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On the Spectral Radius of Unicyclic Graphs *

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Abstract

Let $U(n,m)$ be the set of all unicyclic graphs on n vertices with a maximum matching of cardinality m ($m \geq 2$). Denote by $U^1(n,m)$ the graph on n vertices obtained from C_3 by attaching $n-2m+1$ pendant edges and $m-2$ paths of length 2 together to one of three vertices of C_3. Denote by $U^2(n,m)$ the graph on n vertices obtained from C_3 by attaching $n-2m+1$ pendant edges and $m-3$ paths of length 2 together to one of three vertices, and two pendant edges to the other two vertices of C_3, respectively. In this paper, we prove that $U^1(n,m)$ and $U^2(n,m)$ have the largest and the second largest spectral radius among the graphs in $U(n,m)$, respectively, when $m \geq 4$. We also discuss the corresponding results when $m = 2, 3$.

1. Introduction

In quantum chemistry the skeletons of certain non-saturated hydrocarbons are represented by graphs. By Hückel molecular orbital (HMO) theory, energy levels of electrons in such a molecule are, in fact, the eigenvalues of the corresponding graph. The stability of the molecule as well as other chemically relevant facts are closely connected with the graph eigenvalues [6, 17]. In particular, following a suggestion by Lovász and Pelikán [24], Cvetković and Gutman [8] proposed that the spectral radius of the molecular graph (of a saturated hydrocarbon) be used as a measure of branching of the underlying molecule. This direction of research was eventually further elaborated, with emphasis on acyclic polyenes [13], alkanes [18], and benzenoid hydrocarbons [15, 16, 25]. To our best knowledge, the spectral radius of unicyclic graphs was, so far, not considered in the chemical literature. On the other hand, unicyclic graphs represent important classes of molecules (e.g., monocycloalkanes), and their spectral radius was much studied in graph spectral theory (see, e.g., [3, 10, 20, 28]). The evaluation of graph eigenvalues were the topic of numerous papers (see, e.g., [2]-[4], [7]-[11], [13]-[16], [18]-[28]). Here we are concerned with unicyclic graphs.

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In order to describe our results, we need some graph-theoretic notation and terminology. Other undefined notation may refer to [1].

We consider only finite undirected simple graphs. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. A graph $G' = (V(G'), E(G'))$ is a subgraph of G (written $G' \subseteq G$) if $V(G') \subseteq V(G)$ and $E(G') \subseteq E(G)$; If $G' \neq G$, G' is called a proper subgraph of G and written as $G' \subset G$; If $V(G') = V(G)$, G' is called a spanning subgraph of G. If $W \subset V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E' \subset E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v\}$ and $E' = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively.

Two edges of a graph are said to be independent if they are not adjacent. An m-matching M of G is a set of m mutually independent edges. A vertex v is said to be M-saturated, if some edge of M is incident with v; otherwise, v is M-unsaturated. If every vertex of G is M-saturated, the matching M is perfect. If G has no matching M' with $|M'| > |M|$, then M is a maximum matching; clearly, every perfect matching is maximum. We call the number of edges in a maximum matching of G the edge-independence number and denote it by $\alpha'(G)$. An M-alternating path in G is a path whose edges are alternately in $E \setminus M$ and M. An M-augmenting path is an M-alternating path whose origin and terminus are M-unsaturated.

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 $G_1, G_2, \cdots, G_t$, then G is denoted by $\bigcup_{i=1}^{t} G_i$.

Let $A(G)$ the adjacency matrix of G, then $\mathrm{Det}(\lambda I - A(G))$ is called the characteristic polynomial of G and denoted by $p(G;\lambda)$. Since $A(G)$ is real and symmetric, its eigenvalues are real. These eigenvalues of $A(G)$ are independent of the ordering of the vertices of G, so they are also called the eigenvalues of G. The largest eigenvalue of G is called the spectral radius of G and denoted by $\lambda_1(G)$. In particular, if G is connected, $A(G)$ is irreducible and so $\lambda_1(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\lambda_1(G)$ by the Perron-Frobenius theory of non-negative matrices.

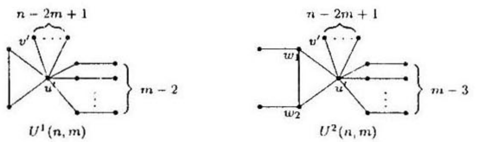


Fig. 1

Unicyclic graphs are connected graphs in which the number of edges equals the number of vertices. Thus a unicyclic graph is either a cycle or a cycle with trees attached. Let $U(n)$ denote the set of all unicyclic graphs on n vertices and $U(n,m)$ the set of all unicyclic graphs on n vertices with $\alpha'(G) = m$ ($m \geq 2$). Let $U^1(n,m)$ denote the graph on n vertices obtained from C_3 by attaching $n - 2m + 1$ pendant edges and $m - 2$ paths of length 2 together to one of three vertices of C_3. Let $U^2(n,m)$ denote the graph on n vertices obtained from C_3 by attaching $n - 2m + 1$ pendant edges and $m - 3$ paths of length 2 together to one of three vertices, and two pendant edges to the other two vertices of C_3, respectively. Both $U^1(n,m)$ and $U^2(n,m)$ are shown in Fig. 1.

The following result, on the spectral radius of unicyclic graphs, is well known.

Theorem 1.1 [2, 28, 20]. *If G is a graph in $U(n)$, then $\lambda_1(C_n) = 2 \leq \lambda_1(G) \leq \lambda_1(S_n^*)$, where S_n^* denotes the graph obtained from S_n by joining any two vertices of degree one in S_n. The lower bound is attained if and only if $G \cong C_n$. The upper bound is attained if and only if $G \cong S_n^*$. Moreover, if $G \ncong S_n^*$, $p(G;\lambda) > p(S_n^*;\lambda)$ for all $\lambda \geq \lambda_1(G)$.*

Since $U(n,m)$ is a subset of $U(n)$, Theorem 1.1 also holds for the graphs in $U(n,m)$. Therefore, C_n alone has the smallest spectral radius among the graphs in $U(n,m)$, where $n = 2m$ or $2m+1$, and $S_n^*(\cong U^1(n,2))$ is the unique graph with the largest spectral radius in $U(n,2)$.

When $n = 2m$, $U(n,m)$ is the set of all unicyclic graphs on $2m$ vertices with perfect matchings. For this case, A. Chang and F. Tian have proved the following result.

Theorem 1.2 [3]. *Among the graphs in $U(2m,m)$, $U^1(2m,m)$ and $U^2(2m,m)$ have the largest and the second largest spectral radius, respectively, when $m \geq 4$.*

The main purpose of this paper is to prove that $U^1(n,m)$ and $U^2(n,m)$ have the largest and the second largest spectral radius among the graphs in $U(n,m)$, respectively, when $m \geq 4$.

2. Preliminaries.

Since the spectral radius of G is the largest root of the equation $p(G;\lambda) = 0$, we have $p(G;\lambda) > 0$ for all $\lambda > \lambda_1(G)$. Then we immediately get the following elementary but useful result.

Lemma 2.1. *Let G_1 and G_2 be two graphs. If $p(G_1;\lambda) < p(G_2;\lambda)$ for $\lambda \geq \lambda_1(G_1)$, then $\lambda_1(G_1) > \lambda_1(G_2)$.*

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

Lemma 2.2 [23, 22, 12].

(1) Let G be a connected graph and G' a proper spanning subgraph of G. Then

$$p(G';\lambda) > p(G;\lambda) \quad for\ \lambda \geq \lambda_1(G).$$

(2) Let G', H' be spanning subgraphs of connected graphs G and H, respectively, where $\lambda_1(G) \geq \lambda_1(H)$ and G' is a proper subgraph of G. Then

$$p(G' \cup H';\lambda) > p(G \cup H;\lambda) \ for\ \lambda \geq \lambda_1(G).$$

The following three results are often used to calculate the characteristic polynomials of unicyclic graphs in our proof.

Lemma 2.3 [6]. *Let v be a vertex of degree 1 in the graph G and u the vertex adjacent to v. Then $p(G;\lambda) = \lambda p(G-v;\lambda) - p(G-\{u,v\};\lambda)$.*

Lemma 2.4 [6, 27]. *Let $e = uv$ be a edge of G and $C(e)$ the set of all cycles containing e. The characteristic polynomial of G satisfies*

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

Lemma 2.5 [6]. *If $G_1, G_2, \cdots, G_t$ are the components of a graph G, we have*

$$p(G;\lambda) = \prod_{i=1}^{t} p(G_i;\lambda).$$

Lemma 2.6 [1]. *A matching M in G is a maximum matching if and only if G contains no M-augmenting path.*

Lemma 2.7 [22]. *Let T be an n-vertex tree with an m-matching, where $n > 2m$. Then there is an m-matching M and a pendant vertex v such that M does not saturate v.*

According to the proof of Theorem 1.2, we have the following two lemmas.

Lemma 2.8 [3]. *Let G be a graph in $U(2m,m)$ $(m \neq 3)$ and $G \not\cong U^1(2m,m)$. Then $p(G;\lambda) > p(U^1(2m,m);\lambda)$ for $\lambda \geq \lambda_1(U^1(2m,m))$. Therefore, $\lambda_1(G) < \lambda_1(U^1(2m,m))$.*

Lemma 2.9 [3]. *Let G be a graph in $U(2m,m)$ $(m \neq 3)$, $G \not\cong U^1(2m,m)$, and $G \not\cong U^2(2m,m)$. Then $p(G;\lambda) > p(U^2(2m,m);\lambda)$ for $\lambda \geq \lambda_1(U^2(2m,m))$. Therefore, $\lambda_1(G) < \lambda_1(U^2(2m,m))$.*

Finally, we list the characteristic polynomials of some graphs which will often be used in our proof.

Let n and m be positive integers and $n \geq 2m$. Denote by $A(n,m)$ the tree obtained from S_{n-m+1} by attaching a pendant edge to each of $m-1$ non-central vertices. For $n > 2m$, denote by $B(n,m)$ the tree obtained from $A(n-1,m)$ by attaching a pendant edge to one vertex of degree 2. Then both $A(n,m)$ and $B(n,m)$ have an m-matching. In Fig. 2, we have drawn $A(14,6)$ and $B(14,6)$.

$A(14,6)$ $B(14,6)$

Fig. 2

Lemma 2.10 [22].
$p(A(n,m);\lambda) = \lambda^{n-2m}(\lambda^2-1)^{m-2} \times [\lambda^4 - (n-m+1)\lambda^2 + (n-2m+1)]$;

$p(B(n,m);\lambda) = \lambda^{n-2m}(\lambda^2-1)^{m-3} \times [\lambda^6 - (n-m+2)\lambda^4 + (3n-4m-1)\lambda^2 - 2(n-2m)]$.

Lemma 2.11 [27].
$p(P_n;\lambda) = \lambda p(P_{n-1};\lambda) - p(P_{n-2};\lambda)$.

By Lemma 2.11, we immediately get $p(P_3;\lambda) = \lambda(\lambda^2-2)$ and $p(P_4;\lambda) = \lambda^4 - 3\lambda^2 + 1$.

3. Main results

Lemma 3.1. *Let G be a graph in $U(n,m)$ and $G \not\cong C_n$, where $n > 2m$. Then there is an m-matching M and a pendant vertex v such that M does not saturate v.*

Proof. Since G is a graph in $U(n,m)$ and $G \not\cong C_n$, G is a cycle attached by some trees. We denote this cycle by C_G. Let M' be a maximum matching of G and u an arbitrary vertex of C_G where some trees are attached. Among the two edges in $E(C_G)$ incident with u, there must be one edge belonging to $E(G)\setminus M'$. We denote this edge by uu_1, then $T = G - uu_1$ is an n-vertex tree with an m-matching M', where $n > 2m$. Furthermore, $\alpha'(T) = \alpha'(G) = m$. (Since $T \subset G$, $\alpha'(T) \leq \alpha'(G) = m$. Noting that M' is an m-matching of T, we have $\alpha'(T) \geq m$. Therefore, $\alpha'(T) = m$.)

For the graph T, by Lemma 2.7, there is an m-matching M and a pendant vertex v such that M does not saturate v. If $v \neq u_1$, then v is also a pendant vertex of G. Noting that M is also an m-matching of G, the result holds. If $v = u_1$, let u_2 be the unique vertex of C_G adjacent to u_1 in T. The vertex u_2 must be saturated. (Otherwise, $M \cup \{u_1u_2\}$ is an $(m+1)$-matching of T, which contradicts $\alpha'(T) = m$.) Let $P = u_1u_2\cdots u_t$ $(t \geq 3)$ be the longest M-alternating path of T which starts from u_1. Then u_t is M-saturated for otherwise P is an M-augmenting path of T contradicting Lemma 2.6. Moreover, u_t is a pendant vertex of T. Otherwise, it contradicts the choice of P. Therefore, the symmetric difference $M \triangle P$ is an m-matching M'' of G and $u_t(\neq u_1)$ is an M''-unsaturated pendant vertex of G. This completes the proof of Lemma 3.1. ∎

Theorem 3.2 *Let G be a graph in $U(n,m)$, $m \geq 4$, and $G \ncong U^1(n,m)$. Then $\lambda_1(G) < \lambda_1(U^1(n,m))$.*

Proof. Let G be a graph in $U(n,m)$, $m \geq 4$, and $G \ncong U^1(n,m)$. If G is a cycle, the result holds immediately. So we suppose G is not a cycle. By Lemma 2.1, it is sufficient to prove $p(G;\lambda) > p(U^1(n,m);\lambda)$ for $\lambda \geq \lambda_1(U^1(n,m))$. We prove this by induction on n.

When $n = 2m$, the result holds by Lemma 2.8. Now we suppose $n > 2m$ and the result holds for graphs in $U(n-1,m)$ which are not isomorphic to $U^1(n-1,m)$. By Lemma 3.1, G has an m-matching M and a pendant vertex v such that M does not saturate v. Let u be the vertex of G adjacent to v and $v'u'$ a pendant edge of $U^1(n,m)$ attached to C_3 (see Fig. 1).

By Lemma 2.3, we have

$$\begin{aligned} p(G;\lambda) &= \lambda p(G-v) - p(G-\{u,v\};\lambda), \\ p(U^1(n,m);\lambda) &= \lambda p(U^1(n,m)-v';\lambda) - p(U^1(n,m)-\{v',u'\};\lambda). \end{aligned}$$

It is easy to see that $G - v \in U(n-1,m)$ and $U^1(n,m) - v' \cong U^1(n-1,m)$. By the induction hypothesis,

$$p(G-v;\lambda) \geq p(U^1(n,m)-v';\lambda) \text{ for } \lambda \geq \lambda_1(U^1(n,m)-v').$$

By Lemma 2.1, $\lambda_1(U^1(n,m)-v') \geq \lambda_1(G-v)$. Since $U^1(n,m)-\{v',u'\} \cong (m-1)K_2 \cup (n-2m)K_1$, $G \ncong U^1(n,m)$ and $G-\{u,v\}$ has an $(m-1)$-matching, $U^1(n,m)-\{v',u'\}$ is a proper spanning subgraph of $G-\{u,v\}$. By Lemma 2.2,

$$p(G-\{u,v\};\lambda) < p(U^1(n,m)-\{v',u'\};\lambda) \text{ for } \lambda \geq \lambda_1(G-\{u,v\}).$$

Since $\lambda_1(U^1(n,m)) > \lambda_1(U^1(n,m)-v') \geq \lambda_1(G-v) > \lambda_1(G-\{u,v\})$, we get

$$p(G;\lambda) > p(U^1(n,m);\lambda) \text{ for } \lambda \geq \lambda_1(U^1(n,m)).$$

∎

It is known that the graph $S_n^* \cong U^1(n,2)$ has the largest spectral radius among the graphs in $U(n,2)$, and so we have

Theorem 3.3. *The graph $U^1(n,m)$ alone has the largest spectral radius in $U(n,m)$, when $m \neq 3$.*

Before proving that $U^2(n,m)$ has the second largest spectral radius in $U(n,m)$, we give the characteristic polynomials of some graphs which will be used in our proof.

Lemma 3.4. *Let n and m be two integers such that $n > 2m$ and $m \geq 4$. Denote by G_a, G_b, G_c, G_d and G_e the graphs shown in Fig. 3 and 4, respectively. Then*

$$\begin{aligned}
p(U^2(n,m);\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6-2\lambda^5+(4n-5m+3)\lambda^4 \\
&\quad +2\lambda^3-(4n-7m+4)\lambda^2+(n-2m+1)] \\
p(G_a;\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6-2\lambda^5+(4n-5m+5)\lambda^4 \\
&\quad +6\lambda^3-(5n-8m+3)\lambda^2-4\lambda+(2n-4m+1)] \\
p(G_b;\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6-2\lambda^5+(4n-5m+4)\lambda^4 \\
&\quad +6\lambda^3-(5n-8m+1)\lambda^2-4\lambda+(2n-4m)] \\
p(G_c;\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6-2\lambda^5+(4n-5m+4)\lambda^4 \\
&\quad +4\lambda^3-(5n-8m+2)\lambda^2-2\lambda+(2n-4m+1)] \\
p(G_d;\lambda) &= (\lambda^2-1)^{m-4}[\lambda^9-(m+5)\lambda^7-2\lambda^6+(3m+9)\lambda^5+6\lambda^4-(3m+7)\lambda^3 \\
&\quad -6\lambda^2+(m+2)\lambda+2] \\
p(G_e;\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6+(4n-5m+3)\lambda^4 \\
&\quad -(5n-8m)\lambda^2+(2n-4m)].
\end{aligned}$$

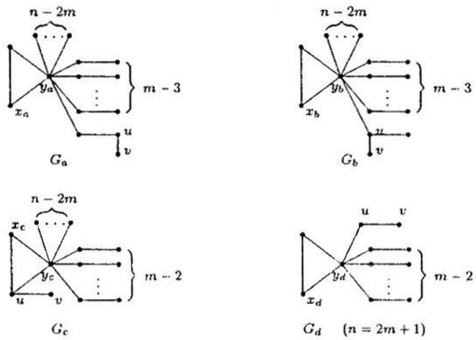


Fig. 3

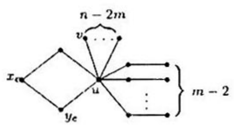


Fig. 4

Proof. For the graph $U^2(n,m)$, let w_1 and w_2 be two vertices of C_3 shown in Fig. 1. By Lemma 2.4, we have

$$p(U^2(n,m);\lambda) = p(U^2(n,m)-w_1w_2;\lambda) - p(U^2(n,m)-\{w_1,w_2\};\lambda) -2p((n-2m+3)K_1 \cup (m-3)K_2;\lambda).$$

Noting that $U^2(n,m) - w_1w_2 \cong A(n,m)$ and $U^2(n,m) - \{w_1,w_2\} \cong 2K_1 \cup A(n-4,m-2)$, by Lemmas 2.5 and 2.10, we have

$$p(U^2(n,m);\lambda) = \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6-2\lambda^5+(4n-5m+3)\lambda^4 +2\lambda^3-(4n-7m+4)\lambda^2+(n-2m+1)].$$

For the graph G_a, let x_a, y_a, v and u be the vertices shown in Fig. 3, by Lemmas 2.3 and 2.4, we have

$$\begin{aligned} p(G_a;\lambda) &= \lambda p(G_a-v;\lambda) - p(G_a-\{v,u\};\lambda) \\ &= \lambda p(U^1(n-1,m);\lambda) - p(U^1(n-2,m-1);\lambda) \\ &= \lambda[p(U^1(n-1,m)-x_ay_a;\lambda) - p(U^1(n-1,m)-\{x_a,y_a\};\lambda) \\ &\quad -2p((n-2m)K_1 \cup (m-2)K_2;\lambda)] - [p(U^1(n-2,m-1)-x_ay_a;\lambda) \\ &\quad -p(U^1(n-2,m-1)-\{x_a,y_a\};\lambda) - 2p((n-2m+1)K_1 \cup (m-3)K_2;\lambda]. \end{aligned}$$

Noting that $U^1(n-1,m)-x_ay_a \cong A(n-1,m)$, $U^1(n-1,m)-\{x_a,y_a\} \cong (n-2m+1)K_1 \cup (m-2)K_2$, $U^1(n-2,m-1)-x_ay_a \cong A(n-2,m-1)$ and $U^1(n-2,m-1)-\{x_a,y_a\} \cong (n-2m+2)K_1 \cup (m-3)K_2$, by Lemmas 2.5 and 2.10, we have

$$p(G_a;\lambda) = \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^8-(n-m+4)\lambda^6-2\lambda^5+(4n-5m+5)\lambda^4 +6\lambda^3-(5n-8m+3)\lambda^2-4\lambda+(2n-4m+1)].$$

Similarly, we can calculate the characteristic polynomials of graphs G_b, G_c, G_d and G_e, by using Lemmas 2.3, 2.4, 2.5, 2.10 and 2.11. ■

Theorem 3.5. *Let G be a graph in $U(n,m)$, $G \ncong U^1(n,m)$ and $G \ncong U^2(n,m)$, where $m \geq 4$. Then $\lambda_1(G) < \lambda_1(U^2(n,m))$.*

Proof. Let G be a graph in $U(n,m)$, $G \ncong U^1(n,m)$ and $G \ncong U^2(n,m)$, where $m \geq 4$. If G is a cycle, the result holds immediately. So we suppose G is not a cycle. By Lemma 2.1, it is sufficient to prove $p(G;\lambda) > p(U^2(n,m);\lambda)$ for $\lambda \geq \lambda_1(U^2(n,m))$. We prove this by induction on n.

When $n = 2m$, the result holds by Lemma 2.9. Now we suppose $n > 2m$ and the result holds for graphs in $U(n-1,m)$ which are isomorphic to neither $U^1(n-1,m)$ nor $U^2(n-1,m)$. By Lemma 3.1, G has an m-matching M and a pendant vertex v such that M does not saturate v. Let u be the vertex of G adjacent to v and $v'u'$ a pendant edge of $U^2(n,m)$ attached to C_3 together with $m-2$ paths of length 2 (see Fig. 1).

Case 1. $G - v \cong U^1(n-1,m)$.

Since $G - v \cong U^1(n-1,m)$ and $G \ncong U^1(n,m)$, G must be isomorphic to one of the graphs shown in Fig. 3.

If $G \cong G_a$, we have

$$\begin{aligned} p(G_a;\lambda) - p(U^2(n,m);\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[2\lambda^4 + 4\lambda^3 - (n-m-1)\lambda^2 - 4\lambda \\ &\quad +n-2m] \\ &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^4 - (n-m)\lambda^2 + n - 2m + f_a(\lambda)], \end{aligned}$$

where $f_a(\lambda) = \lambda^4 + 4\lambda^3 + \lambda^2 - 4\lambda$.

Since $A(n-1,m)$ is a proper subgraph of $U^2(n,m)$, $\lambda_1(U^2(n,m)) > \lambda_1(A(n-1,m))$. Thus $p(A(n-1,m);\lambda) > 0$ for $\lambda \geq \lambda_1(U^2(n,m))$. It follows that

$$\lambda^4 - (n-m)\lambda^2 + n - 2m > 0 \ for \ \lambda \geq \lambda_1(U^2(n,m)).$$

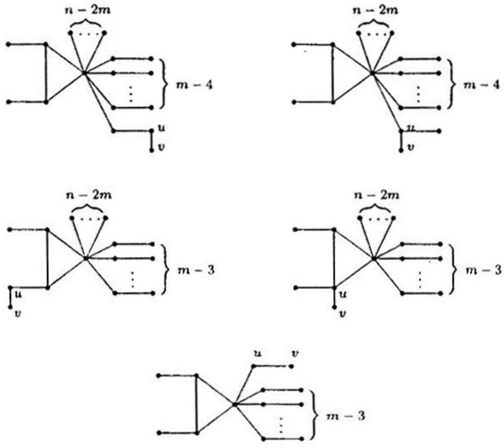
Since $f_a'(\lambda) = 4\lambda^3 + 12\lambda^2 + 2\lambda - 4 > 0$ for $\lambda \geq 2$ and $f_a(2) = 44 > 0$, we have $f_a(\lambda) > 0$ for $\lambda \geq 2$. By Theorem 1.1, $\lambda_1(U^2(n,m)) > 2$. So $f_a(\lambda) > 0$ for $\lambda \geq \lambda_1(U^2(n,m))$. Thus

$$p(G_a;\lambda) > p(U^2(n,m);\lambda) \ for \ \lambda \geq \lambda_1(U^2(n,m)).$$

For the remaining three cases, the proofs are similar.

Case 2. $G - v \cong U^2(n-1,m)$.

Since $G - v \cong U^2(n-1,m)$ and $G \not\cong U^2(n,m)$, then G is isomorphic to one of the graphs shown in Fig. 5.



(n = 2m + 1)

Fig. 5

By Lemma 2.2, we have

$$\begin{aligned} p(G;\lambda) &= \lambda p(G-v;\lambda) - p(G-\{u,v\};\lambda), \\ p(U^2(n,m);\lambda) &= \lambda p(U^2(n,m)-v';\lambda) - p(U^2(n,m)-\{v',u'\};\lambda). \end{aligned}$$

Obviously, $G - v \cong U^2(n,m) - v' \cong U^2(n-1,m)$ and $U^2(n,m) - \{v',u'\} \cong (m-3)K_2 \cup (n-2m)K_1 \cup P_4$. Then $p(G-v;\lambda) = p(U^2(n,m) - v';\lambda)$. It is easy to see that $U^2(n,m) - \{v',u'\}$ is a proper spanning subgraph of $G - \{u,v\}$. So by Lemma 2.3, we have

$$p(U^2(n,m) - \{v',u'\};\lambda) > p(G - \{u,v\};\lambda) \text{ for } \lambda \geq \lambda_1(G - \{u,v\}).$$

Since $\lambda_1(U^2(n,m)) > \lambda_1(G-v) > \lambda_1(G - \{u,v\})$, we have

$$p(G;\lambda) > p(U^2(n,m);\lambda) \ for \ \lambda \geq \lambda_1(U^2(n,m)).$$

Case 3. $G - v \ncong U^1(n-1,m)$ and $G - v \ncong U^2(n-1,m)$.

Since $G - v \in U(n-1,m)$, $G - v \ncong U^1(n-1,m)$ and $G - v \ncong U^2(n-1,m)$, by the induction hypothesis, we have

$$P(G-v;\lambda) > p(U^2(n,m) - v';\lambda)) \ for \ \lambda \geq \lambda_1(U^2(n,m) - v').$$

If $U^2(n,m) - \{v',u'\}$ is a proper spanning subgraph of $G - \{v,u\}$, the result holds by Lemma 2.3. If $U^2(n,m) - \{v',u'\}$ is not a proper spanning subgraph of $G - \{v,u\}$, $G - \{v,u\}$ is isomorphic to one of the graphs shown in Fig. 6 or to a graph G' on $n-2$ vertices with $\alpha'(G') = m-1$. Furthermore, at least one component of G' has more than two vertices and no component contains P_4. Such a component of G' must be a star S_t $(t \geq 2)$.

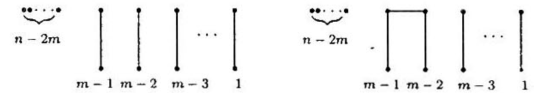
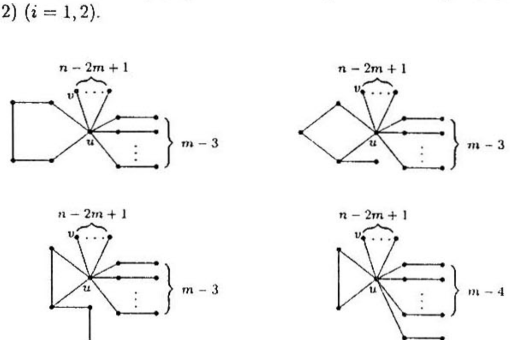


Fig. 6

Since $G \ncong U^1(n,m)$, $G \ncong U^2(n,m)$, $G - v \ncong U^1(n-1,m)$ and $G - v \ncong U^2(n-1,m)$, G must be one of the graphs shown in Fig. 7 and Fig. 8. In Fig. 8, G_i is a graph on n vertices which is not isomorphic to $U^1(n,m)$ and each box represents a component of $G_i - \{v,u\}$, i.e. a star S_t $(t \geq 2)$ $(i = 1,2)$.



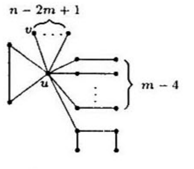


Fig. 7

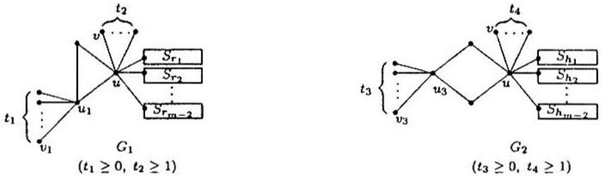


Fig. 8

For the graphs G in Fig. 7, we have $p(G-v;\lambda) > p(U^2(n,m)-v';\lambda)$ for $\lambda \geq \lambda_1(U^2(n,m)-v')$ and $p(G-\{u,v\};\lambda) = p(U^2(n,m)-\{v',u'\};\lambda)$, since $G-\{u,v\} \cong U^2(n,m)-\{v',u'\} \cong (m-3)K_2 \cup (n-2m)K_1 \cup P_4$. Thus the result holds.

For the graph G_1, we distinguish the following two cases:

(1) $G_1 \cong G_a$ or $G_1 \cong G_b$ or $G_1 \cong G_c$.

By the proof of Case 1, the result holds.

(2) $G_1 \ncong G_a$, $G_1 \ncong G_b$ and $G_1 \ncong G_c$.

When $t_1 \geq 1$, we replace vertices v, u by v_1, u_1 (as shown in Fig. 8) , respectively; When $t_1 = 0$, since $G_1 \ncong U^1(n,m)$, at least one component of $G_1 - \{u,v\}$ has more than two vertices. In other words, there must be a star $S_{r_i}(r_i \geq 3)$. Then we choose a pendant vertex v_2 of G_1 $(v_2 \in V(S_{r_i}))$ and the vertex u_2 adjacent to v_2, and replace v, u by v_2, u_2, respectively. Since $G_1 \ncong G_a$, $G_1 \ncong G_b$ and $G_1 \ncong G_c$, $G_1 - v \in U(n-1,m)$, $G_1 - v \ncong U^1(n-1,m)$, $G_1 - v \ncong U^2(n-1,m)$ and $U^2(n,m) - \{v',u'\}$ is a proper spanning subgraph of $G_1 - \{v,u\}$. Then the result holds.

For the graph G_2, we also distinguish two cases:

(1) $G_2 \cong G_e$.

Here we have

$$\begin{aligned} p(G_e;\lambda) - p(U^2(n,m);\lambda) &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[2\lambda^5 - 2\lambda^3 - (n-m-4)\lambda^2 \\ &\quad +n-2m-1] \\ &= \lambda^{n-2m}(\lambda^2-1)^{m-4}[\lambda^4 - (n-m+1)\lambda^2 + n - 2m + 1 \\ &\quad +f_c(\lambda)], \end{aligned}$$

where $f_c(\lambda) = 2\lambda^5 - \lambda^4 - 2\lambda^3 + 5\lambda^2 - 2$.

Since $A(n,m)$ is a proper subgraph of $U^2(n,m)$, $\lambda_1(U^2(n,m)) > \lambda_1(A(n,m))$. It follows that

$$\lambda^4 - (n-m+1)\lambda^2 + n - 2m + 1 > 0.$$

Thus $p(A(n,m);\lambda) > 0$ for $\lambda \geq \lambda_1(U^2(n,m))$. Since $f_e'(\lambda) = 10\lambda^4 - 4\lambda^3 - 6\lambda^2 + 10\lambda = 2\lambda^2(5\lambda^2 - 2\lambda - 3) + 10\lambda > 0$ for $\lambda \geq 2$ and $f_e(2) = 50 > 0$, we have $f_e(\lambda) > 0$ for $\lambda \geq 2$. By Theorem 1.1, $\lambda_1(U^2(n,m)) > 2$. So $f_e(\lambda) > 0,\ for\ \lambda \geq \lambda_1(U^2(n,m))$. Thus

$$p(G_e;\lambda) > p(U^2(n,m);\lambda)\ for\ \lambda \geq \lambda_1(U^2(n,m)).$$

(2) $G_2 \ncong G_e$.

If $t_3 \geq 1$, we replace vertices v, u by v_3, u_3 (as shown in Fig. 8), respectively; If $t_3 = 0$, then at least one component of $G_2 - \{u,v\}$ has more than two vertices. In other words, there must be a star $S_{h_i}(h_i \geq 3)$. Then we choose a pendant vertex v_4 of $G_1(v_4 \in V(S_{h_i}))$ and the vertex u_4 adjacent to v_4, and replace v, u by v_4, u_4, respectively. Then $G_2 - v \in U(n-1,m)$, $G_2 - v \ncong U^1(n-1,m)$, $G_2 - v \ncong U^2(n-1,m)$ and $U^2(n,m) - \{v', u'\}$ is a proper spanning subgraph of $G_2 - \{v,u\}$. Then the result holds. This completes the proof of Theorem 3.5. ■

Remark

From the table of the spectra of connected graphs on six vertices in [9], we known that $U^2(6,3)$ and $U^1(6,3)$ have the largest and the second largest spectral radius among the graphs in $U(6,3)$. So Theorem 3.3 and 3.5 do not hold when $n = 6$ and $m = 3$. However, when $n = 7$ and $m = 3$, Theorem 3.3 and 3.5 hold, by the table of the spectra of graphs on seven vertices in [5]. In fact, with proofs similar to those of Theorems 3.3 and 3.5, we can obtain the following result.

$U^1(n,3)$ and $U^2(n,3)$ have the largest and the second largest spectral radius among the graphs in $U(n,3)$, where $n \geq 7$.

From the table of the spectra of connected graphs on n vertices ($2 \leq n \leq 5$) in [6], C_4 has the second largest spectral radius among the graphs in $U(4,2)$. When $n \geq 5$ and $m = 2$, with a proof similar to that of Theorem 3.5, we can prove the following result.

$U^3(n,2)$ has the second largest spectral radius among the graphs in $U(n,2)$ ($n \geq 5$), where $U^3(n,2)$ is the graph on n vertices formed from C_3 by attaching $n-4$ pendant edges to one of three vertices and one pendant edge to another vertex of C_3 (as shown in Fig. 9).

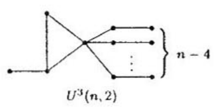


Fig. 9

Acknowledgements

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