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QUADRATIC FORMS ON GRAPHS WITH APPLICATION TO MINIMIZING THE LEAST EIGENVALUE OF SIGNLESS LAPLACIAN OVER BICYCLIC GRAPHS*

GUI-DONG YU†, YI-ZHENG FAN‡, AND YI WANG‡

Abstract. Given a graph and a vector defined on the graph, a quadratic form is defined on the graph depending on its edges. In order to minimize the quadratic form on trees or unicyclic graphs associated with signless Laplacian, the notion of basic edge set of a graph is introduced, and the behavior of the least eigenvalue and the corresponding eigenvectors is investigated. Using these results a characterization of the unique bicyclic graph whose least eigenvalue attains the minimum among all non-bipartite bicyclic graphs of fixed order is obtained.

Key words. Graph, Bicyclic graph, Quadratic form, Least eigenvalue, Signless Laplacian.

AMS subject classifications. 05C50, 15A18.

1. Introduction. Let G be a simple graph of order n with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The *adjacency matrix* of G is defined as the $n \times n$ matrix $A(G) = [a_{ij}]$ given by: $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. Denote by $D(G) = \mathrm{diag}\{d_G(v_1), d_G(v_2), \ldots, d_G(v_n)\}$ the diagonal matrix of vertex degrees, where $d_G(v)$, or simply $d(v)$, denotes the degree of the vertex v. The matrix $Q = Q(G) = D(G) + A(G)$ is called the *signless Laplacian* of G (see [29]), and is also known as the *unoriented Laplacian* (see [22, 27, 36]). Evidently, $Q(G)$ is symmetric and positive semidefinite, so its eigenvalues can be arranged as $0 \le \lambda_1(G) \le \lambda_2(G) \le \cdots \le \lambda_n(G)$. In this paper, the eigenvalue $\lambda_1(G)$ and the corresponding eigenvectors for a given graph G are simply called the *least eigenvalue* and the *first eigenvectors* of G, respectively.

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The matrix $L(G) = D(G) - A(G)$, known as the standard *Laplacian* of G, and is studied extensively in the literature; see e.g. [33, pp. 113–136]. A more generalized matrix associated with graphs, the Laplacian of mixed graphs or signed graphs are discussed in [1, 21, 30, 44].

Recently the eigenvalues of the signless Laplacian have received a lot of attention, especially the spectral radius. The papers [6, 8, 9, 10, 11] provide a comprehensive survey on this topic. There are a number of works discussing the relationships between the spectral radius of $Q(G)$ and certain graph parameters of G, such as chromatic number [3], order and size [5], pendant vertices [24], maximum clique [32], connectivity [42], matching number [43], degree [34] or degree sequence [45], and hamiltonicity [46].

On the other hand, there is far less work on the least eigenvalue of the signless Laplacian. It is well known that for a connected graph G, the least eigenvalue is zero if and only if G is bipartite. So connected non-bipartite graphs are considered here. In [13], the least eigenvalue was used to reflect the 'non-bipartiteness' of graphs. Some results on minimizing or maximizing the least eigenvalue of mixed graphs are given in [16]. The paper [37] introduces a parameter called *edge singularity* to reflect the singularity of Laplacian of mixed graphs. The structure of the eigenvectors corresponding the least eigenvalue is also discussed in [16, 17, 37]. In [20], the authors introduce the *characteristic set* of mixed graphs, and determine the unique graph with minimum least eigenvalue among all nonsingular unicyclic mixed graphs with fixed order. Their results can be easily applied to the signless Laplacian of graphs. Independently, Cardoso et al. [4] determine the unique graph (surely being unicyclic) with minimum least eigenvalue among all non-bipartite graphs of fixed order with respect to the signless Laplacian of graphs.

In this paper, we focus on the least eigenvalues of the signless Laplacian of graphs, especially the least eigenvalue of non-bipartite bicyclic graphs. We determine the unique graph whose least eigenvalue attains the minimum among all non-bipartite bicyclic graphs with fixed order. The optimal graph is obtained from a triangle and a square by connecting a path between them. We begin the discussion from the quadratic form defined on graphs, as many problems of graph eigenvalues can be translated to maximizing or minimizing quadratic form on graphs. This will be discussed in next section.

We finally remark that the signless Laplacian of a graph is maybe more closely related to the graph structures than the adjacency matrix and the Laplacian of that graph. The papers [12, 29] provide *spectral uncertainties* with respect to the adjacency matrix, with respect to the Laplacian, and with respect to the signless Laplacian of sets of all graphs on n vertices for $n \leq 11$. It was found that the spectral uncertainty with respect to the signless Laplacian is smallest when $7 \leq n \leq 11$.

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2. Quadratic forms on graphs. Many problems arising from the spectra of graphs can be viewed as those of minimizing or maximizing quadratics of associated matrices of graphs. As these matrices are defined on graphs, the corresponding quadratics are also defined on graphs. Formally, given a graph G of order n, a vector $X \in \mathbb{R}^n$ is called to be defined on G, if there is a 1-1 map φ from $V(G)$ to the entries of X, simply written $X_u := \varphi(u)$ for each $u \in V(G)$. A function defined on G with respect to X, denoted by $f(G,X)$, is defined as

$$f(G,X) = \sum_{uw \in E(G)} f_{uw},$$

where f_{uw} is a symmetric function in two variables X_u, X_w. Particularly, $f(G,X)$ is a quadratic form on G when f_{uw} is a symmetric polynomial of degree 2. For example, if f_{uw} equals $2X_uX_w$ or $(X_u - X_w)^2$ or $(X_u + X_w)^2$, then the function is exactly the quadratic form of the adjacency matrix or the Laplacian or the signless Laplacian of G with respect to X.

The Courant-Fischer-Weyl min-max principle, for a real symmetric matrix A of order n, implies

$$\lambda_k^{\uparrow} = \min_{S_k} \max_{X \in S_k, \|x\|=1} X^T A X, \quad \lambda_k^{\downarrow} = \max_{S_k} \min_{X \in S_k, \|x\|=1} X^T A X,$$

where S_k denotes a k dimensional subspace of $\mathbb{R}^n$, and $\uparrow$ or $\downarrow$ indicates it is the kth eigenvalue in the increasing or decreasing order. So, the eigenvalue of (the adjacency matrix, Laplacian, signless Laplacian) of a graph is exactly a optimal solution obtained by maximizing or minimizing the quadratic form on the graph in a certain subspace.

This viewpoint has been applied to many topics, such as the algebraic connectivity [15, 31] related to the Laplacian, the spectral radius [5, 22, 36, 42] and the least eigenvalue [20] related to the signless Laplacian, and the least eigenvalue [23, 38, 39, 41] related to the adjacency matrix. Consider an example of minimizing the least eigenvalue of the signless Laplacian over a certain class $\mathscr{G}$ of graphs. Let $f(G,X) = X^TQ(G)X$ defined on graphs $G \in \mathscr{G}$. If we find a graph $H \in \mathscr{G}$ such that $f(G,X) \geq f(H,X)$, or also a vector Y with length not less than X such that $f(G,X) \geq f(H,Y)$, then $\lambda_1(G) \geq \lambda_1(H)$ whenever X is a first eigenvector of G. This can be done by locally changing the graph structure and keeping the resulting graph in $\mathscr{G}$.

We often ignore the ordering of the vertices of G and the entries of X. The quadratic $X^TQ(G)X$ may be written as

$$f_Q(G,X) := \sum_{uw \in E(G)} (X_u + X_w)^2.$$

The eigen-equation $Q(G)X = \lambda X$ is interpreted as

$$[\lambda - d_G(v)]X_v = \sum_{u \in N(v)} X_u, \quad \text{for each } v \in V(G), \tag{2.1}$$

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where $N_G(v)$, or simply $N(v)$, denotes the neighborhood of the vertex v in G.

2.1. Basic edge sets of graphs. In this section, we introduce the notion of basic edge set of a graph, and use it to investigate the property of first eigenvectors.

With respect to a real vector X defined on a graph G, the *value*, *modulus*, *sign* of a vertex $u \in V(G)$ is X_u, $|X_u|$, $\text{sgn}(X_u)$, respectively. A vertex of G is called *zero* (*nonzero*) if its sign is zero (nonzero). An edge uw of G is called *positive* or *nonnegative* or *negative* if $X_uX_w > 0$ or $X_uX_w \geq 0$ or $X_uX_w < 0$.

A *basic edge set* of G with respect to X, denoted by $\mathcal{B}_X$, is a set with a minimum number of nonnegative edges whose deletion yields a bipartite graph. In particular, when G is bipartite, then $\mathcal{B}_X = \emptyset$. The basic edge set $\mathcal{B}_X$ may not be unique, but this does not cause any difficulties with our discussion.

The *edge bipartiteness* of G, denoted by $\epsilon_b(G)$, is the minimum number of edges G whose deletion yields a bipartite graph, which was introduced in [14] to measure how close a graph is to being bipartite. The notion was used in [18] to confirm a conjecture on minimum signless Laplacian spread [7].

We find that the basic edge set of a graph is closely related to the edge bipartiteness; see Lemma 2.1 below. A *resigning* X' of a real vector X is a vector obtained from X by changing the signs of some (possibly none or all) entries of X, that is, $X' = DX$ for some signature matrix D (a diagonal matrix with 1 or -1 on its diagonals).

LEMMA 2.1. *Let G be a connected non-bipartite graph with n vertices and m edges, and let X be a vector defined on $V(G)$. Then the following hold:*

(1) *$G - \mathcal{B}_X$ is connected, and each edge of $\mathcal{B}_X$ lies on an odd cycles.*

(2) *$1 \leq |\mathcal{B}_X| \leq m - n + 1$.*

(3) *$\epsilon_b(G) = \min_{X'} |\mathcal{B}_{X'}|$, where X' is taken over all resignings of X.*

Proof. (1) If $G - \mathcal{B}_X$ is disconnected, say with components $C_1, \ldots, C_k$ (each of which must be bipartite), then there exists an edge $e \in \mathcal{B}_X$ such that e connects C_i and C_j for some i, j, as G is connected. It is clear that the addition of the edge e to $G - \mathcal{B}_X$ still yields a bipartite graph. Thus, $G - (\mathcal{B}_X - e)$ is still bipartite, which contradicts the definition of basic edge set. So $G - \mathcal{B}_X$ is connected.

Let (U, W) be the bipartition of $G - \mathcal{B}_X$. Then each edge of $\mathcal{B}_X$ lies within the same part U or W, and the addition of this edge to $G - \mathcal{B}_X$ will yield an odd cycle of G as $G - \mathcal{B}_X$ is connected.

(2) Note that G contains a spanning tree and the deletion of the edges complementary to this tree will produce a bipartite graph. Hence, any basic edge set $\mathcal{B}_X$

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contains at most $m-n+1$ elements. Surely $\mathcal{B}$ contains at least 1 element as G is non-bipartite.

(3) Clearly, $\epsilon_b(G) \le |\mathcal{B}_X|$. Let F be a set of $\epsilon_b(G)$ edges such that $G-F$ is bipartite. By a similar discussion as in (1), $G-F$ is connected. Let (U,W) be a bipartition of $G-F$. Then the edges of F lies within the same part U or W. Let X' be a resigning of X such that the value of each vertex in U is given by its modulus and the value of each vertex in W is given by the negative of its modulus. Then $|\mathcal{B}_{X'}| \le \epsilon_b(G)$, and hence, $|\mathcal{B}_{X'}| = \epsilon_b(G)$. The result follows. ◻

A bipartite graph G is called *bi-signed* with respect to a vector X defined on G if there exists a bipartition for G such that the vertices in one part of the bipartition are nonnegative and the vertices in the other part are nonpositive.

Let G be a connected graph and let X be a real vector defined on G. If G is bipartite, there is a resigning X' of X such that G is bi-signed with respect to X', and

$$f_Q(G,X) \ge f_Q(G,X'),$$

where the equality holds if and only if G contains no positive edges with respect to X. The vector X' is defined as follows: reassign the value of each vertex in one part of the bipartition for G by its modulus and the value of each vertex in the other part by the negative of its modulus.

If G is non-bipartite, then $G-\mathcal{B}_X$ is connected and bipartite by Lemma 2.1(1). By the above discussion, there exists a resigning X' of X such that $G-\mathcal{B}_X$ is bi-signed with respect to X', and $f_Q(G-\mathcal{B}_X, X) \ge f_Q(G-\mathcal{B}_X, X')$. As the edges of $\mathcal{B}_X$ join the vertices within same part of the bipartition for $G-\mathcal{B}_X$, $\mathcal{B}_X$ is still a basic edge set of G with respect to X', and consequently, $(X_u+X_w)^2 = (X'_u+X'_w)^2$ for each edge $uw \in \mathcal{B}_X$. Hence,

$$\begin{aligned} f_Q(G,X) &= f_Q(G-\mathcal{B}_X, X) + \sum_{uw\in\mathcal{B}_X} (X_u+X_w)^2 \\ &\ge f_Q(G-\mathcal{B}_X, X') + \sum_{uw\in\mathcal{B}_X} (X'_u+X'_w)^2 = f_Q(G,X'). \end{aligned}$$

In the above, we have established the following result, which includes the case of G being bipartite whence $\mathcal{B}_X = \emptyset$.

Lemma 2.2. *Let G be a connected graph and let X be a real vector defined on G. For any basic edge set $\mathcal{B}_X$, there exists a resigning X' of X such that $f_Q(G,X) \ge f_Q(G,X')$, $G-\mathcal{B}_X$ is bi-signed with respect to X' and $\mathcal{B}_X$ is a also basic edge set with respect to X'. Furthermore, $f_Q(G,X) = f_Q(G,X')$ if and only if $G-\mathcal{B}_X$ contains no positive edges with respect to X.*

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If considering the basic edge sets with respect to the first eigenvectors of a graph, we will obtain some properties of the first eigenvectors.

LEMMA 2.3. *Let G be a connected non-bipartite graph and let X be a first eigenvector of G. Then the following results hold:*

(1) *$G - \mathcal{B}_X$ contains no positive edges with respect to X.*

(2) *There exists a first eigenvector X' (as a resigning of X) of G such that, with respect to X', $\mathcal{B}_X$ is also a basic edge set and $G - \mathcal{B}_X$ is bi-signed.*

(3) *If a vertex is not adjacent to any vertices with smaller moduli, then this vertex and its neighbors must all have zero values, unless it is incident with an edge in $\mathcal{B}_X$.*

(4) *If the minimum modulus is positive, then any vertex with the minimum modulus is incident with an edge in $\mathcal{B}_X$; if the minimum modulus is zero, then there exists a zero vertex incident with an edge in $\mathcal{B}_X$.*

Proof. By Lemma 2.2, there exists a resigning X' of X such that $f_Q(G, X) \geq f_Q(G, X')$, $G - \mathcal{B}_X$ is bi-signed with respect to X' and $\mathcal{B}_X$ is a basic edge set with respect to X'. As X corresponds to the least eigenvalue of G, we have $f_Q(G, X) = f_Q(G, X')$, by Lemma 2.2, $G - \mathcal{B}_X$ contains no positive edges with respect to X. From the equality, X' is also a first eigenvector of G. So the assertions (1) and (2) follow.

Let $G - \mathcal{B}_X$ have a bipartition (U, W). Note that $\mathcal{B}_X$ is a basic edge set with respect to X', and X' differs to X only at the signs of its entries. We prove the assertions (3) and (4) using X'. Assume that there exists a vertex, say $u \in U$ with $X'_u \geq 0$, and adjacent to vertices of moduli greater than or equal to $|X'_u|$ such that the edges incident with u are all not in $\mathcal{B}_X$. Then $N(u) \subset W$, and for each $v \in N(u)$, $X'_v \leq -X'_u \leq 0$. By the eigen-equation (2.1) for X' at u,

$$[\lambda_1(G) - d(u)]X'_u = \sum_{v \in N(u)} X'_v \leq -d(u)X'_u.$$

As G is connected and non-bipartite, $\lambda_1(G) > 0$. So $X'_u = 0$ from the above equation, and then $X'_v = 0$ for each $v \in N(u)$. The assertion (3) follows.

By the result (3), the first part of the assertion (4) follows. Now assume that u is a zero vertex but not incident with any edge of $\mathcal{B}_X$. Then all neighbors of u have zero values. As $G - \mathcal{B}_X$ is connected, there must exist a zero vertex joining a nonzero vertex by an edge of $G - \mathcal{B}_X$. By (2.1) at this zero vertex, it must be adjacent to another nonzero vertex by an edge of $\mathcal{B}_X$. ☐

COROLLARY 2.4. *Let G be a connected non-bipartite graph and let X be a first eigenvector of G. If vw is a cut edge of G, then $X_v X_w \leq 0$.*

Proof. By Lemma 2.1(1), a cut edge cannot be contained in any basic edge set

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$\mathcal{B}_X$ of G, and is hence contained in $G-\mathcal{B}_X$. The result follows from Lemma 2.3(1). ☐

The *coalescence* of two disjoint nontrivial graphs G_1, G_2 with respect to $v_1 \in V(G_1), v_2 \in V(G_2)$, denoted by $G_1(v_1) \diamond G_2(v_2)$, is obtained by identifying v_1 with v_2 and forming a new vertex u, and is also written as $G_1(u) \diamond G_2(u)$. Let X be a vector defined on a graph G and let H be a subgraph of G. Denote by X_H the subvector of X indexed by the vertices of H.

Corollary 2.5. [40] *Let $G = G_1(u) \diamond B(u)$, where G_1 is a connected graph, B is a connected bipartite graph. Let X be a first eigenvector of G.*

(1) *If $X_u = 0$, then $X_B = 0$.*

(2) *If $X_u \neq 0$, then $X_p \neq 0$ for every vertex $p \in V(B)$. Furthermore, for every vertex $p \in V(B)$, X_pX_u is either positive or negative, depending on whether p is or is not in the same part of the bipartite graph B as u; consequently, $X_pX_q < 0$ for each edge $pq \in E(B)$.*

Note that in Corollary 2.4, if G is connected and bipartite, then 0 is a simple least eigenvalue of G and a corresponding eigenvector takes the same value at each vertex of one part of the bipartition for G and takes its negative value at each vertex of the other part. So Corollary 2.4 still holds in this case. In addition, Corollary 2.5 can also be proved by using Lemma 2.3 and the eigen-equation (2.1).

We finally remark that the idea of basic edge set with respect to a first eigenvector is similar to that of 'characteristic set' (a set consisting of characteristic edges and characteristic vertices), which is used for standard Laplacian with respect to a Fiedler vector [2] or other eigenvector [19, 26, 35], and is also used for Laplacian of mixed graphs with respect to a first eigenvector [20].

2.2. Quadratic forms on trees and unicyclic graphs. In this section, by the notion of basic edge set, we minimize of the quadratic forms on unicyclic graphs associated with signless Laplacian. We begin with trees as a preliminary work, though the basic edge sets of this kind of graphs are empty.

Denote by $P_n : v_1v_2 \cdots v_n$, a path on distinct vertices $v_1, v_2, \ldots, v_n$ with edges v_iv_{i+1} for $i = 1, 2, \ldots, n-1$. Let

$$f_L(G, X) := \sum_{uw \in E(G)} (X_u - X_w)^2,$$

be the quadratic form on G associated with Laplacian.

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LEMMA 2.6. [15] *Let T be a tree of order n, and let $X \in \mathbb{R}^n$ defined on T whose entries are arranged as $X_1 \le X_2 \le \cdots \le X_n$. Then*

$$f_L(T, X) = \sum_{uw \in E(T)} (X_u - X_w)^2 \ge \sum_{i=1}^{n-1} (X_i - X_{i+1})^2 = f_L(P_n, Y),$$

where Y is defined on $P_n : v_1 v_2 \cdots v_n$ such that $Y_{v_i} = X_i$ for $i = 1, 2, \ldots, n$. Furthermore, if $X_u \ne X_w$ for each edge $uw \in E(T)$, then the equality holds if and only if $X_1 < X_2 < \cdots < X_n$ and $T = P_n$.

It was proved by Fiedler [25] that $\alpha(T) \ge \alpha(P_n)$, where $\alpha(G)$ denotes the *algebraic connectivity* of a graph G, which is defined as the second smallest eigenvalue of the Laplacian of G. Using Lemma 2.6, the inequality can be obtained directly. Furthermore, the equality holds if and only if $T = P_n$. For a vector $X = (X_1, X_2, \ldots, X_n)$, denote $|X| := (|X_1|, |X_2|, \ldots, |X_n|)$.

COROLLARY 2.7. *Let T be a tree of order n, and let $X \in \mathbb{R}^n$ defined on T whose entries are arranged as $|X_1| \le |X_2| \le \cdots \le |X_n|$. Then*

$$f_Q(T, X) \ge \sum_{i=1}^{n-1} (|X_{i+1}| - |X_i|)^2 = f_Q(P_n, Y),$$

where Y is defined on $P_n : v_1 v_2 \cdots v_n$ such that $Y_{v_i} = (-1)^{i+1}|X_i|$ for $i = 1, 2, \ldots, n$. Furthermore, if $|X_u| \ne |X_w|$ for each edge $uw \in E(T)$, then the equality holds if and only if T contains no positive edges, $|X_1| < |X_2| < \cdots < |X_n|$, and $T = P_n$.

Proof. By Lemma 2.2, there exists a vector X' (as a resigning of X) such that T is bi-signed with respect to X', and $f_Q(T, X) \ge f_Q(T, X')$ with equality if and only if T contains no positive edges with respect to X. Let (V_+, V_-) be the bipartition of T, and let D be the signature matrix with a 1 for the vertices of V_+ and a -1 for V_-. Then $Q(T) = DL(T)D$, and $f_Q(T, X') = f_L(T, |X'|)$. By Lemma 2.6,

$$f_L(T, |X'|) \ge \sum_{i=1}^{n-1} (|X_i| - |X_{i+1}|)^2 = f_Q(P_n, Y).$$

The second claim follows from the above discussion and Lemma 2.6. ∎

LEMMA 2.8. *Let G be an odd-unicyclic graph of order n, and let $X \in \mathbb{R}^n$ defined on G. In addition, assume that if there exists an edge of $\mathcal{B}_X$ whose end vertices have the smallest and the 2nd smallest moduli respectively, then one of the end vertices has degree 2. Then we have*

$$f_Q(G, X) \ge f_Q(G_\triangle, Y),$$

where $G_\triangle$ is the graph of order n and Y is defined on $G_\triangle$ as shown in Fig. 2.1.

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Proof. Arrange the entries of X as $|X_1| \le |X_2| \le \cdots \le |X_n|$. Note that $\mathcal{B}_X$ must contain an edge, say uw, necessarily on the odd cycle. By Lemma 2.2, there exists a vector X' (as a resigning of X) such that $f_Q(G,X) \ge f_Q(G,X')$, and with respect to X', $G-uw$ is bi-signed and $\{uw\}$ is still a basic edge set. If one of $|X_u|, |X_w|$ is greater than or equal to $|X_3|$, then by Corollary 2.7,

$$\begin{aligned} f_Q(G,X') &= f_Q(G-uw,X') + (|X_u|+|X_w|)^2 \\ &\ge \sum_{i=1}^{n-1}(|X_i|-|X_{i+1}|)^2 + (|X_1|+|X_3|)^2 \\ &\ge \sum_{i=2}^{n-1}(|X_i|-|X_{i+1}|)^2 + (|X_1|+|X_2|)^2 + (|X_1|-|X_3|)^2 \\ &= f_Q(G_\triangle, Y). \end{aligned}$$

Otherwise, assume that $|X_u| = |X_1| \le |X_w| = |X_2| < |X_3|$. By the assumption, u or w has degree 2. If u has degree 2, letting v be its other neighbor, we have

$$\begin{aligned} f_Q(G,X') &= f_Q(G-u,X'_{G-u}) + (|X_u|+|X_w|)^2 + (|X_u|-|X_v|)^2 \\ &\ge \sum_{i=2}^{n-1}(|X_i|-|X_{i+1}|)^2 + (|X_1|+|X_2|)^2 + (|X_1|-|X_3|)^2 \\ &= f_Q(G_\triangle, Y). \end{aligned}$$

The argument is similar if w has degree 2. ☐

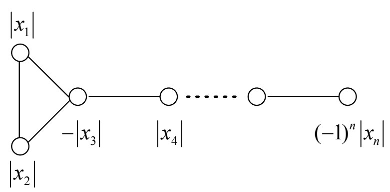

Fig. 2.1. The graph $G_\triangle$ of order n with a vector Y defined on it.

Lemma 2.9. *Let G be an even-unicyclic graph of order n, and let $X \in \mathbb{R}^n$ defined on G where the cycle of G contains a vertex with minimum or maximum modulus. In addition, assume that if the vertex with minimum modulus (maximum modulus, respectively) has two neighbors on the cycle with the 2nd and the 3rd smallest moduli respectively (the 2nd and the 3rd largest moduli respectively), then one of these neighbors has degree 2. Then we have*

$$f_Q(G,X) \ge f_Q(G_\Box, Y),$$

where $G_\Box$ is the graph of order n and Y is defined on $G_\Box$ without boxes (in the minimum case) or within the boxes (for the maximum case) as shown in Fig. 2.2.

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Proof. Arrange the entries of X as $|X_1| \le |X_2| \le \cdots \le |X_n|$. By Lemma 2.2, there exists a vector X' (a resigning of X) such that $f_Q(G, X) \ge f_Q(G, X')$ and G is bi-signed with respect to X'. Assume that u is a vertex with minimum modulus defined on the cycle. If one neighbor w of u on the cycle satisfies $|X_w| \ge |X_4|$, then by Corollary 2.7,

$$\begin{aligned} f_Q(G, X') &= f_Q(G - uw, X') + (|X_u| - |X_w|)^2 \\ &\ge \sum_{i=1}^{n-1} (|X_i| - |X_{i+1}|)^2 + (|X_1| - |X_4|)^2 \\ &\ge \sum_{i=3}^{n-1} (|X_i| - |X_{i+1}|)^2 + (|X_1| - |X_3|)^2 + (|X_1| - |X_2|)^2 + (|X_2| - |X_4|)^2 \\ &= f_Q(G_\square, Y), \end{aligned}$$

where $G_\square$ is in Fig. 2.2 and Y is defined on $G_\square$ without boxes.

Otherwise, both neighbors of u, say v, w, on the cycle have moduli less than $|X_4|$, say, $|X_1| = |X_u| \le |X_2| = |X_v| \le |X_3| = |X_w| < |X_4|$. If v has degree 2, letting v' be another neighbor of v other than u, considering $G - v$ (a tree), we have

$$\begin{aligned} f_Q(G, X') &= f_Q(G - v, X'_{G-v}) + (|X_v| - |X_u|)^2 + (|X_v| - |X_{v'}|)^2 \\ &\ge (|X_1| - |X_3|)^2 + \sum_{i=3}^{n-1} (|X_i| - |X_{i+1}|)^2 + (|X_1| - |X_2|)^2 + (|X_2| - |X_4|)^2 \\ &= f_Q(G_\square, Y). \end{aligned}$$

If w has degree 2, the argument is similar and is omitted.

If a vertex with maximum modulus is defined on the cycle, the discussion is also similar and the corresponding graph is $G_\square$ with a vector Y defined on $G_\square$ within the boxes; see Fig. 2.2. ∎

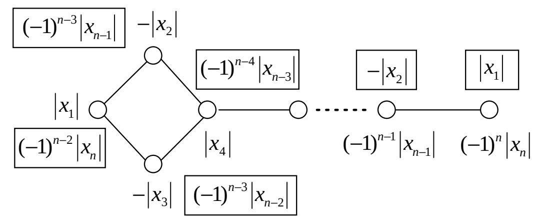

Fig. 2.2. The graphs $G_\square$ with a vector Y defined on it without or within boxes.

2.3. Perturbations of least eigenvalue. In this section, we use the quadratic forms on graphs to establish a perturbation result for the least eigenvalues. Though

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Lemma 2.10 was already given in [40], the proof idea is still related to it.

Note that if a graph G contains a pendant edge, say uw with $d_u = 1$, then $\lambda_1(G) < 1$. Let A be the 2×2 principal submatrix of $Q(G)$ indexed by u, w. From the interlacing of eigenvalues (see [28]) it follows that

$$\lambda_1(G) \le \lambda_1(A) = (d(w) + 1 - \sqrt{[d(w) - 1]^2 + 4}\,)/2 < 1, \tag{2.2}$$

where $\lambda_1(A)$ denotes the least eigenvalue of A. In particular, if $d(w) = 2$, then $\lambda_1(G) \le (3 - \sqrt{5})/2$.

Lemma 2.10. [40] *Let $G = G_0(v_1) \diamond B(u)$ and $\bar{G} = G_0(v_2) \diamond B(u)$, where G_0 is a connected graph containing two distinct vertices v_1, v_2, and B is connected bipartite graph. If there exists a first eigenvector X of G such that $|X_{v_2}| \ge |X_{v_1}|$, then*

$$\lambda_1(G) \ge \lambda_1(\bar{G})$$

with equality only if $|X_{v_2}| = |X_{v_1}|$ and $d_B(u)X_u = -\sum_{v \in N_B(u)} X_v$.

Lemma 2.11. [40] *Let $G = G_1(u) \diamond T(u)$, where G_1 is a connected non-bipartite graph and T is a tree. Let X be a first eigenvector of G, which gives a nonzero value at some vertex of T. Then $|X_q| < |X_p|$ whenever p, q are vertices of T such that q lies on the unique path from u to p.*

Lemma 2.12. *Let $G = G_1(u) \diamond T(u)$, where G_1 is a connected non-bipartite graph and T is a tree of order m. Let X be a unit first eigenvector of G, which gives a nonzero value at some vertex of T. Then there exists a unit vector Y such that*

$$f_Q(G_1(u) \diamond T(u), X) \ge f_Q(G_1(u) \diamond P_m(u), Y),$$

where P_m has u as an end vertex. Hence, $\lambda_1(G) \ge \lambda_1(G_1(u) \diamond P_m(u))$. Both equalities hold if and only if $T = P_m$ having u as an end vertex.

Proof. By Corollary 2.5(2) and Lemma 2.11, we may arrange the moduli of vertices of T as $0 < |X_u| =: |X_0| < |X_1| \le |X_2| \le \cdots \le |X_{m-1}|$. By Corollary 2.7,

$$\begin{aligned} f_Q(G, X) &= f_Q(G_1, X_{G_1}) + f_Q(T, X_T) \\ &\ge f_Q(G_1, X_{G_1}) + \sum_{i=0}^{m-2} (|X_i| - |X_{i+1}|)^2 \\ &= f_Q(G_1(u) \diamond P_m(u), Y), \end{aligned}$$

where Y is defined as: $Y_v = X_v$ if $v \in V(G_1)$, and $Y_{u_i} = (-1)^i \mathrm{sgn}(X_u)|X_i|$ for $i = 1, 2, \ldots, m-1$ if P_m is the path on vertices $u, u_1, u_2, \ldots, u_{m-1}$. So $\lambda_1(G) \ge \lambda_1(G_1(u) \diamond P_m(u))$. Note that the end vertices of each edge of T must have different moduli by Lemma 2.11 and different signs by Corollary 2.5(2). The last claim now follows from Corollary 2.7. ∎

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A graph G is called *minimizing* among all graphs in a graph class $\mathscr{C}$ if $\lambda_1(G) = \min_{H\in\mathscr{G}} \lambda_1(H)$.

Corollary 2.13. [4, 20] *Let G be an odd-unicyclic graph of order n. Then*

$$\lambda_1(G) \geq \lambda_1(G_\triangle),$$

with equality if and only if $G = G_\triangle$, where $G_\triangle$ is the graph in Fig. 2.1.

Proof. It suffices to prove if G is a minimizing graph among all odd-unicyclic graphs of order n, then $G = G_\triangle$. Suppose G contains a cycle C_m. Let X be a unit first eigenvector of G, and let u be the vertex with maximum modulus among all vertices of C_m. Surely $X_u \neq 0$; otherwise $X = 0$ by Corollary 2.5(1). If there exists a tree T attached at $w \neq u$, relocating T from w to u, we arrive at a graph G' holding that $\lambda_1(G) \geq \lambda_1(G')$ by Lemma 2.10. As G is minimizing, $\lambda_1(G) = \lambda_1(G')$, which implies $|X_w| = |X_u| > 0$ and $d_T(w) = -\sum_{v\in N_T(w)} X_v$ by the last part of Lemma 2.10. But the latter cannot hold by Lemma 2.11. So $G = C_m(u) \diamond T(u)$ for some tree T, where u is the unique (nonzero) vertex with maximum modulus among all vertices of C_m. By Lemma 2.12, $G = C_m(u) \diamond P_{n-m}(u)$, where u is an end vertex of P.

Now by Lemma 2.8, there exists a graph $G_\triangle$ of order n and a unit vector Y defined on it (see Fig. 2.1), such that

$$\lambda_1(G) = f_Q(G, X) \geq f_Q(G_\triangle, Y) \geq \lambda_1(G_\triangle).$$

If the equality holds, then Y is a first eigenvector of $G_\triangle$. By Lemma 2.11 and from the eigen-equation of Y for the graph $G_\triangle$, $|X_1| = |X_2| < |X_3| < \cdots < |X_n|$. If $G \neq G_\triangle$, then G will have two or more pairs of vertices with same moduli. The result now follows. ▯

3. Minimum of the least eigenvalue over bicyclic graphs. Using the result in Section 2, we will minimize the least eigenvalue over all non-bipartite bicyclic graphs of fixed order. A graph G on n vertices is a *bicyclic graph* if it is a connected graph with exactly $n + 1$ edges. Observe that G is obtained from a ∞-graph or a θ-graph G_0 (possibly) by attaching trees to some of its vertices, where a ∞*-graph* is a union of two cycles that share exactly one vertex or is obtained from two disjoint cycles by connecting a path between them, and a θ*-graph* is a union of three internally disjoint paths with common end vertices, which are distinct, and such that at most one of the paths has length 1. We also call G_0 the *kernel* of G.

3.1. Least eigenvalues of special bicyclic graphs. We first discuss the least eigenvalues of some special bicyclic graphs, which will be used for our main result.

Lemma 3.1. *Let G be a non-bipartite bicyclic graph whose kernel is a ∞-graph and contains an even cycle. Then $\lambda_1(G) < 1$.*

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Proof. Let G_0 be the kernel of G, and let C be an odd cycle of G_0. Let v be a vertex of C such that $d_{G_0}(v) > 2$, and let e be an edge of C which is incident with v. By the interlacing property (see [4]), $\lambda_1(G) \leq \lambda_2(G-e)$. As $G-e$ is bipartite, $Q(G-e)$ is similar to $L(G-e)$, and $\lambda_2(G-e)$ is exactly the algebraic connectivity of $G-e$. Furthermore, the graph $G-e$ has vertex connectivity 1 with v as a cut vertex, so $\lambda_2(G-e) < 1$ by [31, Theorem 1] as v cannot be adjacent to all other vertices of $G-e$. □

We introduce four bicyclic graphs on $n \geq 9$ vertices in Fig. 3.1, and list some properties on the first eigenvectors and least eigenvalues for them. Observe that in Fig. 3.1, all graphs have least eigenvalue less than 1 by Lemma 3.1 and (2.2).

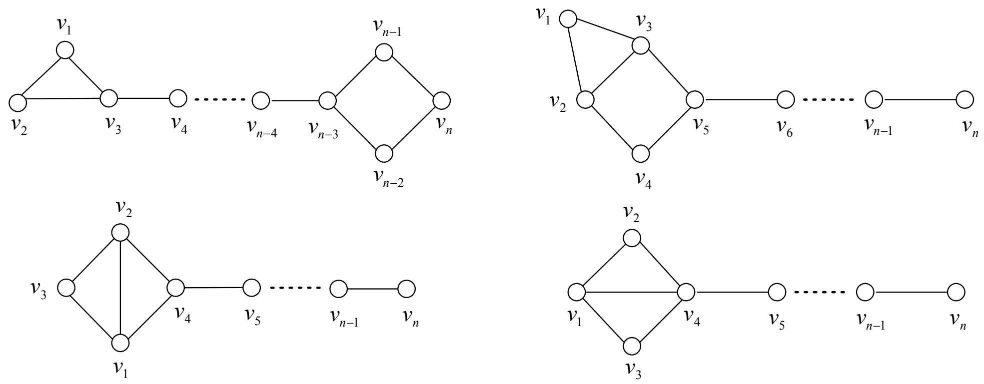

Fig. 3.1. The graph $\mathbf{G_1}$(left-upper), $\mathbf{G_2}$(right-upper), $\mathbf{G_3}$(left-lower), $\mathbf{G_4}$(right-lower.)

Lemma 3.2. *Let G be one graph of order $n \geq 9$ in Fig. 3.1, and let X be a first eigenvector of G. Then we have the following results.*

(1) *If $G = \mathbf{G}_1$, then $X_{v_1} = X_{v_2} \neq 0$, $|X_{v_2}| < |X_{v_3}|$, and v_1, v_2, v_3 are the vertices with the smallest, the 2nd smallest and the 3rd smallest moduli, respectively.*

(2) *If $G = \mathbf{G}_3$, then X contains no zero entries.*

(3) $\lambda_1(\mathbf{G}_4) > \lambda_1(\mathbf{G}_3)$.

Proof. We simply write X_{v_i} as X_i for $i = 1, 2, \ldots, n$. Assume $G = \mathbf{G}_1$. Then $\mathcal{B}_X$ contains only one edge necessarily on the triangle. By Lemma 2.10, $|X_3| \geq \max\{|X_1|, |X_2|\}$. So $X_3 \neq 0$; otherwise $X = 0$ by Corollary 2.5(1). By the eigen-equations (2.1) of X at v_1 and v_2 respectively, together with the fact $\lambda_1(\mathbf{G}_1) < 1$ by Lemma 3.1, $X_1 = X_2 \neq 0$. So there exists a basic edge set $\mathcal{B}_X = \{v_1v_2\}$. By Lemma 2.3(4), v_1 or v_2 is a nonzero vertex with minimum modulus. So X contains no zero entries, and $\mathbf{G}_1 - v_1v_2$ contains only negative edges by Lemma 2.3(1), which

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also implies $\mathcal{B}_X$ is unique. Considering (2.1) at v_2, we have $(\lambda_1(\mathbf{G}_1) - 3)X_2 = X_3$, which implies $|X_2| < |X_3|$. We assert v_3 must have the 3rd modulus. Otherwise, there exists a vertex of the 3rd modulus which is not adjacent to the edge of $\mathcal{B}_X$, and this vertex is zero by Lemma 2.3(3), a contradiction.

Assume $G = \mathbf{G}_3$. By the eigen-equations (2.1) of X at v_1 and v_2 respectively, $X_1 = X_2$. If $X_1 = 0$, then $X_2 = 0$, and $X_3 = X_4 = 0$ by using (2.1), which implies $X = 0$ by Corollary 2.5(1). So $X_1 = X_2 \neq 0$, and $\{v_1v_2\}$ is a basic edge set. By Lemma 2.3(4), v_1 or v_2 is a vertex with minimum modulus. So X contains no zero entries.

Finally, we prove $\lambda_1(\mathbf{G}_4) > \lambda_1(\mathbf{G}_3)$. Let X be a first eigenvector of $\mathbf{G}_4$. Similar to the above discussion, $|X_4| \geq |X_1|$, $X_4 \neq 0$, and $X_2 = X_3$. In addition, $|X_4| > |X_1|$ by the last part of Lemma 2.10, and then $X_2 \neq 0$ by (2.1) at v_2. If assuming $X_2 > 0$, then $X_4 < 0$ also by (2.1) at v_2. Considering (2.1) at v_1 and v_2 respectively, we get

$$\lambda_1(\mathbf{G}_4)X_2 = [\lambda_1(\mathbf{G}_4) - 2]X_1,\ X_4 = \left(\lambda_1(\mathbf{G}_4) - 2 - \frac{\lambda_1(\mathbf{G}_4)}{\lambda_1(\mathbf{G}_4) - 2}\right) X_2.$$

From the first equality, we have $X_1 < 0$, which implies $\{v_1v_4\}$ is a basic edge set. So X contains no zero entries, and $\mathbf{G}_4 - v_1v_4$ contains only negative edges by Lemma 2.3(1). By the second equality, $|X_4| > |X_2|$ if $\lambda_1(\mathbf{G}_4) - 1 - \frac{\lambda_1(\mathbf{G}_4)}{\lambda_1(\mathbf{G}_4)-2} < 0$. This can be assured as $\lambda_1(\mathbf{G}_4) \leq (3 - \sqrt{5})/2$ by (2.2).

In the graph $\mathbf{G}_4$, deleting the edge v_2v_4 and adding a new edge v_2v_3, we derive a graph G' isomorphic to $\mathbf{G_3}$. Define a vector Y on G' such that $Y_{v_1} = -X_1$, $Y_{v_2} = -X_2$, and $Y_u = X_u$ for other vertices u. Then

$$f_Q(\mathbf{G}_4, X) - f_Q(G', Y) = (|X_4| - |X_2|)^2 + 4|X_1|(|X_4| - |X_3|) > 0,$$

which implies the desired conclusion. ☐

Lemma 3.3. *Let $\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3$ be the graphs of order $n \geq 9$ in Fig. 3.1. Then*

$$\lambda_1(\mathbf{G}_2) > \lambda_1(\mathbf{G}_3) > \lambda_1(\mathbf{G}_1).$$

Proof. The result follows from the following two assertions.

Assertion 1: $\lambda_1(\mathbf{G}_2) > \lambda_1(\mathbf{G}_3)$. Simply denote $f(x) = \det(Q(\mathbf{G}_2) - x\mathbf{I})$ and $g(x) = \det(Q(\mathbf{G}_3) - x\mathbf{I})$, denote $f[a : b]$ or $g[a : b]$ the contiguous principal minor of the determinant $f(x)$ or $g(x)$ indexed by vertices v_i for $i = a, a+1, \ldots, b$, where $1 \leq a \leq b \leq n$. Expanding $f(x)$ and $g(x)$ with respect to the edge v_5v_6, respectively, and noting that $f[a : n] = g[a : n]$ when $6 \leq a \leq n$, we have

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$$\begin{aligned} f(x)-g(x) &= f[1:5]f[6:n]-f[1:4]f[7:n]-\big(g[1:5]g[6:n]-g[1:4]g[7:n]\big)\\ &= \big(f[1:5]-g[1:5]\big)f[6:n]-\big(f[1:4]-g[1:4]\big)f[7:n]\\ &= -3(x-1)(x-3)f[6:n]-(x-1)(x-3)^2f[7:n]\\ &= (x-1)(x-3)\big(-3f[6:n]-(x-3)f[7:n]\big). \end{aligned}$$

Note that if $0 < x \le \lambda_1(\mathbf{G}_2)(< 1)$, then by interlacing theorem $f[a:b] \ge 0$ for $1 \le a \le b \le n$. From the recursion relation that $f[6:n] = (2-x)f[7:n] - f[8:n]$, for $0 < x \le \lambda_1(\mathbf{G}_2) < 1$,

$$\begin{aligned} f[7:n]-f[6:n] &= f[8:n]-f[7:n]+xf[7:n] \ge f[8:n]-f[7:n]\\ &\ge \cdots \ge f[n:n]-f[n-1:n] > 0. \end{aligned}$$

Hence,

$$f(x)-g(x) = (x-1)(x-3)\big\{3(f[8:n]-f[7:n])+2xf[7:n]\big\} > 0,$$

which implies the desired assertion.

Assertion 2: $\lambda_1(\mathbf{G}_3) > \lambda_1(\mathbf{G}_1)$. Simply denote $f(x) = \det(Q(\mathbf{G}_3) - x\mathbf{I})$ and $g(x) = \det(Q(\mathbf{G}_1) - x\mathbf{I})$. Denote by p_m the principal minor of f or g indexed by the vertices of an induced path of order m which contains vertices all of degree 2. The notation $f[a:b], g[a:b]$ are as defined in Assertion 2. Expanding $f(x)$ first with respect to the edge v_4v_5 and then with respect to the edge $v_{n-4}v_{n-3}$, we have

$$\begin{aligned} f(x) &= f[1:4]f[5:n]-f[1:3]f[6:n]\\ &= f[1:4]\big(f[5:n-4]f[n-3:n]-f[5:n-5]f[n-2:n]\big)\\ &\quad -f[1:3]\big(f[6:n-4]f[n-3:n]-f[6:n-5]f[n-2:n]\big)\\ &= f[1:4]f[n-3:n]p_{n-8}+f[1:3]f[n-2:n]p_{n-10}\\ &\quad -\big(f[1:4]f[n-2:n]+f[1:3]f[n-3:n]\big)p_{n-9}, \end{aligned}$$

where $p_{n-9} = 1, p_{n-10} = 0$ if $n = 9$, and $p_{n-10} = 1$ if $n = 10$.

Using a similar expansion for $g(x)$, we compute the difference

$$\begin{aligned} f(x)-g(x) &= \big(f[1:4]f[n-3:n]-g[1:4]g[n-3:n]\big)p_{n-8}\\ &\quad +\big(f[1:3]f[n-2:n]-g[1:3]g[n-2:n]\big)p_{n-10}\\ &\quad -\big(f[1:4]f[n-2:n]+f[1:3]f[n-3:n]\big)p_{n-9}\\ &\quad +\big(g[1:4]g[n-2:n]+g[1:3]g[n-3:n]\big)p_{n-9}\\ &= -(x-1)^2(x-2)^4p_{n-8}-(x-2)^4p_{n-10}-2(x-1)(x-2)^4p_{n-9}\\ &= -(x-2)^4\big\{(x-1)^2p_{n-8}+p_{n-10}+2(x-1)p_{n-9}\big\}\\ &= x(x-2)^4p_{n-7}, \end{aligned}$$

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where the last equality is obtained by using the recursion relations for p_{n-8}, p_{n-7}. We assert $p_{n-7} > 0$ if $0 < x \le \lambda_1(\mathbf{G}_3)$; otherwise $\lambda_1(\mathbf{G}_3)$ is a least eigenvalue of some proper principal submatrix of $Q(\mathbf{G}_3)$, but then $\mathbf{G}_3$ has a first eigenvector containing zero entries by the interlacing theorem (see [28, Theorem 2.1]), a contradiction of Lemma 3.2(2). ◻

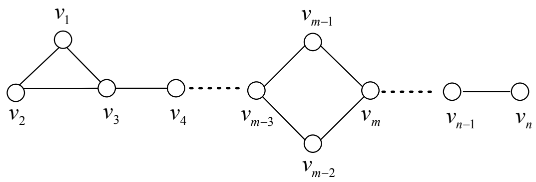

Fig. 3.2. The graph $\bar{\mathbf{G}}_1$.

Lemma 3.4. *Let $\bar{\mathbf{G}}_1$ be the graph of order n in Fig. 3.2. If $m < n$, then $\lambda_1(\bar{\mathbf{G}}_1) > \lambda_1(\mathbf{G}_1)$.*

Proof. Let X be a first eigenvector of $\bar{\mathbf{G}}_1$. We simply write X_{v_i} as X_i for $i = 1, 2, \ldots, n$. By a similar argument as in the proof of Lemma 3.2 for the graph $\mathbf{G}_1$, $\mathcal{B}_X$ consists of the positive edge v_1v_2, and $G - v_1v_2$ contains only negative edges, $X_{m-2} = X_{m-1}$, and $0 < |X_m| < |X_{m+1}| < \cdots < |X_n|$ by Lemma 2.11. Considering the eigen-equations (2.1) at v_m, v_{m-1} respectively, we have $|X_{m-3}| < |X_{m-1}| < |X_m|$. Deleting the edges of the square and also the edge $v_{n-1}v_n$, joining v_{m-3} to v_m and joining each of v_{m-2}, v_{m-1} to both v_{n-1}, v_n, we form a graph G' isomorphic to $\mathbf{G}_1$. Now define a vector Y on G' such that $Y_{v_{m-2}} = Y_{v_{m-1}} = (X_{n-1} - X_n)/2$, $Y_{v_i} = -X_{v_i}$ for $i = m, m+1, \ldots, n-1$, and $Y_u = X_u$ for any other vertices u. Then

$$\begin{aligned} f_Q(\bar{\mathbf{G}}_1, X) - f_Q(G', Y) &= 2[(|X_{m-1}| - |X_{m-3}|)^2 + (|X_m| - |X_{m-1}|)^2] \\ &\quad -(|X_m| - |X_{m-3}|)^2 \ge 0. \end{aligned}$$

If equality holds, then $2|X_{m-1}| = |X_{m-3}| + |X_m|$. By (2.1) at v_{m-1}, we get $X_{m-1} = 0$ and then $X_{m-3} = X_m = 0$, a contradiction. So $f_Q(\bar{\mathbf{G}}_1, X) > f_Q(G', Y)$ and the desired result follows as $\|Y\| > \|X\|$. ◻

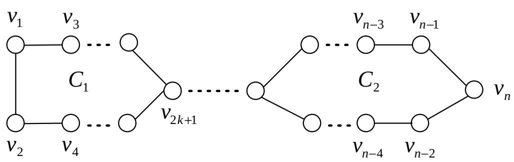

Fig. 3.3. The graph $\hat{\mathbf{G}}_1$.

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LEMMA 3.5. *Let $\hat{\mathbf{G}}_1$ be a ∞-graph of order n in Fig. 3.3, which is obtained from an odd cycle C_1 and an even cycle C_2 connected by a (possibly trivial) path. If C_1 contains at least 5 vertices or C_2 contains at least 6 vertices, then there exists a non-bipartite bicyclic graph G whose kernel is a ∞-graph such that $\lambda_1(\hat{\mathbf{G}}_1) > \lambda_1(G)$.*

Proof. First note that $0 < \lambda_1(\hat{\mathbf{G}}_1) < 1$ by Lemma 3.1. Let X be a first eigenvector of $\hat{\mathbf{G}}_1$. By Lemma 2.10, v_{2k+1} has the maximum modulus among all vertices of C_1. So $X_{v_{2k+1}} \neq 0$; otherwise $X = 0$ by Corollary 2.5(1). This implies every vertex of C_2 is nonzero by Corollary 2.5(2). We divide the discussion into two cases: (1) C_1 contains at least 5 vertices, (2) C_2 contains at least 6 vertices. From the graph symmetry and the fact $X_{v_{2k+1}} \neq 0$, we may assume X holds that $X_{v_1} = X_{v_2}$, $X_{v_3} = X_{v_4}$ (if case (1) occurs), $X_{v_{n-1}} = X_{v_{n-2}}$.

If case (1) occurs, deleting the edge v_1v_3 and adding a new edge v_1v_4, we will get a new graph G with the same quadratic form as $\hat{\mathbf{G}}_1$ associated with X. So $\lambda_1(\hat{\mathbf{G}}_1) \geq \lambda_1(G)$. If the equality holds, then X is also a first eigenvector of G. By the eigen-equations (2.1) of X for $\hat{\mathbf{G}}_1$ and G both at v_3, we have $X_{v_1} = -X_{v_3}$. Also by (2.1) for $\hat{\mathbf{G}}_1$ at v_1, we have $X_{v_1} = 0$, and then $X_{v_{2k+1}} = 0$ by repeatedly using (2.1), a contradiction. Hence, $\lambda_1(\hat{\mathbf{G}}_1) > \lambda_1(G)$.

If case (2) occurs, deleting the $v_{n-1}v_{n-3}$ and adding a new edge $v_{n-1}v_{n-4}$, we also get a new graph G' with the same quadratic form as $\hat{\mathbf{G}}_1$ associated with X. So $\lambda_1(\hat{\mathbf{G}}_1) \geq \lambda_1(G')$. If the the equality holds, then X is also a first eigenvector of G'. By a similar discussion to the first case, we have $X_{v_{n-3}} = -X_{v_{n-1}}$. Considering (2.1) for $\hat{\mathbf{G}}_1$ at v_{n-1} and v_n respectively, we get $\lambda_1(\hat{\mathbf{G}}_1)$ equals 0 or 3, a contradiction. ◻

LEMMA 3.6. *Let G be a non-bipartite bicyclic graph and let X be a first eigenvector of G. Suppose G contains a triangle on vertices $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, where $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ have the smallest, the 2nd smallest and the 3rd smallest moduli respectively, and $\mathcal{B}_X$ contains only $\mathbf{v}_1\mathbf{v}_2$ or $\mathbf{v}_1\mathbf{v}_3$. In addition, assume G is obtained from a θ-graph by attaching at most one path at some vertex other than one of $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$. Then $\lambda_1(G) \geq \lambda_1(\mathbf{G}_2)$ or $\lambda_1(G) \geq \lambda_1(\mathbf{G}_3)$, where $\mathbf{G}_2, \mathbf{G}_3$ are the graphs in Fig. 3.1.*

Proof. Let X be a first eigenvector of G, whose entries are arranged as $|X_1| \leq |X_2| \leq \cdots \leq |X_n|$. We only discuss the case of $\mathbf{v}_1\mathbf{v}_2 \in \mathcal{B}_X$. The case of $\mathbf{v}_1\mathbf{v}_3 \in \mathcal{B}_X$ can be argued similarly and is omitted. Let G_0 be the kernel of G. We have three cases according to the structure of G_0; see Fig. 3.4.

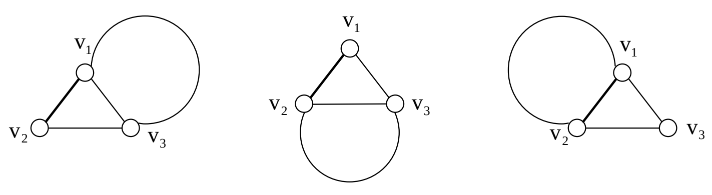

Fig. 3.4. An illustration in the proof of Lemma 3.6.

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If G_0 is of the first graph in Fig. 3.4, then by Lemma 2.9,

$$f_Q(G,X) = f_Q(G - \mathbf{v}_2, X_{G-\mathbf{v}_2}) + S \geq f_Q(G_\Box, Y_{G_\Box}) + S = f_Q(\mathbf{G}_2, Y),$$

where $\mathbf{G}_2$ is the graph in Fig. 3.1, $G_\Box = \mathbf{G}_2 - v_1$, and $S = (|X_1| + |X_2|)^2 + (|X_2| - |X_3|)^2$. Here Y is defined as: $Y_{v_1} = |X_2|$, $Y_{v_2} = |X_1|$, $Y_{v_i} = -|X_i|$ for $i = 3, 4$ and $Y_{v_i} = (-1)^{i-5}|X_i|$ for $i = 5, \ldots, n$. So, $\lambda_1(G) \geq \lambda_1(\mathbf{G}_2)$.

If G_0 is of the second graph in Fig. 3.4, we also get $\lambda_1(G) \geq \lambda_1(\mathbf{G}_2)$ by a similar discussion to the above. If G_0 is of the third graph in Fig. 3.4, then by Lemma 2.8,

$$f_Q(G,X) = f(G - \mathbf{v}_3, X_{G-\mathbf{v}_3}) + S \geq f_Q(G_\triangle, Y_{G_\triangle}) + S = f_Q(\mathbf{G}_3, Y),$$

where $\mathbf{G}_3$ is the graph in Fig. 3.1, $G_\triangle = \mathbf{G}_3 - v_3$, $S = (|X_1| - |X_3|)^2 + (|X_2| - |X_3|)^2$. Here Y is defined as: $Y_{v_i} = |X_i|$ for $i = 1, 2$, $Y_{v_3} = -|X_3|$, and $Y_{v_i} = (-1)^{i-3}|X_i|$ for $i = 4, \ldots, n$. So, $\lambda_1(G) \geq \lambda_1(\mathbf{G}_3)$. □

3.2. Minimum of least eigenvalues of bicyclic graphs. In this section, we will get the main result of this paper, namely a characterization of the unique minimizing non-bipartite bicyclic graphs of order n.

LEMMA 3.7. *Let G be a minimizing graph among all non-bipartite bicyclic graphs of order $n \geq 9$, and let X be a first eigenvector of G. Then*

(1) *G is formed from a ∞-graph or θ-graph G_0 by attaching at most one path P at some vertex w_0, where w_0 is the unique vertex with (nonzero) maximum modulus among all vertices of G_0 (if P exists).*

(2) *$\mathcal{B}_X$ contains exactly one edge $\mathbf{v}_1 u$, where $\mathbf{v}_1$ has the minimum modulus.*

(3) *There exists a vertex $\mathbf{v}_2$ with the 2nd smallest modulus such that $\mathbf{v}_2$ is adjacent to $\mathbf{v}_1$.*

(4) *If $\mathbf{v}_1\mathbf{v}_2 \in \mathcal{B}_X$, then there exists a vertex $\mathbf{v}_3$ of the 3rd smallest modulus such that $\mathbf{v}_3$ is adjacent to $\mathbf{v}_1$ or $\mathbf{v}_2$.*

(5) *If $\mathbf{v}_1$ has degree 2, then u has the 2nd smallest modulus.*

Proof. (1) The argument is similar to the first paragraph of the proof of Corollary 2.13.

(2) By Lemma 2.3(2), we may assume X be such that $G - \mathcal{B}_X$ is bi-signed. Arrange the entries of X as $|X_1| \leq |X_2| \leq \cdots \leq |X_n|$. Assume to the contrary, $\mathcal{B}_X$ contains two edges, both of which necessarily lie on odd cycles by Lemma 2.1(1).

If one edge in $\mathcal{B}_X$, say vw, incident with a vertex with modulus not less than $|X_4|$, we will prove $\lambda_1(G) \geq \lambda_1(\mathbf{G}_3)$, and hence, $\mathbf{G}_3$ is also minimizing. However, this

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is impossible by Lemma 3.3. Observe that $G - vw$ is a unicyclic graph containing an odd cycle. If the odd cycle of $G - vw$ contains the other basic edge, say $v'w'$ of $\mathcal{B}_X$, such that v', w' have the smallest and the 2nd smallest moduli respectively, and $d_{G-vw}(v')$ and $d_{G-uv}(w')$ are both greater than 2, noting that the path P in (1) cannot be attached at v' or w', then G_0 (the kernel of G) has the structure as the graph in Fig. 3.5, where C_1 is an odd cycle and C_2 is an even cycle. In this case, deleting the edge pv' and adding a new edge pw', we arrive at a graph G' for which v' has degree 2. As $|X_p| \geq \max\{|X_{v'}|, |X_{w'}|\}$ and $G - \mathcal{B}_X$ contains no positive edges, $f_Q(G, X) \geq f_Q(G', X)$.

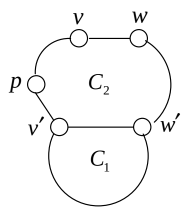

Fig. 3.5. An illustration in the proof of Lemma 3.7(2).

From the above discussion, we may assume $G - vw$ holds the condition of Lemma 2.8 (otherwise taking G' as G). Now by Lemma 2.8

$$\begin{aligned} f_Q(G, X) &\geq f_Q(G - vw, X) + (X_v + X_w)^2 \\ &\geq f_Q(G_\triangle, Y) + (|X_1| + |X_4|)^2 = f_Q(\mathbf{G}_3, Y), \end{aligned}$$

where $G_\triangle$ is the graph in Fig. 2.1 with the vector Y defined on it, $\mathbf{G_3}$ is the graph in Fig. 3.1. Thus, $\lambda_1(G) \geq \lambda_1(\mathbf{G}_3)$. However, $\mathbf{G}_3$ is not minimizing by Lemma 3.3.

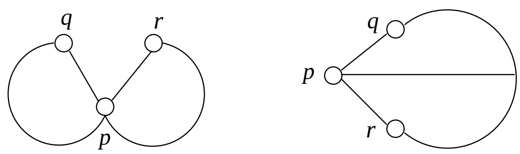

Fig. 3.6. An illustration in the proof of Lemma 3.7(2).

So the two edges of $\mathcal{B}_X$ share a common vertex, say p, and have the other two end vertices, say q, r, which have the moduli $|X_1|$, $|X_2|$, $|X_3|$ respectively (regardless of their order) and same signs (including zero), all lying on odd cycles; see Fig. 3.6 for their positions. Let u be a vertex with minimum modulus among all neighbors of p, q, r other than themselves. If u joins p, q, r, by the assertion (1), $G = \mathbf{G}_4$, which is impossible as $\mathbf{G}_4$ is not minimizing by Lemma 3.2(3). Otherwise, we have a graph G' for which u is adjacent to p, q, r and $f_Q(G', X) \leq f_Q(G, X)$. Thus, $\lambda_1(G') = \lambda_1(G)$ and G' is a minimizing graph. By the assertion (1), $G' = \mathbf{G}_4$, also a contradiction.

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Hence, $\mathcal{B}_X$ contains exactly one basic edge, which must be incident with a vertex, say $\mathbf{v}_1$, with minimum modulus by Lemma 2.3(4).

(3) Let $\mathbf{v}_1 u$ be the only edge of $\mathcal{B}_X$. If $\mathbf{v}_2$, a vertex with the second modulus, is not adjacent to $\mathbf{v}_1$, by Lemma 2.3(3), $\mathbf{v}_2$ and its neighbors all have zero values. In addition $\mathbf{v}_1$ has a zero value. If $X_u \neq 0$, noting that $G - \mathcal{B}_X = G - \mathbf{v}_1 u$ is bi-signed, delete $\mathbf{v}_1 u$ and add a new edge $\mathbf{v}_1\mathbf{v}_2$ or $\mathbf{v}_1 u'$ depending on whether $\mathbf{v}_1, \mathbf{v}_2$ are in the same part of the bipartition for $G - \mathcal{B}_X$ or not, where u' is a neighbor of $\mathbf{v}_2$ in $G - \mathcal{B}_X$. A non-bipartite bicyclic graph G' follows having $f_Q(G', X) < f_Q(G, X)$, a contradiction as G is minimizing. So the vertex u must have a zero value, and is taken as $\mathbf{v}_2$.

(4) If $\mathbf{v}_3$, a vertex with the third modulus, is not adjacent to $\mathbf{v}_1$ or $\mathbf{v}_2$, then $\mathbf{v}_3$ and all its neighbors have zero values. In addition $\mathbf{v}_1$ and $\mathbf{v}_2$ have zero values. Note that $\mathbf{v}_1$ lies on an odd cycle. If one of the neighbors of $\mathbf{v}_1$ other than $\mathbf{v}_2$, say w, has nonzero value, then delete $\mathbf{v}_1 w$ and add a new edge $\mathbf{v}_1\mathbf{v}_3$ or $\mathbf{v}_1 w'$ depending on whether $\mathbf{v}_1, \mathbf{v}_3$ are in different part of the bipartition for $G - \mathcal{B}_X$ or not, where w' is a neighbor of $\mathbf{v}_3$ in $G - \mathcal{B}_X$. A non-bipartite graph G'' follows having $f_Q(G'', X) < f_Q(G, X)$, a contradiction as G is minimizing. So w must have zero value, and is taken as $\mathbf{v}_3$.

(5) Let $\mathbf{v}_1 u$ be the only edge in $\mathcal{B}_X$, where $d(\mathbf{v}_1) = 2$. Assume to the contrary that $|X_u| > |X_2|$. Now $\mathbf{v}_1$ has two neighbors: u and the vertex $\mathbf{v}_2$ by the assertion (3). Re-assigning the value of $\mathbf{v}_1$ by its minus, denoted the resulting vector as X', we have $f_Q(G, X) \geq f_Q(G, X')$ with equality only if $X_{\mathbf{v}_1} = 0$, and consequently, $X_{\mathbf{v}_2} = -X_u$ by the eigen-equation at $\mathbf{v}_1$ for the graph G, a contradiction. □

THEOREM 3.8. *Let G be a non-bipartite bicyclic graph of order $n \geq 9$. Then*

$$\lambda_1(G) \geq \lambda_1(\mathbf{G}_1),$$

with equality if and only if $G = \mathbf{G}_1$, where $\mathbf{G}_1$ is depicted as in Fig. 3.1.

Proof. Suppose G is a minimizing non-bipartite bicyclic graph of order n. The result will follow if we prove $G = \mathbf{G}_1$. Let X be a first eigenvector of G, arranged as $|X_1| \leq |X_2| \leq \cdots \leq |X_n|$. By Lemma 3.7(1), we may assume G is obtained from a ∞-graph or a θ-graph G_0 by attaching at most one path P. By Lemma 2.3(2) we may assume X be such that $G - \mathcal{B}_X$ is bi-signed. By Lemma 3.7(2), $\mathcal{B}_X$ contains exactly one edge $\mathbf{v}_1 u$, where $\mathbf{v}_1$ has the minimum modulus.

Case 1. G_0 is a ∞-graph. We will prove $G = \mathbf{G}_1$.

Firstly we will show $G = G_0$, that is, no path is attached to G_0. Otherwise, let $G = G_0(w_0) \diamond P_{n-m+1}(w_0)$, where G_0 has order $m < n$, and w_0 is the unique vertex with (nonzero) maximum modulus among all vertices of G_0. By Lemma 2.11, we have $|X_{m-1}| < |X_{w_0}| = |X_m| < |X_{m+1}| < \cdots < |X_n|$, where $X_m, X_{m+1}, \ldots, X_n$ are the

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values of the vertices of P starting from w_0.

As $\mathcal{B}_X$ contains exactly one edge, we may assume C_1, C_2 are the two cycles of G_0, where C_1 is odd and C_2 is even. The vertex w_0 must lie on C_2; otherwise, removing C_2 and attaching it at w_0, we could get a graph whose least eigenvalue is less than G by Lemma 2.10. Similarly, by Lemma 2.10, C_1 contains exactly one vertex, say p, with degree greater than 2 and also with maximum modulus among all vertices of C_1. So $X_p \neq 0$, by Corollary 2.5(1). If $p = \mathbf{v}_1$, then all vertices of C_1 have same moduli as $\mathbf{v}_1$, and the vertex u is chosen as $\mathbf{v}_1$.

Thus, $G_0 - \mathbf{v}_1$ is a unicyclic graph of order $m-1 (\geq 5)$, which contains an even cycle with w_0 (the vertex of maximum modulus) on the cycle. Now letting r, s be two neighbors of $\mathbf{v}_1$, by Lemma 2.9 and its proof, we have

$$\begin{aligned} f_Q(G,X) &= f_Q(G_0 - \mathbf{v}_1, X_{G_0-\mathbf{v}_1}) + f_Q(P, X_P) + (X_{\mathbf{v}_1} + X_r)^2 + (X_{\mathbf{v}_1} + X_s)^2 \\ &\geq f_Q(G_\Box, Y_{G_\Box}) + \sum_{i=m}^{n-1} (|X_i| - |X_{i+1}|)^2 + (|X_1| + |X_2|)^2 + (|X_1| - |X_3|)^2 \\ &= f_Q(\bar{\mathbf{G}}_1, Y), \end{aligned}$$

where $\bar{\mathbf{G}}_1$ is the graph in Fig. 3.2, $G_\Box$ is the subgraph of $\bar{\mathbf{G}}_1$ induced by $v_2, v_3, \ldots, v_m$, and Y is defined as: $Y_{v_i} = |X_i|$ for $i = 1, 2$, $Y_{v_i} = (-1)^i |X_i|$ for $i = 3, \ldots, m-2$, $Y_{v_{m-1}} = (-1)^{m-2} |X_{m-1}|$, $Y_{v_i} = (-1)^{i-1} |X_i|$ for $i = m, \ldots, n$. So, $\lambda_1(G) \geq \lambda_1(\bar{\mathbf{G}}_1)$. As G is minimizing, $\bar{\mathbf{G}}_1$ is also minimizing, where the path P is also attached at v_m now. However, by Lemma 3.4, $\lambda_1(\bar{\mathbf{G}}_1) > \lambda_1(\mathbf{G}_1)$, a contradiction.

So $G = G_0$, that is, G is obtained from C_1, C_2 connected by a (possibly trivial) path, i.e., G is the graph $\hat{\mathbf{G}}_1$ in Fig. 3.3. If $\hat{\mathbf{G}}_1$ contains an odd cycle of order at least 5 or an even cycle of order at least 6, then $\hat{\mathbf{G}}_1$ is not minimizing by Lemma 3.5. So we get the desired assertion in this case.

Case 2. G_0 is a θ-graph. We will prove $\lambda_1(G)$ is one of $\lambda_1(\mathbf{G}_2)$, $\lambda_1(\mathbf{G}_3)$ and $\lambda_1(\mathbf{G}_4)$. However, by Lemma 3.2(3) and Lemma 3.3, $\lambda_1(G) > \lambda_1(\mathbf{G}_1)$, a contradiction. So this case cannot occur. Recall that $\mathcal{B}_X = \{\mathbf{v}_1 u\}$.

Case 2.1. $|X_u| \leq |X_3|$. In this case, we will show there exists a minimizing graph H whose kernel is a θ-graph and contains a C_3 made by vertices $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, where $\mathbf{v}_2, \mathbf{v}_3$ have the 2nd smallest and the 3rd smallest moduli, respectively. Furthermore $\lambda_1(H)$ equals $\lambda_1(\mathbf{G}_2)$ or $\lambda_1(\mathbf{G}_3)$.

Case 2.1.1. $|X_u| = |X_2|$. Denote u as $\mathbf{v}_2$. By Lemma 3.7(4), there exists a vertex with third smallest modulus, say $\mathbf{v}_3$, adjacent to $\mathbf{v}_1$ or $\mathbf{v}_2$. If $\mathbf{v}_3$ is adjacent to $\mathbf{v}_1$ but not $\mathbf{v}_2$, letting u be a neighbor of $\mathbf{v}_2$ other than $\mathbf{v}_1$, and deleting $\mathbf{v}_2 u$ and adding $v_2 \mathbf{v}_3$, we would get a graph G' containing C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, and holding $f_Q(G,X) \geq f_Q(G',X)$, which implies G' is also minimizing with X as a first

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eigenvector. If G' contains a ∞-graph as its kernel, then from the discussion of Case 1, $G' = \mathbf{G}_1$ with X as a first eigenvector. By the eigen-equations of X for G and G' both at $\mathbf{v}_3$, we get $X_{\mathbf{v}_2} = -X_{\mathbf{v}_3}$, a contradiction to Lemma 3.2(1). So G' contains a θ-graph as its kernel, and also a triangle C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$.

Similarly, if $\mathbf{v}_3$ is adjacent to $\mathbf{v}_2$ but not $\mathbf{v}_1$, letting w be a neighbor of $\mathbf{v}_1$ other than $\mathbf{v}_2$, and deleting $\mathbf{v}_1 w$ and adding $v_1\mathbf{v}_3$, we would get a graph G'' containing C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, and holding $f_Q(G, X) \geq f_Q(G'', X)$, which implies G'' is also minimizing. By a discussion similar to the above, G'' contains a θ-graph as its kernel, and also a triangle C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$.

Case 2.1.2. $|X_u| = |X_3| > |X_2|$. Denote u as $\mathbf{v}_3$. By Lemma 3.7(3), there exists a vertex with the 2nd smallest modulus, say $\mathbf{v}_2$, adjacent to $\mathbf{v}_1$. In addition, $\mathbf{v}_2$ lies on cycle; otherwise, $|X_2| > |X_{w_0}| > |X_3|$, a contradiction. If $\mathbf{v}_2$ is not adjacent to $\mathbf{v}_3$, letting v be a neighbor of $\mathbf{v}_2$ other than $\mathbf{v}_1$, deleting $\mathbf{v}_2 v$ and adding $\mathbf{v}_2 v_3$, we would get a graph G''' containing C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, and holding $f_Q(G, X) \geq f_Q(G''', X)$, which implies G''' is also minimizing. By a discussion similar to Case 2.1.1, G''' contains a θ-graph as its kernel, and also a triangle C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$.

From the above discussion, we arrive at a minimizing graph H with X as a first eigenvector, which contains a θ-graph as its kernel, and a triangle C_3 made by $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$. By Lemma 3.7(2), the basic edge set $\mathcal{B}_X$ of H contains only one edge, which is incident to a vertex of minimal modulus by Lemma 2.3(4). So the basic edge set $\mathcal{B}_X$ of H contains only $\mathbf{v}_1\mathbf{v}_2$ or $\mathbf{v}_1\mathbf{v}_3$. By Lemma 3.6, $\lambda_1(H)$ equals $\lambda_1(\mathbf{G}_2)$ or $\lambda_1(\mathbf{G}_3)$.

Case 2.2. $\mathbf{v}_1 u$ is a basic edge of $\mathcal{B}_X$, where $|X_u| > |X_3|$. Then by Lemma 3.7(5), $\mathbf{v}_1$ has degree 3. Noting that $G - \mathbf{v}_1 u$ is a unicyclic graph containing an even cycle with $\mathbf{v}_1$ (the vertex with minimum modulus) on that cycle, by Lemma 2.9,

$$\begin{aligned} f_Q(G, X) &= f(G - \mathbf{v}_1 u, X_{G - \mathbf{v}_1 u}) + (|X_1| + |X_u|)^2 \\ &\geq f_Q(G_\Box, Y_{G_\Box}) + (|X_1| + |X_4|)^2 = f_Q(\mathbf{G}_4, Y), \end{aligned}$$

where $\mathbf{G}_4$ is the graph in Fig. 3.1, $G_\Box = \mathbf{G}_4 - v_1 v_4$, Y is defined as: $Y_{v_1} = |X_1|$, $Y_{v_i} = -|X_i|$ for $i = 2, 3$, and $Y_{v_i} = (-1)^{i-4}|X_i|$ for $i = 4, \ldots, n$. So $\lambda_1(G) \geq \lambda_1(\mathbf{G}_4)$, and hence, $\lambda_1(G) = \lambda_1(\mathbf{G}_4)$ as G is a minimizing graph.

The result follows from the above discussion. $\square$

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