left(U_{2 k}^{3}-u^{\prime}-w^{\prime}\right)
$$

It is easy to verify that

$$
P\left(3 K_{1} \cup(k-3) K_{2}, \lambda\right)>P\left(K_{1} \cup(k-2) K_{2}, \lambda\right) \quad \text { when } \lambda>1
$$

Since $U_{2 k}^{3}-u^{\prime}-w^{\prime}$ is a proper subgraph of $U_{2 k}^{3}$, we have $\lambda_{1}\left(U_{2 k}^{3}\right)>\lambda_{1}\left(U_{2 k}^{3}-u^{\prime}-\right.$ $w^{\prime}$ ). Hence by Eqs. (i) and (ii), we get

$$
P\left(U_{2 k}^{2}, \lambda\right)<P\left(U_{2 k}^{3}, \lambda\right) \quad \text { for all } \lambda \geqslant \lambda_{1}\left(U_{2 k}^{3}\right)
$$

Thus we have the result. The proof is completed.
Let $G$ be a graph in $\mathscr{U}_{2 k}^{+}, k \geqslant 4$, and let $C_{G}$ be the cycle of $G, C_{G} \not \approx C_{3}$. 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 $r v$ is in a perfect matching of $G$.

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

Lemma 3.4. Let $G$ and $G^{\prime}$ be the two graphs in Fig. 4. Then

$$
P(G, \lambda)>P\left(G^{\prime}, \lambda\right) \quad \text { for all } \lambda \geqslant \lambda_{1}(G)
$$

In particular, $\lambda_{1}\left(G^{\prime}\right) \geqslant \lambda_{1}(G)$.
Proof. Consider the edge $e_{1}=v u(u \neq r)$ of $C_{G}$ and the edge and the edge $e_{1}^{\prime}=r u$ of $C_{G^{\prime}}$. Note that $\left|V\left(C_{G^{\prime}}\right)\right|=\left|V\left(C_{G}\right)\right|-1$. By Lemma 2.4, we have

$$
\begin{aligned}
& P(G, \lambda)=P\left(G-e_{1}, \lambda\right)-P(G-v-u, \lambda)-2 P\left(G \backslash V\left(C_{G}\right), \lambda\right) \\
& P\left(G^{\prime}, \lambda\right)=P\left(G^{\prime}-e_{1}^{\prime}, \lambda\right)-P\left(G^{\prime}-r-u, \lambda\right)-2 P\left(G^{\prime} \backslash V\left(C_{G^{\prime}}\right), \lambda\right)
\end{aligned}
$$


$G$

$G^{\prime}$

Fig. 4. The graph $G$ and the resulting graph $G^{\prime}$ in Lemma 3.4.

Moreover, it is easy to see that we have

$$
\begin{aligned}
& G-e_{1} \cong G^{\prime}-e_{1}^{\prime}, \\
& G^{\prime}-r-u \subset G-v-u, \\
& G^{\prime} \backslash V\left(C_{G^{\prime}}\right)=G \backslash V\left(C_{G}\right) \cup\left\{v^{\prime}\right\}
\end{aligned}
$$

Hence,

$$
\begin{aligned}
& P\left(G-e_{1}, \lambda\right)=P\left(G^{\prime}-e_{1}^{\prime}, \lambda\right), \\
& P\left(G^{\prime} \backslash V\left(C_{G^{\prime}}\right), \lambda\right)=\lambda P\left(G \backslash V\left(C_{G}\right), \lambda\right)>P\left(G \backslash V\left(C_{G}\right), \lambda\right) \quad \text { when } \lambda>1,
\end{aligned}
$$

and by Lemma 2.7, we have

$$
P\left(G^{\prime}-r-u, \lambda\right)>P(G-v-u, \lambda) \quad \text { for all } \lambda \geqslant \lambda_{1}(G-v-u) .
$$

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 $P(G, \lambda)>P\left(G^{\prime}, \lambda\right)$ for all $\lambda \geqslant$ $\lambda_{1}(G)$.

The proof is completed.
Theorem 3.5. Let $G$ be a graph in $\mathscr{U}_{2 k}^{+}, k \geqslant 4$. Then

$$
\lambda_{1}(G) \leqslant \lambda_{1}\left(U_{2 k}^{1}\right)
$$

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

Proof. Suppose that $G$ is a graph in $\mathscr{U}_{2 k}^{+}, k \geqslant 4$. If $G \cong C_{2 k}$, the result is obvious. If the cycle $C_{G}$ is $C_{3}$, by Theorem 3.3, the result also holds. So now we assume $G \not \not C_{2 k}$, and $\left|V\left(C_{G}\right)\right| \geqslant 4$. 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 $\lambda_{1}(G)<\lambda_{1}\left(G_{0}\right)$. Therefore, it is sufficient to focus our attention on those unicyclic graphs in $\mathscr{U}_{2 k}^{+}$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 $\lambda_{1}\left(G_{0}\right)<\lambda_{1}\left(G_{1}\right)$. 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 $\lambda_{1}\left(G_{1}\right)<\lambda_{1}\left(U_{0}\right)$. 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 $U_{2 k}^{1}$ and $U_{2 k}^{2}$. By Theorem 3.3, the result holds immediately.
(ii) The cycle $C_{U_{0}}$ of $U_{0}$ is not $C_{3}$. Then we have $\left|V\left(C_{U_{0}}\right)\right| \geqslant 4$. 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 $u v_{0}$ 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 $u v$, is attached, and $\lambda_{1}\left(U_{0}\right)<\lambda_{1}\left(U_{1}\right)$. If $U_{1} \cong U_{2 k}^{2}$, then we have the result by Theorem 3.3; If $\left|V\left(C_{U_{1}}\right)\right| \geqslant 4$, 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 $r u$, and attach a path of length 2 , say $r u^{\prime} v^{\prime}$, 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. $\lambda_{1}\left(U_{1}\right)<\lambda_{1}\left(U_{2}\right)$.
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 $e_{1}=u u_{1}$ of $U_{1}$ and the edge $e_{2}=r u_{1}$ of $U_{2}$. By Lemma 2.4, we have

$$
\begin{aligned}
& P\left(U_{1}, \lambda\right)=P\left(U_{1}-e_{1}, \lambda\right)-P\left(U_{1}-u-u_{1}, \lambda\right)-2 P\left(U_{1} \backslash V\left(C_{U_{1}}\right), \lambda\right), \\
& P\left(U_{2}, \lambda\right)=P\left(U_{2}-e_{2}, \lambda\right)-P\left(U_{2}-r-u_{1}, \lambda\right)-2 P\left(U_{2} \backslash V\left(C_{U_{2}}\right), \lambda\right) .
\end{aligned}
$$

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, $P\left(U_{1}-e_{1}, \lambda\right)=P\left(U_{2}-e_{2}, \lambda\right)$.
And, by Lemma 2.7, we have $P\left(U_{2}-r-u_{1}, \lambda\right)>P\left(U_{1}-u-u_{1}, \lambda\right)$ when $\lambda \geqslant \lambda_{1}\left(U_{1}-u-u_{1}\right)$.

Moreover,

$$
\begin{aligned}
& P\left(U_{1} \backslash V\left(C_{U_{1}}\right), \lambda\right)=\lambda^{s}\left(\lambda^{2}-1\right)^{i} \\
& P\left(U_{2} \backslash V\left(C_{U_{2}}\right), \lambda\right)=\lambda^{s-1}\left(\lambda^{2}-1\right)^{i+1}
\end{aligned}
$$

where $s$ is the number of pendant edges attached to roots of $U_{1}$. Then

$$
P\left(U_{2} \backslash V\left(C_{U_{2}}\right), \lambda\right)-P\left(U_{1} \backslash V\left(C_{U_{1}}\right), \lambda\right)=\lambda^{s-1}\left(\lambda^{2}-1\right)^{i}\left(\lambda^{2}-\lambda-1\right) .
$$

Therefore, $P\left(U_{2} \backslash V\left(C_{U_{2}}\right), \lambda\right)>P\left(U_{1} \backslash V\left(C_{U_{1}}\right), \lambda\right)$ when $\lambda>(1+\sqrt{5}) / 2$.
Since $U_{1}-u-u_{1}$ is a proper subgraph of $U_{1}$, we know that $\lambda_{1}\left(U_{1}\right)>\lambda_{1}\left(U_{1}-\right.$ $\left.u-u_{1}\right)$. Thus, when $\lambda \geqslant \lambda_{1}\left(U_{1}\right)(>(1+\sqrt{5}) / 2)$, we have $P\left(U_{1}, \lambda\right)>P\left(U_{2}, \lambda\right)$. So the Claim is established.

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

The proof is completed.
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 $\mathscr{U}_{2 k}^{+}, k \geqslant 4$, and $G \not \not U_{2 k}^{1}$. Then

$$
\lambda_{1}(G) \leqslant \lambda_{1}\left(U_{2 k}^{2}\right)
$$

and the equality holds if and only if $G \cong U_{2 k}^{2}$, where $\lambda_{1}\left(U_{2 k}^{2}\right)$ 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 $\mathscr{U}_{6}^{+}$, 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 $\mathscr{U}_{2 k}^{+}(k \neq 3)$, two graphs $U_{2 k}^{1}$ and $U_{2 k}^{2}$ have the largest and the second largest spectral radius, respectively.

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