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# THE LEAST EIGENVALUE OF GRAPHS WHOSE COMPLEMENTS ARE UNICYCLIC

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#### Abstract

A graph in a certain graph class is called minimizing if the least eigenvalue of its adjacency matrix attains the minimum among all graphs in that class. Bell *et al.* have identified a subclass within the connected graphs of order n and size m in which minimizing graphs belong (the complements of such graphs are either disconnected or contain a clique of size  $\frac{n}{2}$ ). In this paper we discuss the minimizing graphs of a special class of graphs of order n whose complements are connected and contains exactly one cycle (namely the class  $\mathscr{U}_n^c$  of graphs whose complements are unicyclic), and characterize the unique minimizing graph in  $\mathscr{U}_n^c$  when  $n \geq 20$ .

**Keywords:** unicyclic graph, complement, adjacency matrix, least eigenvalue.

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## 1. INTRODUCTION

Let G = (V, E) be a simple graph with vertex set  $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set E = E(G). The *adjacency matrix* of G is a matrix  $A(G) = [a_{ij}]$  of order n, where  $a_{ij} = 1$  if  $v_i$  is adjacent to  $v_j$ , and  $a_{ij} = 0$  otherwise. Since A(G) is real and symmetric, its eigenvalues are real and can be arranged as:  $\lambda_1(G) \leq \lambda_2(G) \leq \cdots \leq \lambda_n(G)$ . The eigenvalues of A(G) are referred to as the *eigenvalues* of G. The eigenvalue  $\lambda_n(G)$  is the spectral radius of A(G); and there are many results in literatures concerning this eigenvalue of A(G) (see, e.g. [3] for some older results).

The least eigenvalue  $\lambda_1(G)$  is now denoted by  $\lambda_{\min}(G)$ , and the corresponding eigenvectors are called the *first eigenvectors* of G. In contrast to the largest eigenvalue, the least eigenvalue has received much less attention in the literature. In the past the main work on the least eigenvalue of a graph is focused on its bounds; see e.g. [4, 7]. Recently, the problem of minimizing the least eigenvalues of graphs subject to graph parameters has received much more attention, since two papers of Bell *et al.* [1, 2] and one paper of our group [5] appeared in the same issue of the journal Linear Algebra and Its Applications. Ye and Fan [14] discuss the connectivity and the least eigenvalue of a graph. Liu *et al.* [8] discuss the least eigenvalues of unicyclic graphs with given number of pendant vertices. Petrović *et al.* [9, 10] discuss the least eigenvalues of bicyclic graphs and get further results for the graphs of order n and size n + k, where  $0 \le k \le 4$  and  $n \ge k + 5$ . Wang *et al.* [12, 13] discuss the least eigenvalue and the number of cut vertices of a graph. Tan and Fan [11] discuss the least eigenvalue and the vertex/edge independence number, the vertex/edge cover number of a graph.

For convenience, a graph is called *minimizing* in a certain graph class if its least eigenvalue attains the minimum among all graphs in the class. Let  $\mathscr{G}(n,m)$  denote the class of connected graphs of order n and size m. Bell *et al.* (see [1, Theorem 1]) have characterized the structure of the minimizing graphs in  $\mathscr{G}(n,m)$  as follows.

**Theorem 1.** Let G be a minimizing graph in  $\mathcal{G}(n,m)$ . Then G is either

- (i) a bipartite graph, or
- (ii) a join of two nested split graphs (not both totally disconnected).

We observe here that the complements of the minimizing graphs in  $\mathscr{G}(n,m)$  are either disconnected or contain a clique of order at least n/2. This motivates us to discuss the least eigenvalue of graphs whose complements are connected and contain clique of small size. In a recent work [6] we characterized the unique minimizing graph in the class of graphs of order n whose complements are trees.

In this paper, we continue this work on the complements of unicyclic graphs, and determine the unique minimizing graph in  $\mathscr{U}_n^c$  for  $n \ge 20$ , where  $\mathscr{U}_n^c$  denotes the class of the complements of connected unicyclic graphs of order n. It is easily seen that  $\mathscr{U}_n^c \subsetneq \mathscr{G}(n, \binom{n}{2} - n)$ . However, for the minimizing graph in  $\mathscr{U}_n^c$  the conditions of Theorem 1 do not hold.

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### 2. Preliminaries

We begin with some definitions. Given a graph G of order n, we say that a vector  $X \in \mathbb{R}^n$  is *defined* on G, if there is a 1-1 map  $\varphi$  from V(G) to the entries of X; simply written  $X_u = \varphi(u)$  for each  $u \in V(G)$ . If X is an eigenvector of A(G), then it is naturally defined on V(G), *i.e.*  $X_u$  is the entry of X corresponding to the vertex u. One can find that

(2.1) 
$$X^T A X = 2 \sum_{uv \in E(G)} X_u X_v$$
,  
and  $\lambda$  is an eigenvalue of  $G$  corresponding to the eigenvector  $X$  if and only if  $X \neq 0$  and

(2.2)  $\lambda X_v = \sum_{u \in N_G(v)} X_u$ , for each vertex  $v \in V(G)$ , where  $N_G(v)$  denotes the neighborhood of v in G. The equation (2.2) is called  $(\lambda, X)$ -eigenequation of G. In addition, for an arbitrary unit vector  $X \in \mathbb{R}^n$ ,

(2.3) 
$$\lambda_{\min}(G) \le X^T A(G) X,$$

with equality if and only if X is a first eigenvector of G.

In this paper all unicyclic graphs are assumed to be connected. Denote by  $\mathscr{U}_n$  the set of unicyclic graphs of order n, and let  $\mathscr{U}_n^c = \{G^c : G \in \mathscr{U}_n\}$ , where  $G^c$  denotes the complement of G. Note that  $A(G^c) = \mathbf{J} - \mathbf{I} - A(G)$ , where  $\mathbf{J}, \mathbf{I}$  denote the all-ones matrix and the identity matrix both of suitable sizes, respectively. So for any vector  $X \in \mathbb{R}^n$ ,

(2.4) 
$$X^T A(G^c) X = X^T (\mathbf{J} - \mathbf{I}) X - X^T A(G) X.$$



Figure 2.1. The graphs  $\mathbf{U}(p,q)$  (left side) and  $\mathbf{U}'(p)$  (right side).

A star of order n, denoted by  $K_{1,n-1}$ , is a tree of order n with n-1 pendant edges attached to a fixed vertex. The vertex of degree n-1 in  $K_{1,n-1}$  is called the *center* of  $K_{1,n}$ . A cycle and a complete graph both of order n are denoted by  $C_n, K_n$  respectively. Denote by  $S_n^3$  the graph obtained from  $K_{1,n-1}$  by adding a new edge between two pendant vertices. Next, we introduce two special unicyclic graphs denoted by  $\mathbf{U}(p,q)$  and  $\mathbf{U}'(p)$ , respectively (see Figure 2.1).  $\mathbf{U}(p,q)$  is obtained from two disjoint graphs  $K_{1,p}$   $(p \ge 1)$  and  $S_{q+1}^3(q \ge 3)$  by adding a new edge between one pendant vertex of  $K_{1,p}$  and one pendant vertex of  $S_{q+1}^3$ .  $\mathbf{U}'(p)$  is obtained from two disjoint graphs  $K_{1,p}$   $(p \ge 1)$  and  $C_3$  by adding a new edge between one pendant vertex of  $K_{1,p}$  and one vertex of  $C_3$ .

For a graph G containing at least one edge, it holds  $\lambda_{\min}(G) \leq -1$ , with equality if and only if G is a complete graph or a union of disjoint copies of complete graphs, at least one copy being nontrivial (i.e. contains more than one vertices). So, for a unicyclic graph U other than  $C_4$ ,  $\lambda_{\min}(U^c) < -1$ . In addition, if  $U^c$  is disconnected, then U contains a complete multipartite graph as a spanning subgraph, which implies U is  $C_4$  or  $S_n^3$ . When  $n \geq 4$ ,  $(S_n^3)^c$  consists of an isolated vertex and a connected non-complete subgraph of order n-1.

At the end of this section, we will discuss the least eigenvalues of  $\mathbf{U}(p,q)^c$ and  $\mathbf{U}'(p)^c$ . Let X be a first eigenvector of the graph  $\mathbf{U}(p,q)^c$  with some vertices labeled as in Figure 2.1. By eigenequations (2.2), as  $\lambda_{\min}(\mathbf{U}(p,q)^c) < -1$ , all the pendant vertices attached at  $v_2$  have the same value as  $v_1$  given by X, say  $X_1$ . Similarly, all the pendant vertices attached at  $v_5$  have the same value as  $v_7$ , say  $X_7$ ; two vertices of degree 2 on the triangle have the same value as  $v_6$ , say  $X_6$ . Write  $X_{v_i} =: X_i$  for the vertices  $v_i$ 's in  $\mathbf{U}(p,q)^c$  for i = 2, 3, 4, 5 and  $\lambda_{\min}(\mathbf{U}(p,q)^c) =: \lambda_1$  for simplicity. Then by the eigenequations (2.2) on  $v_i$  for  $i = 1, 2, \ldots, 7$ , we have

$$(2.5) \begin{cases} \lambda_1 X_1 = (p-2)X_1 + X_3 + X_4 + X_5 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_2 = X_4 + X_5 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_3 = (p-1)X_1 + X_5 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_4 = (p-1)X_1 + X_2 + 2X_6 + (q-3)X_7, \\ \lambda_1 X_5 = (p-1)X_1 + X_2 + X_3, \\ \lambda_1 X_6 = (p-1)X_1 + X_2 + X_3 + X_4 + 2X_6 + (q-4)X_7. \end{cases}$$

Transform (2.5) into a matrix equality  $(B - \lambda_1 \mathbf{I})X' = 0$ , where  $X' = (X_1, X_2, \dots, X_7)^T$  and the matrix B of order 7 is easily seen. We have

$$\begin{aligned} f(\lambda;p,q) &:= \det(B-\lambda \mathbf{I}) = (-8+2p+2q) \\ (2.6) &+ (13-11p-7q+4pq)\lambda + (20-6q-4qp)\lambda^2 \\ &+ (-1+11p+7q-7pq)\lambda^3 + (-20+12p+12q-2pq)\lambda^4 \\ &+ (-16+6p+6q)\lambda^5 + (-6+p+q)\lambda^6 - \lambda^7. \end{aligned}$$

So  $\lambda_1$  is the least root of the polynomial  $f(\lambda; p, q)$ .

Let Y be a first eigenvector of the graph  $\mathbf{U}'(p)^c$  with some vertices labeled as in Figure 2.1. By a similar discussion, all the pendant vertices attached at  $v_2$ have the same values given by Y, say  $Y_1$ . Two vertices of degree 2 on the triangle have the same values, say  $Y_5$ . Write  $Y_{v_i} =: Y_i$  for the vertices  $v_i$ 's in  $\mathbf{U}'(p)^c$  for i = 2, 3, 4 and  $\lambda_{\min}(\mathbf{U}'(p)^c) =: \lambda'_1$  for simplicity. Then by the eigenequations (2.2) on  $v_i$  for i = 1, 2, ..., 5,

(2.7) 
$$\begin{cases} \lambda_1' Y_1 = (p-2)Y_1 + Y_3 + Y_4 + 2Y_5, \\ \lambda_1' Y_2 = Y_4 + 2Y_5, \\ \lambda_1' Y_3 = (p-1)Y_1 + Y_4 + 2Y_5, \\ \lambda_1' Y_4 = (p-1)Y_1 + Y_2, \\ \lambda_1' Y_5 = (p-1)Y_1 + Y_2 + Y_3. \end{cases}$$

It is easily found that  $\lambda'_1$  is the least root of the following polynomial:

(2.8) 
$$g(\lambda;p) := (-4+2p) + (3-5p)\lambda + (6-p)\lambda^{2} + (1+4p)\lambda^{3} + (-2+p)\lambda^{4} - \lambda^{5}.$$

**Lemma 2.** If  $n \ge 13$ , then  $\lambda_{\min}(\mathbf{U}(n-5,3)^c) < \lambda_{\min}(\mathbf{U}'(n-4)^c)$ .

**Proof.** Write  $\lambda_{\min}(\mathbf{U}(n-5,3)^c) =: \lambda_1, \ \lambda_{\min}(\mathbf{U}'(n-4)^c) =: \lambda'_1$  for simplicity. By the above discussion,  $\lambda_1$  (respectively,  $\lambda'_1$ ) is the least root of  $f(\lambda; n-5,3)$  (respectively,  $g(\lambda; n-4)$ ). Denote

$$\bar{g}(\lambda; n-4) := (\lambda+1)^2 g(\lambda; n-4).$$

Since  $\lambda'_1 < -1$ ,  $\lambda'_1$  is also the least root of  $\bar{g}(\lambda; n-4)$ . From (2.8), g(-3; n-4) = 171 - 19(-4 + n), and consequently  $\bar{g}(n-4, -3) \leq 0$  if  $n \geq 13$ . Furthermore, when  $\lambda \to -\infty$ ,  $\bar{g}(\lambda; n-4) \to +\infty$ , which implies  $\lambda'_1 \leq -3$ . Obverse that when  $\lambda \leq -3$ ,

$$\bar{g}(\lambda; n-4) - f(\lambda; n-5, 3) = (-6+n)\lambda(1+\lambda)(-2+5\lambda+2\lambda^2) > 0.$$

In particular,  $f(\lambda'_1; n-5, 3) < 0$ , which implies  $\lambda_{\min}(\mathbf{U}(n-5, 3)^c) < \lambda'_1$ . The result follows.

**Lemma 3.** Given a positive integer  $n \ge 20$ , for any positive integers p, q such that  $p \ge 1, q \ge 3$  and p + q = n - 2,

$$\lambda_{\min}(\mathbf{U}(p,q)^c) \ge \lambda_{\min}(\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c),$$

with equality if and only if  $p = \lceil (n-2)/2 \rceil$  and  $q = \lfloor (n-2)/2 \rfloor$ .

**Proof.** Write  $\lambda_{\min}(\mathbf{U}(p,q)^c) =: \lambda_1$  for simplicity. By (2.6), we have

$$\begin{split} f(\lambda;p,q) &- f(\lambda;p+1,q-1) = -\lambda(2+\lambda)(-1+2\lambda)[(p-q+1)(2+\lambda)+2], \\ f(\lambda;p,q) &- f(\lambda;p-1,q+1) = \lambda(2+\lambda)(-1+2\lambda)[(p-q-1)(2+\lambda)+2]. \end{split}$$

In addition, f(-2; p, q) = -10 < 0, which implies  $\lambda_1 < -2$ .

If  $q \ge p+1$ , then for  $\lambda < -2$  we have  $f(\lambda; p, q) - f(\lambda; p+1, q-1) > 0$ . In particular,  $f(\lambda_1; p+1, q-1) < 0$ , which implies

$$\lambda_{\min}(\mathbf{U}(p+1,q-1)^c) < \lambda_1 = \lambda_{\min}(\mathbf{U}(p,q)^c).$$

If  $p \ge q + 3(\ge 6)$ , then, by (2.6), we have f(-3; p, q) = 241 - 19p + 23q - 21pq = 241 - 19(p - q) + (4 - 21p)q < 0, which implies  $\lambda_1 < -3$ . Observe that  $f(\lambda; p, q) - f(\lambda; p - 1, q + 1) > 0$  when  $\lambda < -3$ . In particular,  $f(\lambda_1; p - 1, q + 1) < 0$ , which implies

$$\lambda_{\min}(\mathbf{U}(p-1,q+1)^c) < \lambda_1 = \lambda_{\min}(\mathbf{U}(p,q)^c).$$

To complete the proof, we need to prove  $\lambda_{\min}(\mathbf{U}(p-1,q+1)^c) < \lambda_{\min}(\mathbf{U}(p,q)^c)$ when p = q + 2. In this case,  $p = \frac{n}{2}$ ,  $q = \frac{n}{2} - 2$ , and

$$f(\lambda; p, q) - f(\lambda; p - 1, q + 1) = \lambda(2 + \lambda)(-1 + 2\lambda)(4 + \lambda).$$

So it is enough to prove  $\lambda_1 < -4$  or

$$f\left(-4;\frac{n}{2},\frac{n}{2}-2\right) = 2376 + 582n - 36n^2 < 0.$$

If  $n \ge 20$ , then the above inequality holds, and hence the result follows.

## 3. Main Results

By rearranging the edges of graphs, we first give a maximization of the quadratic form  $X^T A(G)X$  among all trees or all unicyclic graphs G of order n, where X is a non-negative or non-positive real vector defined on G.

**Lemma 4.** Let T be a tree of order n, and let X be a non-negative or non-positive real vector defined on T whose entries are ordered so that  $|X_1| \ge |X_2| \ge \cdots \ge |X_n|$ , i.e. with respect to their moduli. Then

$$\sum_{uv \in E(T)} X_u X_v \le \sum_{i=2}^n X_1 X_i = \sum_{uv \in E(K_{1,n-1})} X_u X_v,$$

where X is defined on  $K_{1,n-1}$  such that the center has value  $X_1$ . If, in addition, X is positive or negative, and  $|X_1| > |X_2|$ , then the above equality holds only if  $T = K_{1,n-1}$ .

**Proof.** We may assume X is non-negative; otherwise we consider -X. Let w be a vertex with value  $X_1$  given by X. If there exists a vertex v not adjacent of w, letting v' be the neighbor of v on a path of T connecting v and w, and deleting the edge vv' and adding a new edge wv, we will arrive at a new graph (tree) T', which holds

(3.1) 
$$\sum_{uv \in E(T)} X_u X_v \leq \sum_{uv \in E(T')} X_u X_v.$$

Repeating the process on the tree T' for the non-neighbors of w, and so on, we at last arrive at a star  $K_{1,n-1}$  with w as its center, and

(3.2)  $\sum_{uv \in E(T)} X_u X_v \leq \sum_{uv \in E(K_{1,n-1})} X_u X_v = \sum_{i=2}^n X_1 X_i.$  If X is positive,  $X_1 > X_2$ , and w is not adjacent to all other vertices in T, then the

**Lemma 5.** Let U be a unicyclic graph of order n, and let X be a non-negative I

inequality (3.1), and hence (3.2), cannot hold as an equality. The result follows.

**Lemma 5.** Let U be a unicyclic graph of order n, and let X be a non-negative or non-positive real vector defined on U whose entries are ordered so that  $|X_1| \ge$  $|X_2| \ge \cdots \ge |X_n|$ , i.e. with respect to their moduli. Then

$$\sum_{uv \in E(U)} X_u X_v \le \sum_{i=2}^n X_1 X_i + X_2 X_3 = \sum_{uv \in E(S_n^3)} X_u X_v,$$

where X is defined on  $S_n^3$  such that the vertex with degree n-1 has value  $X_1$ , and the other two vertices on the triangle have values  $X_2, X_3$  respectively. If, in addition, X is positive or negative, and  $|X_1| > |X_2|$ , then the above equality holds only if  $T = S_n^3$ .

**Proof.** We may assume X is non-negative; otherwise we consider -X. Let w be a vertex with value  $X_1$  given by X. By a similar discuss to the proof of Lemma 4, we have a graph U' of order n, in which the vertex w is adjacent to all other vertices, and

(3.3)  $\sum_{uv \in E(U)} X_u X_v \leq \sum_{uv \in E(U')} X_u X_v = \sum_{i=2}^n X_1 X_i + X_{u'} X_{v'},$ where u'v' is an edge of U' not incident to w. Surely,

 $(3.4) X_{u'} X_{v'} \le X_2 X_3.$ 

So,

3.5) 
$$\sum_{uv \in E(U)} X_u X_v \le \sum_{i=2}^n X_1 X_i + X_2 X_3 = \sum_{uv \in E(S^3_{+})} X_u X_v.$$

If X is positive, and  $X_1 > X_2$ , then the equality (3.5) holds only if (3.3) holds, which implies w is adjacent to all other vertices and consequently  $U = S_n^3$ . The result follows.

**Lemma 6.** Let U be a unicyclic graph of order  $n \ge 5$  such that  $U^c$  is a minimizing graph in  $\mathscr{U}_n^c$ , and let X be a first eigenvector of  $U^c$ . Then X contains no zero entries and has at least two positive entries and two negative entries.

**Proof.** As  $U^c$  is a minimizing graph in  $\mathscr{U}_n^c$ ,  $U \neq S_n^3$ . We first prove that each entry of X is nonzero. One the contrary, let  $X_v = 0$  for some v. As  $U \neq S_n^3$ , there exists two vertices  $w \in N_U(v)$  and  $w' \notin N_U(v)$  such that w, w' belong to the same component of U-v, say  $U_1$ . Let  $\hat{U}^c = U - vw + vw'$ , which is also unicyclic. Since  $X_v = 0$ , we have  $\lambda_{\min}(\hat{U}^c) = \lambda_{\min}(U^c)$  by the choice of  $U^c$  and the minimality principle based on Rayley quotient. Therefore, X is as well the first eigenvector of  $\hat{U}^c$ . But then, by the eigenequation at v, it follows that  $X_w = X_{w'}$ . So, for any vertex  $u \notin N_U(v)$  in the component  $U_1, X_u = X_w$ . This holds for any other neighbors of v in  $U_1$  if taking each of them in the role of w. Hence all vertices in  $U_1$  have the same values.

If there is a nontrivial component of U - v, say  $U_2$ , such that v is adjacent to all vertices in  $U_2$ , then  $U_2$  consists of exactly one edge, say pq, as U is unicyclic. By the eigenequations on p, q, we also get  $X_p = X_q$ . So, the vertices of each component of U - v have the same values.

(i) If v is not a cut vertex of U (e.g. a pendant vertex), then U - v is connected, and hence  $X \ge 0$  or  $X \le 0$ , a contradiction.

(ii) Now suppose v is a cut vertex of U. Let  $U_1, U_2, \ldots, U_k$   $(k \ge 2)$  be the components of U - v, which consist of vertices with same values given by X, respectively. Note that one component of U - v, say  $U_1$ , contains the vertices of the (unique) cycle C of U, and all other components contain pendant vertices of U. Each vertex of  $U_2 \cup \cdots \cup U_k$  has nonzero value; otherwise a pendant vertex will have zero value which yields a contradiction as in (i). If all vertices of  $U_1$  are zero valued, then we take a vertex from  $U_1$  lying on C in the role of v, and also obtain a contradiction as in (i). By the above discussion, all vertices but v have nonzero values.

Next if  $X_r X_s > 0$ , where  $r \in U_i, s \in U_j$  for some distinct i, j, then let  $\overline{U} = U - vw + rs$ , where  $w \in N_U(v)$  lies in  $U_i$ . But then  $\lambda_{\min}(\overline{U}^c) < \lambda_{\min}(U^c)$ , a contradiction. So U - v has exactly two components  $U_1$  and  $U_2$ , one having positive valued vertices and the other having negative valued vertices.

Finally, recalling that all vertices in  $U_i$  have the same values for i = 1, 2, so, by the eigenequations, all vertices in  $U_i$  have the same number of neighbors (or non-neighbors) in  $U_i$  for i = 1, 2. This implies  $U = \mathbf{U}'(1)$  if v lies on the cycle and  $U = \mathbf{U}'(2)$  otherwise. It is easily check the first eigenvector of  $\mathbf{U}'(1)$  or  $\mathbf{U}'(2)$ has no zero entries. So we proved the first assertion.

Now we show the second assertion. On the contrary, assume that only one vertex, say v with positive value given by X. Then any other vertex u is adjacent to v in  $U^c$ , since otherwise an eigenequation does not hold at u. So v is adjacent to all other vertices in  $U^c$ , which implies U is disconnected, a contradiction.

We now arrive at the main result of this paper.

**Theorem 7.** Let U be a unicyclic graph of order  $n \ge 20$ . Then

$$\lambda_{\min}(U^c) \ge \lambda_{\min}(\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c),$$

with equality if and only if  $U = \mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)$ .

**Proof.** Suppose that  $U^c$  is a minimizing graph in  $\mathscr{U}_n^c$  for  $n \ge 20$ . The result will follow if we can show that U is the unique graph  $\mathbf{U}(\lceil (n-2)/2 \rceil, \lceil (n-2)/2 \rceil)$ .

Let X be the first eigenvector of  $U^c$  with unit length. By Lemma 6, X contains no zero entries. Denote  $V_+ = \{v \in V(U^c) : X_v > 0, \}, V_- = \{v \in V(U^c) : X_v > 0, \}$ 

 $V(U^c): X_v < 0$ , both containing at least 2 elements by Lemma 6. Denote by  $U_+$  (respectively,  $U_-$ ) the subgraph of U induced by  $V_+$  (respectively,  $V_-$ ), by E' the set of edges between  $V_+$  and  $V_-$  in U. Since U is connected,  $E' \neq \emptyset$ . Obviously,

(3.6) 
$$\sum_{vv' \in E(U)} X_v X_{v'} = \sum_{vv' \in E(U_+)} X_v X_{v'} + \sum_{vv' \in E(U_-)} X_v X_{v'} + \sum_{vv' \in E'} X_v X_{v'}.$$

First assume  $|V_-| \geq 3$ . The cycle of U may contain the edges of E', or is contained in one of  $U_+, U_-$ . Without loss of generality, we assume that the cycle of U is not contained in  $U_+$ ; otherwise we consider the vector -X instead. Let  $U^*$  be a graph obtained from U by possibly adding some edges within  $V^+$  and  $V^-$ , such that the subgraph of  $U^*$  induced by  $V^+$ , denoted by  $U^*_+$ , is a tree, and the subgraph of  $U^*$  induced by  $V^-$ , denoted by  $U^*_-$ , is a unicyclic graph.

In the tree  $U_{+}^{*}$ , choose a vertex, say **u**, with maximum modulus among all vertices of  $U_{+}^{*}$ . By Lemma 4, we will have a star, say  $K_{1,p}$  centered at **u**, where  $p+1 = |V^{+}| \geq 2$ , which holds

(3.7) 
$$\sum_{vv' \in E(U_+)} X_v X_{v'} \le \sum_{vv' \in E(U_+^*)} X_v X_{v'} \le \sum_{vv' \in E(K_{1,p})} X_v X_{v'}.$$

In the unicyclic graph  $U_{-}^*$ , choosing a vertex, say  $\mathbf{w}$ , with maximum modulus. By Lemma 5, we have a unicyclic graph  $S_{q+1}^3$ , where  $q + 1 = |V_{-}| \ge 3$  and the vertex  $\mathbf{w}$  joins all other vertices of  $S_{q+1}^3$ , which holds

(3.8) 
$$\sum_{vv' \in E(U_{-})} X_v X_{v'} \leq \sum_{vv' \in E(U_{-}^*)} X_v X_{v'} \leq \sum_{vv' \in E(S_{q+1}^3)} X_v X_{v'}.$$

Let  $\mathbf{u}', \mathbf{w}'$  be the vertices of  $U_+, U_-$  with minimum modulus among all vertices of  $U_+, U_-$ , respectively. Then

(3.9) 
$$\sum_{vv' \in E'} X_v X_{v'} \le X_{\mathbf{u}'} X_{\mathbf{w}'},$$

Now by (3.6-3.9), we have

(3.10) 
$$\sum_{vv' \in E(U)} X_v X_{v'} \leq \sum_{vv' \in E(K_{1,p})} X_v X_{v'} + \sum_{vv' \in E(S_{q+1}^3)} X_v X_{v'} + X_{\mathbf{u}'} X_{\mathbf{w}}$$

Since  $p \ge 1$ , the vertex  $\mathbf{u}'$  can be chosen within the pendent vertices of  $K_{1,p}$  by Lemma 4. If  $q \ge 3$ ,  $\mathbf{w}'$  can be chosen within the pendent vertices of  $S_{q+1}^3$  by Lemma 5, then from (3.10) we have

(3.11) 
$$\frac{\frac{1}{2}X^{T}A(U)X}{=\sum_{vv'\in E(U)}X_{v}X_{v'}} \leq \sum_{vv'\in E(\mathbf{U}(p,q))}X_{v}X_{v'}}{=\frac{1}{2}X^{T}A(\mathbf{U}(p,q))X,}$$

and consequently

(3.12)  

$$\lambda_{\min}(U^{c}) = X^{T}A(U^{c})X = X^{T}(\mathbf{J} - \mathbf{I})X - X^{T}A(U)X$$

$$\geq X^{T}(\mathbf{J} - \mathbf{I})X - X^{T}A(\mathbf{U}(p,q))X$$

$$= X^{T}A(\mathbf{U}(p,q)^{c})X$$

$$\geq \lambda_{\min}(\mathbf{U}(p,q)^{c}).$$

If q = 2, that is,  $S_{q+1}^3 = C_3$ , by a similar discussion, we have  $\lambda_{\min}(U^c) \ge \lambda_{\min}(\mathbf{U}'(n-4)^c)$ . By Lemma 2,  $\lambda_{\min}(\mathbf{U}'(n-4)^c) > \lambda_{\min}(\mathbf{U}(n-5,3)^c)$ .

Next we consider the case when  $|V_-| = 2$ . In this case the cycle of U cannot lies in  $U_-$ . We form a graph  $U^{\#}$  from U possibly by adding some edges within  $V^+$ and  $V^-$ , such that the subgraph of  $U^{\#}$  induced by  $V^+$  is a unicyclic graph, and the subgraph of  $U^{\#}$  induced by  $V^-$  is exactly  $K_2$ . Also similar to the discussion for (3.7–3.12), we have  $\lambda_{\min}(U^c) \geq \lambda_{\min}(\mathbf{U}(1, n-3))$ . By Lemma 3 and the above discussion,

(3.13) 
$$\lambda_{\min}(U^c) \geq \lambda_{\min}(\mathbf{U}(p,q)^c) \\ \geq \lambda_{\min}(\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c).$$

By the choice of U, all equalities in (3.13) hold. So  $p = \lceil (n-2)/2 \rceil, q = \lfloor (n-2)/2 \rfloor$  by Lemma 3, and consequently only the case of  $|V_-| \ge 3$  occurs. Also, all equalities in (3.11) and (3.12) hold, which implies that X is a first eigenvector of  $\mathbf{U}(p,q)^c$ . Let  $\mathbf{U}(p,q)$  have some vertices labeled as in Figure 2.1, where  $v_2 = \mathbf{u}, v_3 = \mathbf{u}', v_5 = \mathbf{w}, v_4 = \mathbf{w}'$ .

Assertion 1: The vertices  $v_2 = \mathbf{u}$  and  $v_3 = \mathbf{u}'$  are respectively the unique ones in  $U_+$  with maximum and minimum modulus,  $v_5 = \mathbf{w}$  and  $v_4 = \mathbf{w}'$  are respectively the unique ones in  $U_-$  with maximum and minimum modulus. By Lemma 6, as X is a first eigenvector of the minimizer  $\mathbf{U}(p,q)^c$ ,  $X_{v_i} =: X_i > 0$ for i = 1, 2, 3 and  $X_{v_i} =: X_i < 0$  for i = 4, 5, 6, 7. By (2.5),  $\lambda_1(X_4 - X_7) =$  $-X_3 - X_4 < 0$ ,  $\lambda_1(X_6 - X_7) = -2X_6$ ,  $\lambda_1(X_5 - X_6) = -X_4 - (q - 3)X_7$ , which implies that  $X_5 < X_6 < X_7 < X_4 < 0$ . Also by (2.5),  $\lambda_1(X_1 - X_2) >$  $0, \lambda_1(X_3 - X_1) = X_1 - X_3 - X_4 > X_1 - X_3$ , which implies  $X_3 < X_1 < X_2$ .

Assertion 2:  $U_+ = U_+^* = K_{1,p}$ ,  $U_- = U_-^* = S_{q+1}^3$ ,  $E_1 = \{\mathbf{u'w'}\}$ , *i.e.*  $U = \mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)$ . By the Assertion 1 and the equality in (3.11), retracing the discussion for (3.8–3.9) and applying Lemmas 4 and 5, we get  $U_+ = U_+^* = K_{1,p}$ ,  $U_- = U_-^* = S_{q+1}^3$ . From the discussion for (3.9–3.11), also by Assertion 1,  $E_1$  consists of exactly one edge, i.e.  $\mathbf{u'w'}$ .

It was proved in [5] that  $S_n^3$  is the unique minimizing graph in  $\mathscr{U}_n$  when  $n \ge 6$ . However, when  $n \ge 20$ , by Theorem 7, the graph  $\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)^c$  is the unique minimizing graph in  $\mathscr{U}_n^c$ . So there exists some difference on the least eigenvalue of unicyclic graphs and its complements.

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