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THE LEAST EIGENVALUE OF THE SIGNLESS LAPLACIAN OF NON-BIPARTITE UNICYCLIC GRAPHS WITH K PENDANT VERTICES*

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Abstract. Let $\mathcal{U}(n,k)$ be the set of non-bipartite unicyclic graphs with n vertices and k pendant vertices, where $n \geq 4$. In this paper, the unique graph with the minimal least eigenvalue of the signless Laplacian among all graphs in $\mathcal{U}(n,k)$ is determined. Furthermore, it is proved that the minimal least eigenvalue of the signless Laplacian is an increasing function in k. Let $\mathcal{U}_n$ denote the set of non-bipartite unicyclic graphs on n vertices. As an application of the above results, the unique graph with the minimal least eigenvalue of the signless Laplacian among all graphs in $\mathcal{U}_n$ is characterized, which has recently been proved by Cardoso, Cvetković, Rowlinson, and Simić.

Key words. Non-bipartite unicyclic graph, Signless Laplacian, Least eigenvalue, Pendant vertices.

AMS subject classifications. 05C50.

1. Introduction. All graphs considered are simple, undirected, and connected. The vertex set and edge set of the graph G are denoted by $V(G)$ and $E(G)$, respectively. The distance between vertices u and v of a graph G is denoted by $d_G(u,v)$. The degree of a vertex v, written by $d_G(v)$ or $d(v)$, is the number of edges incident with v. A pendant vertex is a vertex of degree 1. The set of the neighbors of a vertex v is denoted by $N_G(v)$ or $N(v)$. The *girth* $g(G)$ of a graph G is the length of the shortest cycle in G, with the girth of an acyclic graph being infinite. Denote by C_n and P_n the cycle and the path, respectively, on n vertices.

The *adjacency matrix* of G is defined to be the matrix $A(G) = (a_{ij})$, where $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. The degree matrix of G is denoted by $D(G) = \mathrm{diag}(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$. The matrix $Q(G) = D(G) + A(G)$ is called the *signless Laplacian* or the $Q-$*matrix* of G. Note that $Q(G)$ is nonnegative, symmetric and positive semidefinite, so its eigenvalues are real and can be arranged

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ELA

in non-increasing order as follows:

$$q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G) \geq 0,$$

where $q_1(G)$ is the signless Laplacian spectral radius of graph G, and the least eigenvalue $q_n(G)$, denoted by $q(G)$ or q for short, is called the *least eigenvalue of the signless Laplacian* or the *least Q-eigenvalue* of G. It is well known [3] that $q(G) = 0$ of a connected graph G if and only if G is bipartite.

Recently, the signless Laplacian matrix of G has received much attention. As pointed out by Haemers and Spence [7], sometimes the matrix Q is more informative about G than the adjacency matrix A or the Laplacian matrix $L(G) = D - A$. Computer investigations of graphs with up to 11 vertices [4] suggest that the spectrum of $D + A$ performs better than the spectrum of A or $D - A$ in distinguishing non-isomorphic graphs.

There has been a lot of work on the signless Laplacian spectral radius of a graph in recent years, however relatively few results on the least eigenvalue of the signless Laplacian $q(G)$ have appeared in the literature. In [8], Li and Wang proposed the following problem concerning the least eigenvalue of the signless Laplacian:

Given a set of graphs $\mathcal{G}$, find a lower bound for the least eigenvalue of the signless Laplacian and characterize the graphs in which the minimal least eigenvalue of the signless Laplacian is attained.

The above problem is actually one of the signless Laplacian version of the classical Brualdi-Solheid problem [1] for the adjacency matrix. Cardoso et al. [2] determined the unique graph with the minimum value of the least eigenvalue of the signless Laplacian of a connected non-bipartite graph with a prescribed number of vertices. Fan et al. [6] minimized the least eigenvalue among all nonsingular unicyclic mixed graphs in the setting of Laplacian of mixed graphs. Their result can be applied to signless Laplacian of graphs directly. Li and Wang [8] characterized the unique graph whose least eigenvalue of the signless Laplacian attains the minimum among all graphs in the complements of trees on n vertices. In [9], Wang and Fan minimized the least eigenvalue of the signless Laplacian among the class of connected graphs with fixed order which contains a given non-bipartite graph as an induced subgraph. In this paper, we focus on the same question for $\mathcal{U}(n, k)$, the set of non-bipartite unicyclic graphs with n vertices and k pendant vertices.

A connected graph is said to be *non-bipartite unicyclic*, if it has a unique odd cycle, and the same number of vertices and edges. Let $\triangle_n^k$ be the non-bipartite unicyclic graph obtained from C_3 and a star $K_{1,k}$ by joining the center of $K_{1,k}$ and a vertex of C_3 by the path of length $n - k - 3$ (see Fig. 1.1). The main result of this

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paper is as follows:

THEOREM 1.1. *Let U^* have the minimal least eigenvalue of the signless Laplacian among all graphs in $\mathcal{U}(n,k)$. Then U^* is isomorphic to $\triangle_n^k$ for $1 \leq k \leq n-3$. Furthermore, the minimal least eigenvalue of the signless Laplacian $q(\triangle_n^k)$ is an increasing function on k, i.e., $q(\triangle_n^k) < q(\triangle_n^{k+1})$ for $1 \leq k \leq n-4$.*

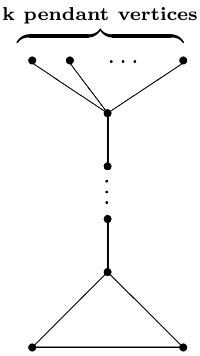

FIG. 1.1. *Graph* $\triangle_n^k$.

2. Preliminaries. Denote the least eigenvalue of $Q(G)$ by $q(G)$. The corresponding eigenvectors are called the *least Q-eigenvectors* of graph G. Let $X = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n$, and G be a graph on vertices $v_1, v_2, \ldots, v_n$. Then X can be considered as a function defined on G, that is, each vertex v_i is mapped to $x_i = x_{v_i}$. If X is an eigenvector of $Q(G)$, then it is naturally defined on $V(G)$, where x_v is the entry of X corresponding to vertex v. One can find that

$$X^T Q(G) X = \sum_{uv \in E(G)} (x_u + x_v)^2.$$

Then q is a signless Laplacian eigenvalue of G corresponding to the eigenvector X if and only if $X \neq 0$ and for each vertex $v \in V(G)$,

$$(q - d_G(v))x_v = \sum_{u \in N_G(v)} x_u. \tag{2.1}$$

In addition, by the Rayleigh-Ritz Theorem, for an arbitrary unit vector $X \in \mathbb{R}^n$,

$$q(G) = \min(X^T Q(G) X) \leq X^T Q(G) X$$

with equality if and only if X is an eigenvector corresponding to the least Q-eigenvalue $q(G)$.

Electronic Journal of Linear Algebra ISSN 1081-3810
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Before giving the proof of Theorem 1.1, we introduce some lemmas in this section.

Lemma 2.1. (**[5]**) *Let G be a connected non-bipartite graph with minimal degree δ, then $0 < q(G) < \delta$. In particular, if G contains a pendant vertex, then $0 < q(G) < 1$.*

Let G_1, G_2 be two vertex-disjoint nontrivial connected graphs with $v_1 \in V(G_1)$ and $u \in V(G_2)$. The *coalescence* of G_1 and G_2, denoted by $G_1v_1uG_2$, is obtained from G_1 and G_2 by identifying v_1 with u (see Fig. 2.1), where G_1 and G_2 are called branches of $G_1v_1uG_2$ with roots v_1 and u, respectively. Let X be a vector defined on $V(G)$. A branch H of G is called a zero branch with respect to X if $x_v = 0$ for all $v \in V(H)$, otherwise it is called a nonzero branch with respect to X.

Fig. 2.1. *$G_1v_1uG_2$ and $G_1v_2uG_2$.*

Lemma 2.2. (**[9]**) *Let G_1, G_2 be two vertex-disjoint nontrivial connected graphs with $v_1, v_2 \in V(G_1)$ and $u \in V(G_2)$. Let X be a least Q-eigenvector of $G_1v_1uG_2$. If $|x_{v_1}| \leq |x_{v_2}|$, then*

$$q(G_1v_1uG_2) \geq q(G_1v_2uG_2)$$

with equality only if $|x_{v_1}| = |x_{v_2}|$ and $d_{G_2}(u)x_u = -\sum_{v \in N_{G_2}(u)} x_v$.

Lemma 2.3. (**[9]**) *Let G be a nontrivial non-bipartite connected graph, and let $G_{k,l}$ be the graph obtained by coalescing G with two paths P_{k+1} and P_{l+1} by identifying an end vertex of P_{k+1} and an end vertex of P_{l+1} both with the same vertex v of G. If $k \geq l \geq 1$, then*

$$q(G_{k,l}) \geq q(G_{k+1,l-1}),$$

with strict inequality if $x_v \neq 0$, where X is a least Q-eigenvector of $G_{k,l}$.

Lemma 2.4. (**[9]**) *Let G be a connected graph which contains a bipartite branch H with root w. Let X be a least Q-eigenvector of G.*
(i) If $x_w = 0$, then H is a zero branch of G with respect to X.
(ii) If $x_w \neq 0$, then $x_v \neq 0$ for every vertex $v \in V(H)$. Furthermore, for every vertex $v \in V(H), x_vx_w$ is either positive or negative, depending on whether v is or is not in the same part of the bipartite graph H as w; consequently, $x_ux_v < 0$ for each edge

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ELA

$uv \in E(H)$.

LEMMA 2.5. (**[9]**) *Let G be a connected non-bipartite graph, and let X be a least Q-eigenvector of G. Let T be a tree, which is a nonzero branch of G with respect to X and with root w. Then $|x_u| < |x_v|$ whenever u, v are vertices of T such that u lies on the unique path from w to v.*

Let $\mathcal{U}_n$ denote the set of non-bipartite unicyclic graphs on n vertices. For any $U \in \mathcal{U}_n$, let C_g be the unique odd cycle in U, where g is the girth of U. In [2], Cardoso et al. obtained the following important result.

LEMMA 2.6. (**[2]**) *Let U be a non-bipartite unicyclic graph on n vertices. Let X be a least Q-eigenvector of U. Then*
(i) $x_s x_t \geq 0$ for some edge st of C_g;
(ii) $x_u x_v \leq 0$ for any other edge uv of U;
(iii) if $x_s x_t = 0$, then either x_s or x_t is nonzero;
(iv) if u is a vertex of U other that s or t, then $|x_u| > |x_s|$ or $|x_u| > |x_t|$.

3. Characterization of the extremal graph. Let $\mathcal{U}(n, k)$ be the set of non-bipartite unicyclic graphs with n vertices and k pendant vertices, where $n \geq 4$. Let U^* have the minimal least Q-eigenvalue in $\mathcal{U}(n, k)$. By Lemma 2.1, clearly $0 < q(U^*) < 1$. Let $\triangle_n^k \in \mathcal{U}(n, k)$ be the non-bipartite unicyclic graph obtained from C_3 and a star $K_{1,k}$ by joining the center of $K_{1,k}$ and a vertex of C_3 by the path of length $n - k - 3$.

First, we consider the case of $k = n - 3$.

THEOREM 3.1. *Let U^* have the minimal least Q-eigenvalue in $\mathcal{U}(n, n-3)$. Then U^* is isomorphic to $\triangle_n^{n-3}$.*

Proof. For $U^* \in \mathcal{U}(n, n-3)$, then the non-bipartite unicyclic graph U^* is obtained from C_3 by adding some pendant edges to its vertices. Suppose that U^* is not isomorphic to $\triangle_n^{n-3}$, then there exist two vertices u, v on C_3 in U^*, which have k_1, k_2 pendant edges, respectively. Let w be a vertex of C_3 other than u or v. Let X be a unit Q-eigenvector of U^* corresponding to $q(U^*)$, without loss of generality, we can assume that $|x_u| \geq |x_v|$. Then by Lemma 2.2, $q(U^*) \geq q(U)$, where U is obtained from U^* by shifting k_2 pendant edges from vertex v to vertex u. If the equality holds, by Lemma 2.2, $|x_u| = |x_v|$ and $k_2 x_v = -k_2 x_s$, where $s \in N_{U^*}(v) \setminus \{u, w\}$. The eigenvalue equations at v and w of U^* yield

$$(q - k_2 - 2)x_v = k_2 x_s + x_u + x_w, \tag{3.1}$$

$$(q - 2)x_w = x_u + x_v, \tag{3.2}$$

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ELA

where $q = q(U^*)$. Since $k_2x_v = -k_2x_s$, (3.1) implies that

$$(q-2)x_v = x_u + x_w. \tag{3.3}$$

Note that $x_v \neq 0$ (otherwise $X = 0$ by Lemma 2.2 and the eigenvalue equation (2.1)). If $x_u = x_v$, then we can deduce that $q(U^*) = 1$ or $q(U^*) = 4$ from (3.2) and (3.3), a contradiction. If $x_u = -x_v$, then we can obtain that $q(U^*) = 1$ from(3.2) and (3.3), a contradiction. Thus, there exists $U \in \mathcal{U}(n, n-3)$ such that $q(U^*) > q(U)$. This contradicts the minimality of U^*. ☐

Next we focus on the case of $1 \leq k \leq n-4$.

Let $\mathcal{U}_1(n,k)$ be the subset of $\mathcal{U}(n,k)$ in which the unicyclic graphs are obtained from C_g by attaching k paths at vertex v_0. Let $\mathcal{U}_2(n,k)$ be the subset of $\mathcal{U}(n,k)$ in which the unicyclic graphs are obtained from $P_{l+1} : v_0u_1\cdots u_l$ $(l \geq 1)$ by attaching C_g to one end vertex v_0 and k paths to the other end vertex u_l (see Fig. 3.1).

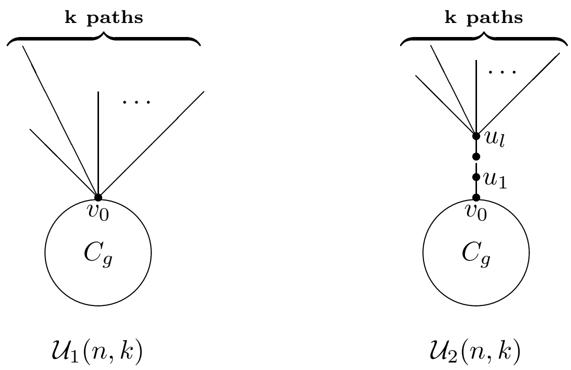

FIG. 3.1. *Two classes of graphs in $\mathcal{U}(n,k)$ with girth g.*

Let $\tilde{U}$ be the non-bipartite unicyclic graph obtained from C_g by attaching k pendant edges at vertex v_0. Clearly $\tilde{U} \in \mathcal{U}_1(n,k)$.

LEMMA 3.2. *For each non-bipartite unicyclic graph $U \in \mathcal{U}(n,k)$, either $q(U) \geq q(\tilde{U})$ or there exists a graph $U_1 \in \mathcal{U}_2(n,k)$ such that $q(U) \geq q(U_1)$.*

Proof. Let C_g be the unique odd cycle in U, where $V(C_g) = \{v_0, v_1, \ldots, v_{g-1}\}$. The unicyclic graph U can be viewed as planting some tree T_i at vertex v_i, where $0 \leq i \leq g-1$. Let X be a unit Q-eigenvector of U corresponding to $q(U)$. Without loss of generality, let $|x_{v_0}| = \max\{|x_{v_i}| : 0 \leq i \leq g-1\}$. Let U_0 be the graph obtained from C_g by planting $T_0, T_1, \ldots, T_{g-1}$ (possibly trivial) at vertex v_0 to form a new big tree T with root v_0, where $d(v_0) \geq 3$. From a repeated use of Lemma 2.2, we have $q(U) \geq q(U_0)$. Consider the graph U_0. Let t be the cardinality of the vertices whose degrees are no less than 3 in $V(T) \setminus \{v_0\}$ and X' be a unit Q-eigenvector of U_0

Electronic Journal of Linear Algebra ISSN 1081-3810
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Volume 26, pp. 333-344, June 2013

ELA

corresponding to $q(U_0)$, and now we distinguish the following three cases:

Case 1. $t = 0$. In this case, $U_0 \in \mathcal{U}_1(n,k)$.

Case 1.1. U_0 is isomorphic to $\tilde{U}$, then $q(U_0) = q(\tilde{U})$.

Case 1.2. U_0 is not isomorphic to $\tilde{U}$, then there exists a vertex $v \in V(T) \setminus \{v_0\}$ with degree 2 in U_0. By Lemmas 2.4 and 2.5, $|x_v^{'}| \geq |x_{v_0}^{'}|$. Denote $N(v_0) = \{v_1, v_{g-1}, w_1, w_2, \ldots, w_p\}$. Assume that w_1 (possibly v) belongs to the unique path joining v_0 and v. Define $U_1 = U_0 - \{v_0w_2, v_0w_3, \ldots, v_0w_p\} + \{vw_2, vw_3, \ldots, vw_p\}$, clearly $U_1 \in \mathcal{U}_2(n,k)$ and by Lemma 2.2, $q(U_0) \geq q(U_1)$.

Case 2. $t = 1$. We can assume that there exists one vertex $v \in V(T) \setminus \{v_0\}$ with $d(v) \geq 3$ in U_0, then there is a unique path with length at least 1 joining v_0 and v. By Lemmas 2.4 and 2.5, $|x_v^{'}| \geq |x_{v_0}^{'}|$.

Case 2.1. $d(v_0) \geq 4$. Denote $N(v_0) = \{v_1, v_{g-1}, w_1, w_2, \ldots, w_p\}$. Assume that vertex w_1 belongs to the unique path joining v_0 and v. Define $U_1 = U_0 - \{v_0w_2, v_0w_3, \ldots, v_0w_p\} + \{vw_2, vw_3, \ldots, vw_p\}$, clearly $U_1 \in \mathcal{U}_2(n,k)$ and by Lemma 2.2, $q(U_0) \geq q(U_1)$.

Case 2.2. $d(v_0) = 3$. In this case, $U_1 = U_0 \in \mathcal{U}_2(n,k)$, and $q(U_0) = q(U_1)$.

Case 3. $t > 1$. Suppose that $u, v \in V(T) \setminus \{v_0\}$ are two vertices of U_0 whose degrees are 3 or greater, and $|x_u^{'}| \geq |x_v^{'}|$. Since T is a tree, there is a path between u and v and only one neighbor of v, say w, is on the path. Assume that $\{v_1, v_2, \ldots, v_{d_v-2}\} \subset N(v) \setminus \{w\}$. Delete the edges (v, v_i) and insert the edges (u, v_i) $(i = 1, 2, \ldots, d_v - 2)$, then we get a new unicycle graph $U_1^{'}$. Obviously $U_1^{'}$ still has k pendant vertices. By Lemma 2.2, we have $q(U_0) \geq q(U_1^{'})$ and the cardinality of the vertices of degree 3 or greater decreases to $t - 1$.

If $t - 1 > 1$, to $U_1^{'}$ repeat the above step until the cardinality is reduced to one. So we get non-bipartite unicyclic graphs

$$U_2^{'}, U_3^{'}, \ldots, U_{t-1}^{'}$$

and

$$q(U_1^{'}) \geq q(U_2^{'}) \geq \cdots \geq q(U_{t-1}^{'}).$$

Moreover, each $U_i^{'}$ has k pendant vertices. Refering to case 2, we always have $U_1 \in \mathcal{U}_2(n,k)$ and $q(U_{t-1}^{'}) \geq q(U_1)$. □

LEMMA 3.3. *Let U^* have the minimal least $Q-$eigenvalue in $\mathcal{U}(n,k)$, where $1 \leq k \leq n-4$. Then $g(U^*) = 3$.*

Electronic Journal of Linear Algebra ISSN 1081-3810
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Volume 26, pp. 333-344, June 2013

Proof. According to Lemma 3.2, we may assume that $U^* \in \mathcal{U}_2(n,k)$ or U^* is isomorphic to $\tilde{U}$.

First consider the case of $U^* \in \mathcal{U}_2(n,k)$. Let C_g be the unique odd cycle in U^*. Suppose that $g(U^*) \geq 5$, and there must exist at least four vertices $v_{i-1}, v_i, v_{i+1}, v_{i+2}$ of C_g in U^*.

Let X be a unit $Q-$eigenvector of U^* corresponding to $q(U^*)$. Since $|x_{v_0}| = \max\{|x_{v_i}| : 0 \leq i \leq g-1\}$, Lemma 2.4 implies $x_{v_0} \neq 0$. According to Lemma 2.6 (i), there must exist an edge $v_iv_{i+1} \in C_g$ such that $x_{v_i}x_{v_{i+1}} \geq 0$. Since $|x_{v_0}| = \max\{|x_{v_i}| : 0 \leq i \leq g-1\}$, by Lemma 2.6 (iv), $v_iv_{i+1} \neq v_0v_1$ and $v_iv_{i+1} \neq v_{g-1}v_0$, i.e., $1 \leq i \leq g-2$. Without loss of generality, we can assume that $|x_{v_i}| \leq |x_{v_{i+1}}|$, by Lemma 2.6 (iii), then $x_{v_{i+1}} \neq 0$. Now we distinguish the following three cases:

Case 1. $(x_{v_{i-1}} - x_{v_{i+2}})(2x_{v_i} + x_{v_{i-1}} + x_{v_{i+2}}) \geq 0$.

Case 1.1. $i = 1$. That is to say, $(x_{v_0} - x_{v_3})(2x_{v_1} + x_{v_0} + x_{v_3}) \geq 0$. Deleting the edge v_1v_0 and inserting the edge v_1v_3, we can get a new graph $U \in \mathcal{U}_2(n,k)$, and

$$\begin{aligned} q(U^*) - q(U) &\geq X^TQ(U^*)X - X^TQ(U)X \\ &= (x_{v_0} + x_{v_1})^2 - (x_{v_1} + x_{v_3})^2 \\ &= (x_{v_0} - x_{v_3})(2x_{v_1} + x_{v_0} + x_{v_3}) \\ &\geq 0. \end{aligned}$$

The equality $q(U^*) = q(U) = q$ holds only if X is also a unit least $Q-$eigenvector of U and $(x_{v_0} - x_{v_3})(2x_{v_1} + x_{v_0} + x_{v_3}) = 0$. By the eigenvalue equations (2.1) of vertices v_0 and v_1 in both U^* and U, we have

$$(q-3)x_{v_0} = x_{u_1} + x_{v_1} + x_{v_{g-1}}, \qquad (q-2)x_{v_1} = x_{v_0} + x_{v_2},$$

$$(q-2)x_{v_0} = x_{u_1} + x_{v_{g-1}}, \qquad (q-2)x_{v_1} = x_{v_2} + x_{v_3}.$$

Hence, $x_{v_1} = -x_{v_0} = -x_{v_3}$. By Lemma 2.6 (iv), $|x_{v_3}| > |x_{v_1}|$, a contradiction. Hence, we find a graph $U \in \mathcal{U}_2(n,k)$ such that $q(U^*) > q(U)$. This contradicts the minimality of U^*.

Case 1.2. $2 \leq i \leq g-2$. Define $\hat{U} = U^* - v_iv_{i-1} + v_iv_{i+2}$, and

$$\begin{aligned} q(U^*) - q(\hat{U}) &\geq X^TQ(U^*)X - X^TQ(\hat{U})X \\ &= (x_{v_i} + x_{v_{i-1}})^2 - (x_{v_i} + x_{v_{i+2}})^2 \\ &= (x_{v_{i-1}} - x_{v_{i+2}})(2x_{v_i} + x_{v_{i-1}} + x_{v_{i+2}}) \\ &\geq 0. \end{aligned}$$

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ELA

At this time, vertex v_{i-1} is a new pendant vertex in $\hat{U}$. Note that $k \geq 1$, there exists an old pendant vertex v in $\hat{U}$. Let $U = \hat{U} - v_1v_0 + v_1v$, clearly $U \in \mathcal{U}_2(n,k)$. Since $|x_{v_0}| < |x_v|$, by Lemma 2.2, $q(\hat{U}) > q(U)$. This contradicts the minimality of U^*.

Case 2. $(x_{v_{i+2}} - x_{v_{i-1}})(2x_{v_{i+1}} + x_{v_{i-1}} + x_{v_{i+2}}) \geq 0$.

Case 2.1. $i = g-2$. That is, $(x_{v_0} - x_{v_{g-3}})(2x_{v_{g-1}} + x_{v_0} + x_{v_{g-3}}) \geq 0$. Deleting the edge $v_{g-1}v_0$ and inserting the edge $v_{g-1}v_{g-3}$, we get a new graph $U \in \mathcal{U}_2(n,k)$, and

$$\begin{aligned} q(U^*) - q(U) &\geq X^TQ(U^*)X - X^TQ(U)X \\ &= (x_{v_0} + x_{v_{g-1}})^2 - (x_{v_{g-1}} + x_{v_{g-3}})^2 \\ &= (x_{v_0} - x_{v_{g-3}})(2x_{v_{g-1}} + x_{v_0} + x_{v_{g-3}}) \\ &\geq 0. \end{aligned}$$

The equality $q(U^*) = q(U) = q$ holds only if X is also a unit least $Q-$eigenvector of U and $(x_{v_0} - x_{v_{g-3}})(2x_{v_{g-1}} + x_{v_0} + x_{v_{g-3}}) = 0$. By the eigenvalue equations (2.1) of vertices v_0 and v_{g-1} in both U^* and U, we have

$$(q-3)x_{v_0} = x_{u_1} + x_{v_1} + x_{g-1}, \qquad (q-2)x_{v_{g-1}} = x_{v_0} + x_{v_{g-2}},$$

$$(q-2)x_{v_0} = x_{u_1} + x_{v_1}, \qquad (q-2)x_{v_{g-1}} = x_{v_{g-3}} + x_{v_{g-2}}.$$

Hence, $x_{v_{g-1}} = -x_{v_0} = -x_{v_{g-3}}$. By Lemma 2.6 (iv), $|x_{v_{g-3}}| > |x_{v_{g-1}}|$, a contradiction. Hence, we find a graph $U \in \mathcal{U}_2(n,k)$ such that $q(U^*) > q(U)$. This contradicts the minimality of U^*.

Case 2.2. $1 \leq i \leq g-3$. Define $\hat{U} = U^* - v_{i+1}v_{i+2} + v_{i+1}v_{i-1}$, and

$$\begin{aligned} q(U^*) - q(\hat{U}) &\geq X^TQ(U^*)X - X^TQ(\hat{U})X \\ &= (x_{v_{i+1}} + x_{v_{i+2}})^2 - (x_{v_{i+1}} + x_{v_{i-1}})^2 \\ &= (x_{v_{i+2}} - x_{v_{i-1}})(2x_{v_{i+1}} + x_{v_{i-1}} + x_{v_{i+2}}) \\ &\geq 0. \end{aligned}$$

At this time, vertex v_{i+2} is a new pendant vertex in $\hat{U}$. Note that $k \geq 1$, there exists an old pendant vertex v in $\hat{U}$. Let $U = \hat{U} - v_{g-1}v_0 + v_{g-1}v$, clearly $U \in \mathcal{U}_2(n,k)$. Since $|x_{v_0}| < |x_v|$, by Lemma 2.2, $q(\hat{U}) > q(U)$. Hence, we find a graph $U \in \mathcal{U}_2(n,k)$ such that $q(U^*) > q(U)$. This contradicts the minimality of U^*.

Case 3. $(x_{v_{i-1}} - x_{v_{i+2}})(2x_{v_i} + x_{v_{i-1}} + x_{v_{i+2}}) < 0$, $(x_{v_{i+2}} - x_{v_{i-1}})(2x_{v_{i+1}} + x_{v_{i-1}} + x_{v_{i+2}}) < 0$. Hence, $2x_{v_i} + x_{v_{i-1}} + x_{v_{i+2}}$ and $2x_{v_{i+1}} + x_{v_{i-1}} + x_{v_{i+2}}$ are of opposite sign. Since we assume that $|x_{v_i}| \leq |x_{v_{i+1}}|$, we have the following two cases:

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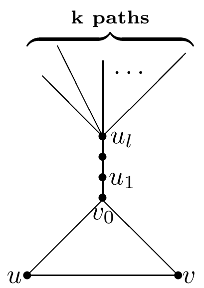
Case 3.1. $x_{v_{i+1}} \geq x_{v_i} \geq 0$. Hence, $2x_{v_{i+1}} + x_{v_{i-1}} + x_{v_{i+2}} > 0$, by Lemma 2.6 (ii), $x_{v_{i-1}}, x_{v_{i+2}} \leq 0$, and $x_{v_{i+1}} > \frac{1}{2}(|x_{v_{i-1}}| + |x_{v_{i+2}}|) \geq \min\{|x_{v_{i-1}}|, |x_{v_{i+2}}|\}$, which is a contradiction to Lemma 2.6 (iv).

Case 3.2. $x_{v_{i+1}} \leq x_{v_i} \leq 0$. It follows that $2x_{v_{i+1}} + x_{v_{i-1}} + x_{v_{i+2}} < 0$, by Lemma 2.6 (ii), $x_{v_{i-1}}, x_{v_{i+2}} \geq 0$, and $|x_{v_{i+1}}| > \frac{1}{2}(x_{v_{i-1}} + x_{v_{i+2}}) \geq \min\{x_{v_{i-1}}, x_{v_{i+2}}\}$, which is a contradiction to Lemma 2.6 (iv).

At last, we consider the case of U^* is isomorphic to $\tilde{U}$.

If U^* is isomorphic to $\tilde{U}$, we have $g(U^*) \geq 5$, since $k + g(U^*) = n \geq k+4$. Similar to the above proof with $U^* \in \mathcal{U}_2(n,k)$, we can always find at least four vertices $v_{i-1}, v_i, v_{i+1}, v_{i+2}$ of C_g in U^* and obtain a contradiction in each case. Hence, it is impossible that U^* is isomorphic to $\tilde{U}$. ◻

Let $\mathcal{U}^*(n,k)$ be the set of non-bipartite unicyclic graphs in $\mathcal{U}_2(n,k)$ which have girth 3 (see Fig. 3.2).



$\mathcal{U}^*(n,k)$

Fig. 3.2. *The class of graphs in* $\mathcal{U}_2(n,k)$ *with girth* 3.

Theorem 3.4. *Let U^* have the minimal least Q-eigenvalue in $\mathcal{U}(n,k)$, where $1 \leq k \leq n-4$. Then U^* is isomorphic to $\triangle_n^k$.*

Proof. According to Lemma 3.3, we can assume without loss of generality that $U^* \in \mathcal{U}^*(n,k)$. If U^* is not isomorphic to $\triangle_n^k$, then $k \geq 2$ and there exists at least a pendant path with length 2 or greater at vertex u_l in U^*. Let X be a unit $Q-$eigenvector of U^* corresponding to $q(U^*)$. From a repeated use of Lemma 2.3, we obtain a new graph $U^{'} \in \mathcal{U}^*(n,k)$ which has one pendant path: $u_l z_1 z_2 \cdots z_{p-1} z_p$ with length $p = n-k-l-2$ and $k-1$ pendant paths with length 1 at vertex u_l in $U^{'}$. Note that $x_{u_l} \neq 0$, by Lemma 2.3, $q(U^*) > q(U^{'})$.

Consider unicyclic graph $U^{'}$, let $X^{'}$ be a unit $Q-$eigenvector of $U^{'}$ corresponding to $q(U^{'})$. Denote $N(u_l) \setminus \{u_{l-1}, z_1\} = \{w_1, w_2, , \ldots, w_{k-1}\}$. Then $\triangle_n^k = U^{'} - w_i u_l +$

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Volume 26, pp. 333-344, June 2013

$w_i z_{p-1}$, where $1 \leq i \leq k-1$. Note that $|x'_{u_l}| < |x'_{z_{p-1}}|$, by Lemma 2.2, then $q(U') > q(\triangle_n^k)$. Hence, we get $q(U^*) > q(\triangle_n^k)$. By the definition of U^*, then U^* is isomorphic to $\triangle_n^k$. □

THEOREM 3.5. *Let $1 \leq k \leq n-4$. Then $q(\triangle_n^k) < q(\triangle_n^{k+1})$.*

Proof. Consider the unicyclic graph $\triangle_n^{k+1}$. Let X be a unit $Q-$eigenvector of $\triangle_n^{k+1}$ corresponding to $q(\triangle_n^{k+1})$. Denote $k+1$ pendant vertices by $v_1, v_2, \ldots, v_k, v_{k+1}$ and their common neighbor u_l. Then $\triangle_n^k = \triangle_n^{k+1} - v_i u_l + v_i v_{k+1}$, where $1 \leq i \leq k$. Note that $|x_{u_l}| < |x_{v_{k+1}}|$, by Lemma 2.2, we have $q(\triangle_n^{k+1}) > q(\triangle_n^k)$. □

Theorem 1.1 follows naturally from Theorems 3.1, 3.4 and 3.5.

Let $\mathcal{U}_n$ be the set of non-bipartite unicyclic graphs on n vertices, where $n \geq 4$. Then $\mathcal{U}_n = \{C_n\} \cup \mathcal{U}(n,1) \cup \mathcal{U}(n,2) \cup \cdots \cup \mathcal{U}(n,n-3)$.

LEMMA 3.6. *Let U^{**} have the minimal least $Q-$eigenvalue in $\mathcal{U}_n$, where $n \geq 4$. Then U^{**} is not isomorphic to C_n.*

Proof. By way of contradiction, suppose that U^{**} is isomorphic to C_n, then we have $n \geq 5$ is odd. Let X be a unit $Q-$eigenvector of U^{**} corresponding to $q(U^{**})$. Using the same techniques as the proof of Lemma 3.3, we can always find at least four vertices $v_{i-1}, v_i, v_{i+1}, v_{i+2}$ of C_n and obtain a contradiction in each case, since $|x_{v_i}| \neq |x_{v_{i-1}}|$ and $|x_{v_{i+1}}| \neq |x_{v_{i+2}}|$. Hence, U^{**} is not isomorphic to C_n. □

According to Lemma 3.6, then $U^{**} \in \mathcal{U}(n,1) \cup \mathcal{U}(n,2) \cup \cdots \cup \mathcal{U}(n,n-3)$. As an immediate consequence of Theorems 1.1, we have the following Corollary 3.7, which is one of the main results in [2].

COROLLARY 3.7. **([2])** *Let $\mathcal{U}_n$ be the set of non-bipartite unicyclic graphs on n vertices, where $n \geq 4$. For any $U \in \mathcal{U}_n$, we have*

$$q(U) \geq q(\triangle_n^1)$$

with equality if and only if U is isomorphic to $\triangle_n^1$.

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