# THE LEAST EIGENVALUE OF GRAPHS WHOSE COMPLEMENTS ARE UNICYCLIC

YI WANG<sup>1</sup>, YI-ZHENG FAN<sup>1</sup>, XIAO-XIN LI<sup>2</sup>

AND

## Fei-Fei Zhang<sup>1</sup>

<sup>1</sup> School of Mathematical Sciences Anhui University, Hefei 230601, P.R. China

<sup>2</sup> Department of Mathematics and Computer Sciences Chizhou University, Chizhou 247000, P.R. China

> e-mail: wangy@ahu.edu.cn fanyz@ahu.edu.cn lxx@czu.edu.cn zhangfeifei2403@126.com

## 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  $\mathcal{U}_n^c$  of graphs whose complements are unicyclic), and characterize the unique minimizing graph in  $\mathcal{U}_n^c$  when  $n \geq 20$ .

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

2010 Mathematics Subject Classification: 05C50, 05D05, 15A18.

## 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  $\mathcal{G}(n,m)$  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  $\mathcal{G}(n,m)$  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  $\mathcal{G}(n,m)$  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  $n \geq 20$ , where  $\mathscr{U}_n^c$  denotes the class of the complements of connected unicyclic graphs of order n. It is easily seen that  $\mathscr{U}_n^c \subseteq \mathscr{G}(n, \binom{n}{2} - n)$ . However, for the minimizing graph in  $\mathscr{U}_n^c$  the conditions of Theorem 1 do not hold.

#### 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) 
$$X^TAX = 2\sum_{uv \in E(G)} X_u X_v,$$
 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) 
$$X^T A(G^c) X = X^T (\mathbf{J} - \mathbf{I}) X - X^T A(G) X.$$

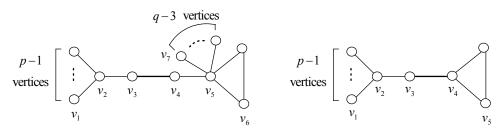


Figure 2.1. The graphs U(p,q) (left side) and U'(p) (right side).

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  $K_{1,p}$  ( $p \geq 1$ ) and  $S_{q+1}^3(q \geq 3)$  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  $v_7$ ; two vertices of degree 2 on the triangle have the same value as  $v_6$ , say  $v_7$ . Write  $v_7$  is in  $v_7$  for the vertices  $v_7$  in  $v_7$  for  $v_7$  for  $v_7$  and  $v_7$  for  $v_7$  for  $v_7$  in  $v_7$  for  $v_7$  for  $v_7$  in  $v_7$  in  $v_7$  for  $v_7$  in  $v_7$  in  $v_7$  in  $v_7$  for  $v_7$  in  $v_7$  in

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

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

$$f(\lambda; p, q) := \det(B - \lambda \mathbf{I}) = (-8 + 2p + 2q)$$

$$(2.6) + (13 - 11p - 7q + 4pq)\lambda + (20 - 6q - 4qp)\lambda^{2} + (-1 + 11p + 7q - 7pq)\lambda^{3} + (-20 + 12p + 12q - 2pq)\lambda^{4} + (-16 + 6p + 6q)\lambda^{5} + (-6 + p + q)\lambda^{6} - \lambda^{7}.$$

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  $\bar{g}(n-4,-3) \le 0$  if  $n \ge 13$ . Furthermore, when  $\lambda \to -\infty$ ,  $\bar{g}(\lambda; n-4) \to +\infty$ , which implies  $\lambda_1' \le -3$ . Obverse that when  $\lambda \le -3$ ,

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

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,

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

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

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

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  $n \geq 20$ , 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

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

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 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)  $X_{u'}X_{v'} \le X_2X_3$ . So,

result follows.

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

**Lemma 6.** Let U be a unicyclic graph of order  $n \geq 5$  such that  $U^c$  is a minimizing graph in  $\mathcal{U}_n^c$ , 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  $X \geq 0$  or  $X \leq 0$ , a contradiction.
- (ii) Now suppose v is a cut vertex of U. Let  $U_1, U_2, \ldots, U_k$   $(k \geq 2)$  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  $X_rX_s>0$ , where  $r\in U_i, s\in U_j$  for some distinct i,j, then let  $\bar{U}=U-vw+rs$ , where  $w\in N_U(v)$  lies in  $U_i$ . But then  $\lambda_{\min}(\bar{U}^c)<\lambda_{\min}(U^c)$ , 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  $n \geq 20$ . 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  $n \geq 20$ . The result will follow if we can show that U is the unique graph  $\mathbf{U}(\lceil (n-2)/2 \rceil, \lfloor (n-2)/2 \rfloor)$ .

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

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  $q+1=|V_{-}|\geq 3$  and the vertex  $\mathbf{w}$  joins all other vertices of  $S_{q+1}^{3}$ , which holds

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

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

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

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

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

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  $\lambda_{\min}(U^c) \geq \lambda_{\min}(\mathbf{U}'(n-4)^c)$ . 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  $|V_-| \geq 3$  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:  $U_+ = U_+^* = K_{1,p}$ ,  $U_- = U_-^* = S_{q+1}^3$ ,  $E_1 = \{\mathbf{u}'\mathbf{w}'\}$ , *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.  $\mathbf{u}'\mathbf{w}'$ .

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

## Acknowledgements

This work is supported by National Natural Science Foundation of China (110710 02, 11371028), Program for New Century Excellent Talents in University (NCET-10-0001), Key Project of Chinese Ministry of Education (210091), Specialized Research Fund for the Doctoral Program of Higher Education (20103401110002), Science and Technological Fund of Anhui Province for Outstanding Youth (100406 06Y33), Scientific Research Fund for Fostering Distinguished Young Scholars of

Anhui University (KJJQ1001), Academic Innovation Team of Anhui University Project (KJTD001B).

The authors would like to thank the anonymous referees for providing a brief proof of the main result of this paper.

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Received 4 November 2013 Revised 6 June 2014 Accepted 9 June 2014