

## DOCTORAL THESIS

### Spectral radius and signless Laplacian spectral radius of $k$ -connected graphs

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# Spectral Radius and Signless Laplacian Spectral Radius of $k$ -connected Graphs

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A thesis submitted in partial fulfillment of the requirements  
for the degree of  
Doctor of Philosophy

Principal Supervisor: Dr. SHIU Wai Chee

Hong Kong Baptist University

November 2016

## DECLARATION

I hereby declare that this thesis represents my own work which has been done after registration for the degree of PhD at Hong Kong Baptist University, and has not been previously included in a thesis or dissertation submitted to this or any other institution for a degree, diploma or other qualifications.

I have read the University's current research ethics guidelines, and accept responsibility for the conduct of the procedures in accordance with the University's Committee on the Use of Human & Animal Subjects in Teaching and Research (HASC). I have attempted to identify all the risks related to this research that may arise in conducting this research, obtained the relevant ethical and/or safety approval (where applicable), and acknowledged my obligations and the rights of the participants.

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# Abstract

The adjacency matrix of a graph is a  $(0, 1)$ -matrix indexed by the vertex set of the graph. And the signless Laplacian matrix of a graph is the sum of its adjacency matrix and its diagonal matrix of vertex degrees. The eigenvalues and the signless Laplacian eigenvalues of a graph are the eigenvalues of the adjacency matrix and the signless Laplacian matrix, respectively. These two matrices of a graph have been studied for several decades since they have been applied to many research fields, such as computer science, communication network, information science and so on.

In this thesis, we study  $k$ -connected graphs and focus on their spectral radius and signless Laplacian spectral radius. Firstly, we determine the graphs with maximum spectral radius among all  $k$ -connected graphs of fixed order with given diameter. As we know, when a graph is regular, its spectral radius and signless Laplacian spectral radius can easily be found. We obtain an upper bound on the signless Laplacian spectral radius of  $k$ -connected irregular graphs. Finally, we give some other results mainly related to the signless Laplacian matrix.

**Keywords:** Irregular graphs; planar graphs;  $k$ -connected; semi-edge walks; adjacency matrix; spectral radius; signless Laplacian matrix; signless Laplacian spectral radius; signless Laplacian characteristic polynomial; coefficient.

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# Chapter 1

## Introduction

This chapter includes four sections. In Section 1.1, some basic notation and definitions on graphs are introduced. Section 1.2 contains some useful results on matrices and introduces three kinds of matrices associated with a graph, which are adjacency matrix, Laplacian matrix and signless Laplacian matrix. Section 1.3 includes the research background of this thesis. And Section 1.4 gives an outline of this thesis.

### 1.1 Graphs

A *graph*  $G = (V(G), E(G))$  consists of a *vertex* set  $V(G)$  and an *edge* set  $E(G)$ , disjoint from  $V(G)$ , where an edge of  $G$  is an unordered pair of vertices (not necessarily distinct) of  $G$ . The cardinalities of  $V(G)$  and  $E(G)$  are known as the *order* and the *size* of  $G$ , usually denoted by  $n$  and  $m$ , respectively. Thus  $n = |V(G)|$  and  $m = |E(G)|$ .

Let  $e = \{u, v\}$  be an edge in  $G$ . The *ends* of  $e$  are  $u$  and  $v$  and they are said to be *incident* with  $e$  and vice versa. Moreover, if  $u$  and  $v$  are distinct, they are called *adjacent* vertices and also *neighbours*. The set of neighbours of a vertex  $v$  in  $G$  is denoted by  $N_G(v)$  (or  $N(v)$  for short). A *loop* is an edge with identical ends. And two or more edges with the same pair of distinct ends are called *parallel edges*. A *simple* graph is a graph without loops and parallel edges.

The number of edges of  $G$  incident with a vertex  $v$  is the *degree* of  $v$  in  $G$ , denoted by  $d_G(v)$  (or  $d_v$  for short). Each loop counts as two edges. In particular, if  $G$  is simple, then  $d_G(v) = |N_G(v)|$ . We denote by  $\delta(G)$  (or  $\delta$  for short) and  $\Delta(G)$  (or  $\Delta$  for short) the minimum and the maximum degrees of the vertices of  $G$ , respectively. A graph  $G$  is said to be *k-regular* if  $d_v = k$  for all  $v \in V(G)$ , in other words,  $\Delta(G) = \delta(G) = k$ . And a graph is *regular* if it is  $k$ -regular for some  $k$ . A simple graph of order  $n$  is called a *complete* graph if any pair of its vertices are adjacent and thus is  $(n - 1)$ -regular, denoted by  $K_n$ . A graph  $G$  is *bipartite* if  $V(G)$  admits a partition into two classes,  $X$  and  $Y$ , such that every edge has one end in  $X$  and one end in  $Y$ . The partition  $(X, Y)$  is called a *bipartition* of  $G$ , and  $X$  and  $Y$  its *parts*.

The following theorem is a fundamental proposition related to the size of  $G$  and the degrees of vertices of  $G$ .

**Theorem 1.1** ([7]). *For any graph  $G$  with size  $m$ ,*

$$\sum_{v \in V(G)} d_G(v) = 2m.$$

A *walk* in  $G$  is an alternating sequence  $W = v_1 e_1 v_2 \cdots v_l e_l v_{l+1}$  of vertices and edges such that  $e_i = \{v_i, v_{i+1}\}$ , for any  $i \in \{1, 2, \dots, l\}$ . A walk  $W$  is called a *path* if all the vertices in  $W$  are distinct. A *connected* graph is one such that any two vertices of the graph are linked by a path, otherwise *disconnected*. A *cycle* is a connected graph where each vertex has exactly two neighbours. A path and a cycle of order  $n$  are usually denoted by  $P_n$  and  $C_n$ , respectively. The number of edges of a path (or a cycle) is its *length*. The *distance* between two distinct vertices  $u$  and  $v$  is the length of a shortest path that contains  $u$  and  $v$ . The maximum distance between any pair of distinct vertices of  $G$  is the *diameter* of  $G$ , denoted by  $d(G)$  (or  $d$  for short).

For two graphs  $G$  and  $H$ , if  $V(H) \subseteq V(G)$  and  $E(H) \subseteq E(G)$ , then  $H$  is called a *subgraph* of  $G$ .  $H$  is a *spanning subgraph* of  $G$  if  $V(H) = V(G)$ . In other words, any spanning subgraph of  $G$  can be constructed by only removing some edges from  $G$ . An *induced subgraph* of  $G$  is a subgraph obtained by vertex deletions from  $G$  only,

together with all edges incident with the vertices that are deleted. Let  $X$  be the set of vertices that are deleted. Then we denote by  $G - X$  the resulting subgraph. Let  $Y$  be the set of remaining vertices, that is  $V \setminus X$ . Then the induced subgraph is called the subgraph of  $G$  *induced by*  $Y$  and denoted by  $G[Y]$ .

Given a graph  $G$ , if  $|V(G)| > k$  ( $k \in \mathbb{N}$ ) and  $G - X$  is connected for any subset  $X \subseteq V(G)$  with  $|X| < k$ , then  $G$  is called *k-connected*. The *connectivity*  $\kappa(G)$  of  $G$  is the largest integer  $k$  such that  $G$  is  $k$ -connected. Therefore,  $G$  is disconnected or a  $K_1$  if and only if  $\kappa(G) = 0$ . By the definition,  $\kappa(K_n) = n - 1$  for all  $n \geq 1$ . Similarly, let  $Y \subseteq E(G)$  and  $G - Y$  be the spanning subgraph by deleting the edges in  $Y$  from  $G$ . If  $|V(G)| > 1$  and  $G - Y$  is connected for every subset  $Y \subseteq E(G)$  with  $|Y| < k$  ( $k \in \mathbb{N}$ ), then  $G$  is *k-edge-connected*. The *edge-connectivity*  $\kappa'(G)$  of  $G$  is the largest integer  $k$  such that  $G$  is  $k$ -edge-connected. In particular,  $\kappa'(G) = 0$  if  $G$  is disconnected. Two graphs are *vertex-disjoint* (or simply *disjoint*) if they have no vertex in common. And if they have no edge in common then they are *edge-disjoint*. We have the following famous Menger's Theorem.

**Theorem 1.2 (Menger's Theorem [32]).** *A graph is k-connected (or k-edge-connected) if and only if it contains k vertex-disjoint (or edge-disjoint) paths between any two vertices.*

Let  $G$  and  $H$  be two simple graphs. The graph  $G \cup H$  with vertex set  $V(G) \cup V(H)$  and edge set  $E(G) \cup E(H)$  is called the *union* of  $G$  and  $H$ . And the union is *disjoint* if  $G$  and  $H$  are disjoint. It can be seen that every graph may be expressed as a disjoint union of connected graphs which are usually called the *connected components*, or simply the *components*.

An *acyclic* graph is a graph with no cycles. And a *tree* is a connected acyclic graph. Each component of an acyclic graph is a tree. Usually, we call acyclic graphs *forests*. A subgraph which is a tree is called a *subtree* of a graph. When this subtree is a spanning subgraph, it is a *spanning tree* of the graph. A tree  $T$  with a specified vertex  $x$ , called the *root* of  $T$ , is a *rooted tree*  $T(x)$ . By the definitions, for any vertex

$v \neq x$  in  $T(x)$ , there is only one path, say  $xTv$ , from  $x$  to  $v$ . Each vertex on the path  $xTv$ , including  $v$ , is called an *ancestor* of  $v$  and a *descendant* of  $v$  is a vertex of which  $v$  is an ancestor. If an ancestor or descendant of a vertex is not the vertex itself, then it is *proper*. The *predecessor* or *parent* of  $v$  other than the root  $x$  is the immediate proper ancestor of  $v$ . And the *successors* or *children* of  $v$  are the vertices whose predecessor is  $v$ .

A graph is called a *planar graph* if it can be drawn in the plane such that no two edges meet at a point other than a common end of them. Obviously, trees and forests are planar graphs.

A family  $\mathcal{F}$  of edge-disjoint subgraphs  $H$  of  $G$  such that

$$\bigcup_{H \in \mathcal{F}} E(H) = E(G)$$

is a *decomposition* of  $G$ . If we restrict  $H$  to be subgraphs such that  $G$  and  $H$  have the same vertex set, then this is a special case of a decomposition of  $G$  which will be used later in this thesis. A graph whose components are paths of length at most  $k$  is called *linear  $k$ -forest*. The least integer  $p$  such that  $E(G)$  can be decomposed into  $p$  linear  $k$ -forests is called the *linear  $k$ -arborocicity* of  $G$ , usually denoted by  $la_k(G)$ .

Sometimes we need a graph whose edges are assigned an orientation, namely a directed graph. A *directed graph* or *digraph*  $F$  is an ordered pair  $(V(F), E(F))$  consisting of a vertex set  $V(F)$  and an *arc* set  $E(F)$ , where an arc of  $F$  is an ordered pair of vertices of  $F$ . Let  $a = (u, v)$  be an arc. Then we say  $u$  *dominates*  $v$ . And  $v$  is the *head* of  $a$  while  $u$  is its *tail*. The *in-neighbours* of a vertex  $v$  are the vertices which dominates  $v$ , its *out-neighbours* are those which are dominated by  $v$ . They are denoted by  $N_F^-(v)$  and  $N_F^+(v)$ , respectively. The *order* and the *size* of  $F$  are the number of its vertices and its arcs, respectively. Given a vertex  $v$  in  $F$ , the number of arcs with head  $v$  is called the *in-degree*, denoted by  $d_F^-(v)$ , of  $v$ . And the number of arcs with tail  $v$  is called the *out-degree*, denoted by  $d_F^+(v)$ , of  $v$ . The minimum in-degree and out-degree of  $F$  are denoted by  $\delta^-(F)$  and  $\delta^+(F)$ , respectively. Similarly, the maximum in-degree and out-degree of  $F$  are denoted by  $\Delta^-(F)$  and  $\Delta^+(F)$ ,

respectively. If the number of arcs of a digraph  $F$  is  $m$ , then we have the following theorem which is similar to Theorem 1.1.

**Theorem 1.3** ([7]). *Let  $F$  be a digraph with size  $m$ , then*

$$\sum_{v \in V(F)} d_F^-(v) = \sum_{v \in V(F)} d_F^+(v) = m.$$

An *orientation* of an undirected graph  $G$  is a digraph  $F$  that is obtained from  $G$  by assigning a direction to each edge of  $G$ . And  $G$  is called the *underlying graph* of  $F$ .

*Infinite graphs* are the graphs defined on infinite sets of vertices and (or) edges. All notation undefined here are referred to the book [7].

## 1.2 Matrices and eigenvalues of a graph

A branch of graph theory that studies graphs by using algebraic properties of associated matrices is known as algebraic graph theory. In particular, spectral graph theory studies the relation between a graph and the spectrum of its adjacency matrix, Laplacian matrix or signless Laplacian matrix. In this section, we first present some useful results on matrices. And then we introduce three kinds of matrices associated with a graph.

### 1.2.1 Some useful results on matrices

Here we assume that readers are familiar with the basic definitions about matrices. Let  $\mathbf{M}_{m,n}(\mathbb{C})$  be the set of all  $m$ -by- $n$  matrices over complex field  $\mathbb{C}$ . For a matrix  $M \in \mathbf{M}_{n,n}(\mathbb{C})$  (or simply  $\mathbf{M}_n(\mathbb{C})$ ), let  $\sigma(M)$  be its spectrum and  $\rho(M)$  be its spectral radius. Then,  $\rho(M) = \max\{|\lambda| : \lambda \in \sigma(M)\}$ .

Let  $M \in \mathbf{M}_n(\mathbb{C})$ . The  $(i, j)$ -*cofactor* is defined by  $(-1)^{i+j} \det M(i, j)$ , where  $M(i, j)$  is the matrix obtained by deleting row  $i$  and column  $j$  from  $M$ . Let  $\mathbf{I}$  de-

note the identity matrix. Then  $\Phi_M(x) = \det(x\mathbf{I} - M)$  is known as the characteristic polynomial of  $M$ .

**Definition 1.1** ([44]). Let  $V$  be a vector space over the field  $\mathbb{R}$  (or  $\mathbb{C}$ ). A function  $\|\cdot\| : V \rightarrow \mathbb{R}$  is a *norm* (sometimes one says *vector norm*) if, for all  $\mathbf{x}, \mathbf{y} \in V$  and all  $c \in \mathbb{R}$  (or  $\mathbb{C}$ ),

- (a)  $\|\mathbf{x}\| \geq 0$ ,
- (b)  $\|\mathbf{x}\| = 0$  if and only if  $\mathbf{x} = 0$ ,
- (c)  $\|c\mathbf{x}\| = |c|\|\mathbf{x}\|$ ,
- (d)  $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ .

We give some examples of useful norms. Let  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  be a vector on  $\mathbb{C}^n$ . The  $l_1$ -norm of  $\mathbf{x}$  is

$$\|\mathbf{x}\|_1 = |x_1| + |x_2| + \dots + |x_n|.$$

The  $l_2$ -norm of  $\mathbf{x}$  on  $\mathbb{C}^n$ ,

$$\|\mathbf{x}\|_2 = \sqrt{|x_1|^2 + |x_2|^2 + \dots + |x_n|^2},$$

is maybe the most familiar norm. And the  $l_\infty$ -norm of  $\mathbf{x}$  on  $\mathbb{C}^n$  is

$$\|\mathbf{x}\|_\infty = \max\{|x_1|, |x_2|, \dots, |x_n|\}.$$

Generally speaking, for  $p \geq 1$ , the  $l_p$ -norm of  $\mathbf{x}$  on  $\mathbb{C}^n$  is

$$\|\mathbf{x}\|_p = (|x_1|^p + |x_2|^p + \dots + |x_n|^p)^{\frac{1}{p}}.$$

Given a Hermitian matrix  $M \in \mathbf{M}_n(\mathbb{C})$ , let  $\sigma(M) = \{\lambda_1(M), \lambda_2(M), \dots, \lambda_n(M)\}$  be its spectrum. Since the eigenvalues of a Hermitian matrix  $M$  are real, we may arrange them in algebraically nondecreasing order. For convenience, we suppose

$$\lambda_{\min}(M) = \lambda_1(M) \leq \lambda_2(M) \leq \dots \leq \lambda_n(M) = \lambda_{\max}(M). \quad (1.1)$$

The first useful result is the following Rayleigh quotient theorem.

**Theorem 1.4 (Rayleigh [44]).** Let  $M \in \mathbf{M}_n(\mathbb{C})$  be Hermitian and let the eigenvalues of  $M$  be ordered as in (1.1). Let  $i_1, i_2, \dots, i_k$  be given integers with  $1 \leq i_1 < i_2 < \dots < i_k \leq n$ . Suppose  $\mathbf{x}_{i_1}, \mathbf{x}_{i_2}, \dots, \mathbf{x}_{i_k}$  are orthonormal such that  $M\mathbf{x}_{i_p} = \lambda_{i_p}\mathbf{x}_{i_p}$  for each  $p \in \{1, 2, \dots, k\}$ . Let  $S = \text{span} \{\mathbf{x}_{i_1}, \mathbf{x}_{i_2}, \dots, \mathbf{x}_{i_k}\}$ . Then

(a)

$$\begin{aligned} \lambda_{i_1} &= \min_{\substack{\mathbf{x} \in S \\ \mathbf{x} \neq \mathbf{0}}} \frac{\mathbf{x}^* M \mathbf{x}}{\mathbf{x}^* \mathbf{x}} = \min_{\|\mathbf{x}\|_2=1} \mathbf{x}^* M \mathbf{x} \\ &\leq \max_{\substack{\mathbf{x} \in S \\ \|\mathbf{x}\|_2=1}} \mathbf{x}^* M \mathbf{x} = \max_{\substack{\mathbf{x} \in S \\ \mathbf{x} \neq \mathbf{0}}} \frac{\mathbf{x}^* M \mathbf{x}}{\mathbf{x}^* \mathbf{x}} = \lambda_{i_k}, \end{aligned}$$

(b)  $\lambda_{i_1} \leq \mathbf{x}^* M \mathbf{x} \leq \lambda_{i_k}$  for any unit vector  $\mathbf{x} \in S$ , with equality in the right hand (or left hand) if and only if  $M\mathbf{x} = \lambda_{i_k}\mathbf{x}$  (or  $M\mathbf{x} = \lambda_{i_1}\mathbf{x}$ ),

(c)  $\lambda_{\min} \leq \mathbf{x}^* M \mathbf{x} \leq \lambda_{\max}$  for any unit vector  $\mathbf{x} \in \mathbb{C}^n$ , with equality in the right hand (or left hand) if and only if  $M\mathbf{x} = \lambda_{\max}\mathbf{x}$  (or  $M\mathbf{x} = \lambda_{\min}\mathbf{x}$ ). Moreover,

$$\lambda_{\max} = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^* M \mathbf{x}}{\mathbf{x}^* \mathbf{x}} = \max_{\|\mathbf{x}\|_2=1} \mathbf{x}^* M \mathbf{x}$$

and

$$\lambda_{\min} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^* M \mathbf{x}}{\mathbf{x}^* \mathbf{x}} = \min_{\|\mathbf{x}\|_2=1} \mathbf{x}^* M \mathbf{x}.$$

The following theorem of Hermann Weyl is very useful when we consider the eigenvalues of a sum of some Hermitian matrices.

**Theorem 1.5 (Weyl [44]).** Let  $A, B \in \mathbf{M}_n(\mathbb{C})$  be Hermitian and let the respective eigenvalues of  $A$ ,  $B$  and  $A + B$  be  $\lambda_i(A)$ ,  $\lambda_i(B)$  and  $\lambda_i(A + B)$  for  $i \in \{1, 2, \dots, n\}$ , each algebraically ordered as in (1.1). Then

$$\lambda_i(A + B) \leq \lambda_{i+j}(A) + \lambda_{n-j}(B),$$

for each  $i \in \{1, 2, \dots, n\}$  and  $j \in \{0, 1, \dots, n - i\}$ , with equality for some pair  $i, j$  if and only if there is a nonzero vector  $\mathbf{x}$  such that  $A\mathbf{x} = \lambda_{i+j}(A)\mathbf{x}$ ,  $B\mathbf{x} = \lambda_{n-i}(B)\mathbf{x}$  and  $(A + B)\mathbf{x} = \lambda_i(A + B)\mathbf{x}$ .



And for each  $i \in \{1, 2, \dots, n\}$  and  $j \in \{1, 2, \dots, i\}$ ,

$$\lambda_{i-j+1}(A) + \lambda_j(B) \leq \lambda_i(A + B),$$

with equality for some pair  $i, j$  if and only if there is a nonzero vector  $\mathbf{x}$  such that  $A\mathbf{x} = \lambda_{i-j+1}(A)\mathbf{x}$ ,  $B\mathbf{x} = \lambda_j(B)\mathbf{x}$  and  $(A + B)\mathbf{x} = \lambda_i(A + B)\mathbf{x}$ .

**Definition 1.2** ([44]). A function  $\|\cdot\| : \mathbf{M}_n(\mathbb{C}) \rightarrow \mathbb{R}$  is a *matrix norm* if, for all  $A, B \in \mathbf{M}_n(\mathbb{C})$  and all  $c \in \mathbb{C}$ ,

- (a)  $\|A\| \geq 0$ ,
- (b)  $\|A\| = 0$  if and only if  $A = 0$ ,
- (c)  $\|cA\| = |c| \cdot \|A\|$ ,
- (d)  $\|A + B\| \leq \|A\| + \|B\|$ ,
- (e)  $\|AB\| \leq \|A\| \cdot \|B\|$

A norm on matrices that does not satisfy property (e) for all  $A$  and  $B$  is obviously a vector norm. There are many kinds of matrix norms. Here we present some usual matrix norms. Note that we may regard  $\mathbf{M}_n(\mathbb{C})$  as a vector space of dimension  $n^2$ , that is  $\mathbb{C}^{n^2}$ . The most familiar examples are the  $l_p$ -norms for  $p = 1, 2, \infty$ . They are already known to be vector norms. The  $l_1$ -norm defined for  $M \in \mathbf{M}_n(\mathbb{C})$  by

$$\|M\|_1 = \sum_{i,j=1}^n |m_{ij}|,$$

where  $m_{ij}$  is the  $(i, j)$ -entry of  $M$ , is a matrix norm. The  $l_2$ -norm defined for  $M \in \mathbf{M}_n(\mathbb{C})$  by

$$\|M\|_2 = \sqrt{\sum_{i,j=1}^n |m_{ij}|^2}$$

is a matrix norm. However, one can show that the  $l_\infty$ -norm defined for  $M \in \mathbf{M}_n(\mathbb{C})$  by

$$\|M\|_\infty = \max_{1 \leq i,j \leq n} |m_{ij}|$$

is a vector norm but not a matrix norm since it does not satisfy the property (e).

The following result is another useful theorem since it gives a relation between the spectral radius of a matrix and its matrix norms.

**Theorem 1.6 (Gelfand Formula [44]).** *Let  $\|\cdot\|$  be a matrix norm on  $\mathbf{M}_n(\mathbb{C})$  and let  $M \in \mathbf{M}_n(\mathbb{C})$ . Then*

$$\rho(M) = \lim_{k \rightarrow \infty} \|\|M^k\|\|^{\frac{1}{k}}.$$

Let  $M = [m_{ij}] \in \mathbf{M}_{m,n}(\mathbb{R})$ . We write  $M \geq 0$  if all  $m_{ij} \geq 0$  and  $M > 0$  if all  $m_{ij} > 0$ . If  $M \geq 0$  then we say  $M$  is a *nonnegative* matrix and if  $M > 0$  then  $M$  is a *positive* matrix. Now let  $M \in \mathbf{M}_n(\mathbb{R})$  be a nonnegative real matrix. If for some  $k \in \mathbb{N}$  we have  $M^k > 0$ , then  $M$  is said to be *primitive*. And if for all  $i$  and  $j$  there is a  $k \in \mathbb{N}$  such that  $(M^k)_{ij} > 0$ , then  $M$  is said to be *irreducible*. Another important theorem is the following Perron-Frobenius theorem.

**Theorem 1.7 (Perron-Frobenius [44]).** *Let  $M \in \mathbf{M}_n(\mathbb{R})$  be irreducible and non-negative, and suppose that  $n > 1$ . Then*

- (a)  $\rho(M) > 0$ ,
- (b)  $\rho(M)$  is an algebraically simple eigenvalue of  $M$ ,
- (c) there is a unique positive real vector  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  such that  $M\mathbf{x} = \rho(M)\mathbf{x}$  and  $x_1 + x_2 + \dots + x_n = 1$ ,
- (d) there is a unique positive real vector  $\mathbf{y} = (y_1, y_2, \dots, y_n)^T$  such that  $\mathbf{y}^T M = \rho(M)\mathbf{y}^T$  and  $x_1 y_1 + x_2 y_2 + \dots + x_n y_n = 1$ .

### 1.2.2 Adjacency matrix of a graph

There exist many kinds of matrices that associated with a graph, such as the adjacency matrix, the Laplacian matrix, the signless Laplacian matrix, the incidence matrix, the distance matrix and so on. Here we only introduce the first three matrices.

Let  $G = (V(G), E(G))$  be a simple graph of order  $n$  and size  $m$  with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ . The *adjacency matrix* of  $G$ , denoted by  $A(G)$ , is defined by  $A(G) = [a_{ij}]$ , where

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent vertices} \\ 0 & \text{otherwise.} \end{cases}$$

It is obvious from the definition that  $A(G)$  is a real symmetric matrix and the trace of  $A(G)$  is zero. Thus  $A(G)$  is diagonalizable and has  $n$  real eigenvalues, denoted by  $\lambda_i(G)$ ,  $i \in \{1, 2, \dots, n\}$ . Usually, we arrange them in the following order,

$$\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G),$$

which is different from (1.1). The characteristic polynomial of  $A(G)$  is known as the *characteristic polynomial* of  $G$ , that is  $\Phi_{A(G)}(x) = \det(x\mathbf{I} - A(G))$ . Thus  $\lambda_i(G)$ ,  $i \in \{1, 2, \dots, n\}$ , are the roots of the equation  $\Phi_{A(G)}(x) = 0$ . The *spectrum* of  $G$ , denoted by  $\sigma(G)$ , is the spectrum of its adjacency matrix  $A(G)$  which is the set of its eigenvalues together with their multiplicities. In other words,

$$\sigma(G) = \{\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)\}.$$

Let  $G$  be a disconnected graph with components  $G_1, G_2, \dots, G_k$ . And let  $A(G_i)$  be the adjacency matrix of  $G_i$ ,  $i \in \{1, 2, \dots, k\}$ . Then  $A(G)$  is a block diagonal matrix. We can label the vertices in  $V(G)$  such that

$$A(G) = A(G_1) \oplus A(G_2) \oplus \dots \oplus A(G_k) = \begin{pmatrix} A(G_1) & 0 & \dots & 0 \\ 0 & A(G_2) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & A(G_k) \end{pmatrix}.$$

Therefore

$$\sigma(G) = \sigma(G_1) \cup \sigma(G_2) \cup \dots \cup \sigma(G_k),$$

which means that we can study the spectrum of  $G$  by studying the spectrum of each component,  $G_i$ , of  $G$ . Thus we just need to consider the connected graphs.

The entries of adjacency matrix can stand for the numbers of walks between vertices in  $G$ . Namely,

**Theorem 1.8** ([65]). *The number of walks of length  $k$ ,  $k \geq 0$ , between vertices  $v_i$  and  $v_j$  in  $G$  is  $(A^k(G))_{ij}$ .*

In particular, the degree of vertex  $v_i$  is  $(A^2(G))_{ii}$ . Hence by Theorem 1.1, we have

$$2m = \sum_{i=1}^n d_{v_i} = \text{Tr}(A^2(G)) = \sum_{i=1}^n \lambda_i^2(G). \quad (1.2)$$

Similarly, the number of triangles in  $G$  is  $\frac{1}{6}\text{Tr}(A^3(G))$ .

For a connected graph  $G$ , there is always a walk of some length  $k$  between any pair of vertices of  $G$ . Thus, by Theorem 1.8, there is an integer  $k$  such that  $(A^k(G))_{ij} > 0$  for all  $i$  and  $j$ , which means the adjacency matrix  $A(G)$  is irreducible. In addition, it is nonnegative. Therefore, by Perron-Frobenius theorem (Theorem 1.7), the spectral radius of  $A(G)$  is an eigenvalue of  $A(G)$ . And then  $\lambda_1(G) \geq -\lambda_n(G)$ , which can imply  $\rho(A(G)) = \lambda_1(G)$ . Now we define the *spectral radius* of  $G$  as the largest eigenvalue  $\lambda_1(G)$  of  $A(G)$ . From Perron-Frobenius theorem, we can also know that the multiplicity of  $\lambda_1(G)$  is 1 and there exists a unit positive eigenvector  $\mathbf{x}$ , which is called the *Perron vector* of  $A(G)$ , such that  $A(G)\mathbf{x} = \lambda_1(G)\mathbf{x}$ . Let  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  be the Perron vector, where the positive number  $x_i$  corresponds to the vertex  $v_i$ ,  $i \in \{1, 2, \dots, n\}$ . Then

$$\lambda_1(G) = \mathbf{x}^T A(G)\mathbf{x} = 2 \sum_{v_i v_j \in E(G)} x_i x_j. \quad (1.3)$$

Moreover,  $\lambda_1(G)$  can be characterized by the Rayleigh quotient (Theorem 1.4),

$$\lambda_1(G) = \max_{\|\mathbf{x}\|_2=1} \mathbf{x}^T A(G)\mathbf{x}. \quad (1.4)$$

One can get a lot of structural properties of a graph  $G$  from its spectrum. For instance, we can determine whether a graph is regular from its spectrum.

**Proposition 1.1** ([8]). *Let  $\bar{d}(G)$  be the average degree of a connected graph  $G$ . Then we have  $\delta(G) \leq \bar{d}(G) \leq \lambda_1(G) \leq \Delta(G)$ , where each equality holds if and only if  $G$  is regular.*

Immediately, by (1.2), we can get

**Proposition 1.2.** *Let  $G$  be a connected graph of order  $n$  with average degree  $\bar{d}(G)$ .*

*Then*

$$\sum_{i=1}^n \lambda_i^2(G) = n\bar{d}(G) \leq n\lambda_1(G),$$

*where the equality holds if and only if  $G$  is regular.*

Another example is to determine whether a graph is bipartite.

**Proposition 1.3** ([58]). *A connected graph  $G$  is bipartite if and only if  $-\lambda_1(G)$  is an eigenvalue of  $G$ , in which case the spectrum is symmetric with respect to 0. If  $G$  is bipartite, then the eigenvector of  $-\lambda_1(G)$  is obtained from its Perron vector by changing signs of the components in one part of the bipartition.*

For more examples, one can see [19, 20] for details.

### 1.2.3 Laplacian matrix of a graph

The Laplacian matrix, denoted by  $L(G)$ , is another important matrix of a graph  $G$ . The *Laplacian matrix* of  $G$  is defined by  $L(G) = D(G) - A(G)$ , where  $D(G) = \text{diag}(d_{v_1}, d_{v_2}, \dots, d_{v_n})$  is the diagonal matrix of vertex degrees. The *Laplacian eigenvalues* of  $G$  are the eigenvalues of  $L(G)$ . Obviously,  $L(G)$  is a real symmetric matrix and thus its eigenvalues, denoted by  $\mu_i(G)$ ,  $i \in \{1, 2, \dots, n\}$ , are real and can be ordered as

$$\mu_1(G) \geq \mu_2(G) \geq \dots \geq \mu_n(G).$$

The characteristic polynomial of  $L(G)$  is known as the *Laplacian characteristic polynomial* of  $G$ , that is,  $\Phi_{L(G)}(x) = \det(x\mathbf{I} - L(G))$ . Thus  $\mu_i(G)$ ,  $i \in \{1, 2, \dots, n\}$ , are the roots of the equation  $\Phi_{L(G)}(x) = 0$ . The *Laplacian spectrum* of  $G$  is the spectrum of its Laplacian matrix  $L(G)$ .

$L(G)$  is a positive semi-definite matrix. Indeed, let  $\mathbf{x}$  be any vector in  $\mathbb{C}^n$ , then

$$\mathbf{x}^T L(G) \mathbf{x} = \sum_{v_i v_j \in E(G)} (x_i - x_j)^2 \geq 0.$$

Therefore  $\mu_i(G) \geq 0$  for  $i \in \{1, 2, \dots, n\}$ . Since all the row sums are 0, 0 is an eigenvalue of  $L(G)$  with the eigenvector  $\mathbf{1} = (1, 1, \dots, 1)^T$ , which implies  $\mu_n(G) = 0$ . The *Laplacian spectral radius* of  $G$  is the largest eigenvalue  $\mu_1(G)$  of  $L(G)$ . And the *algebraic connectivity* of  $G$  is the second smallest eigenvalue  $\mu_{n-1}(G)$ .

Again, if  $G$  is a disconnected graph with components  $G_1, G_2, \dots, G_k$ , then  $L(G)$  is a block diagonal matrix. Thus we have

$$L(G) = L(G_1) \oplus L(G_2) \oplus \dots \oplus L(G_k).$$

And the Laplacian spectrum of  $G$  is the union of the Laplacian spectrum of its components. We can determine the number of components of  $G$  by its smallest Laplacian eigenvalue.

**Proposition 1.4** ([8]). *The multiplicity of 0 as a Laplacian eigenvalue of a graph  $G$  is the number of its components.*

We can obtain the number of spanning trees by the Laplacian spectrum of a graph.

**Proposition 1.5** ([8]). *Let  $G$  be graph of order  $n$ , and Laplacian matrix  $L(G)$  with eigenvalues  $\mu_1(G) \geq \mu_2(G) \geq \dots \geq \mu_n(G) = 0$ . Let  $l_{ij}$  be the  $(i, j)$ -cofactor of  $L(G)$ . Then the number of spanning trees of  $G$  equals*

$$l_{ij} = \det \left( L(G) + \frac{1}{n^2} \mathbf{J} \right) = \frac{1}{n} \mu_1(G) \mu_2(G) \cdots \mu_{n-1}(G),$$

for any  $v_i, v_j \in V(G)$ , where  $\mathbf{J}$  denotes the all-1 matrix.

### 1.2.4 Signless Laplacian matrix of a graph

Given a graph  $G$  with the adjacency matrix  $A(G)$  and the diagonal matrix  $D(G)$ , the *signless Laplacian matrix* of  $G$ , denoted by  $Q(G)$ , is the matrix  $D(G) + A(G)$ . The eigenvalues and the spectrum of  $Q(G)$  are known as the *signless Laplacian eigenvalues* and the *signless Laplacian spectrum* of  $G$ , respectively. Obviously,  $Q(G)$  is a real

symmetric matrix. Hence, its eigenvalues, denoted by  $q_i(G)$ ,  $i \in \{1, 2, \dots, n\}$ , are real and can be arranged as

$$q_1(G) \geq q_2(G) \geq \dots \geq q_n(G).$$

The characteristic polynomial of  $Q(G)$  is known as the *signless Laplacian characteristic polynomial* of  $G$ , that is  $\Phi_{Q(G)}(x) = \det(x\mathbf{I} - Q(G))$ . Thus  $q_i(G)$ ,  $i \in \{1, 2, \dots, n\}$ , are the roots of the equation  $\Phi_{Q(G)}(x) = 0$ .

Let  $\mathbf{x}$  be any vector in  $\mathbb{C}^n$ , then

$$\mathbf{x}^T Q(G) \mathbf{x} = \sum_{v_i v_j \in E(G)} (x_i + x_j)^2 \geq 0.$$

Therefore,  $Q(G)$  is positive semi-definite and  $q_i(G) \geq 0$  for all  $i \in \{1, 2, \dots, n\}$ . The *signless Laplacian spectral radius* of  $G$  is the largest eigenvalue  $q_1(G)$  of  $Q(G)$ .

Similarly to  $A(G)$  and  $L(G)$ , if  $G$  is a disconnected graph with connected components  $G_1, G_2, \dots, G_k$ , then  $Q(G)$  is a block diagonal matrix. Hence

$$Q(G) = Q(G_1) \oplus Q(G_2) \oplus \dots \oplus Q(G_k).$$

And the signless Laplacian spectrum of  $G$  is the union of the signless Laplacian spectrum of its components.

Matrix  $Q(G)$  is nonnegative and irreducible when  $G$  is connected. To see this, we need the definitions of the semi-edge and the semi-edge walk.

**Definition 1.3.** Suppose  $e = uv$  is an edge of a simple graph. A *semi-edge*, denoted by  $u^v u$ , is a ‘walk’ that starts from  $u$  toward  $v$  along  $e$  up to the midpoint of  $uv$  and then returns back to  $u$ .

Note that, for an edge  $uv$ , there are two semi-edges  $u^v u$  and  $v^u v$ .

**Definition 1.4** ([23]). A *semi-edge walk* of length  $k$  in a graph  $G$  is an alternating sequence  $v_1 e_1 v_2 e_2 \dots v_k e_k v_{k+1}$ , where  $v_1, v_2, \dots, v_k, v_{k+1}$  are vertices and  $e_1, e_2, \dots, e_k$  are edges or semi-edges such that for any  $i \in \{1, 2, \dots, k\}$  the vertices  $v_i$  and  $v_{i+1}$  are ends of  $e_i$ .

From Theorem 1.8, we know that the number of walks of length  $k$  from vertex  $v_i$  to vertex  $v_j$  is the  $(i, j)$ -entry of the matrix  $A^k(G)$ . We have a similar theorem for  $Q(G)$ .

**Theorem 1.9** ([23]). *Let  $Q(G)$  be the signless Laplacian matrix of a graph  $G$ . The  $(i, j)$ -entry of the matrix  $Q^k(G)$  is equal to the number of semi-edge walks of length  $k$  starting at vertex  $v_i$  and terminating at vertex  $v_j$ .*

Thus for a connected graph  $G$ , there always exists a semi-edge walk of some length  $k$  between any pair vertices of  $G$ . Thus, by Theorem 1.9, there is an integer  $k$  such that  $(Q^k(G))_{ij} > 0$  for all  $i$  and  $j$ , which means  $Q(G)$  is irreducible. Obviously, it is nonnegative. Therefore, by Perron-Frobenius theorem (Theorem 1.7), the multiplicity of  $q_1(G)$  is 1 and there is a positive eigenvector  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ , which is also called the *Perron vector* of  $Q(G)$ , with  $\sum_{i=1}^n x_i^2 = 1$  such that  $Q(G)\mathbf{x} = q_1(G)\mathbf{x}$ . Moreover,  $q_1(G)$  can be characterized by the Rayleigh quotient (Theorem 1.4),

$$q_1(G) = \max_{\|\mathbf{x}\|_2=1} \mathbf{x}^T Q(G) \mathbf{x}. \quad (1.5)$$

We can learn a lot of information about a graph through its signless Laplacian spectrum. Like the adjacency matrix  $A(G)$ , we can determine whether a graph  $G$  is regular or not from its signless Laplacian matrix  $Q(G)$ .

**Proposition 1.6** ([25]). *A graph  $G$  is regular if and only if its signless Laplacian matrix  $Q(G)$  has an eigenvector all of whose coordinates are equal to 1.*

**Proposition 1.7** ([24]). *For a connected graph  $G$ , we have  $2\delta(G) \leq q_1(G) \leq 2\Delta(G)$ , where equality holds in either place if and only if  $G$  is regular.*

Also, we can know whether a graph is bipartite from its signless Laplacian spectrum. Concerning the least eigenvalue of  $Q(G)$ , we have

**Proposition 1.8** ([23]). *The least eigenvalue of the signless Laplacian matrix of a connected graph is equal to 0 if and only if the graph is bipartite. In this case, 0 is a simple eigenvalue.*



A *bipartite component* of a graph is a connected component of the graph which is a bipartite subgraph.

**Proposition 1.9** ([23]). *In any graph, the multiplicity of the eigenvalue 0 of the signless Laplacian matrix is equal to the number of bipartite components.*

For these three matrices,  $A(G)$ ,  $L(G)$  and  $Q(G)$ , they have some similar properties. For example, regular graphs can be recognized by all of them respectively. The following proposition is another similar property.

**Proposition 1.10** ([8]). *Let  $G$  be a connected graph with diameter  $d(G)$ . Then  $G$  has at least  $d(G) + 1$  distinct eigenvalues, at least  $d(G) + 1$  distinct Laplacian eigenvalues, and at least  $d(G) + 1$  distinct signless Laplacian eigenvalues.*

And there are some relations between the eigenvalues of these three matrices.

**Proposition 1.11** ([75]). *Let  $G$  be a graph with eigenvalues  $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$  and signless Laplacian eigenvalues  $q_1(G) \geq q_2(G) \geq \dots \geq q_n(G)$ . Then for each  $i \in \{1, 2, \dots, n\}$ , we have*

$$q_i(G) \geq 2\lambda_i(G).$$

**Proposition 1.12** ([76]). *Let  $G$  be a simple graph with Laplacian spectral radius  $\mu_1(G)$  and signless Laplacian spectral radius  $q_1(G)$ . Then*

$$q_1(G) \geq \mu_1(G).$$

*If  $G$  is connected, then the equality holds if and only if  $G$  is bipartite.*

**Proposition 1.13** ([8]). *A graph  $G$  is bipartite if and only if the Laplacian spectrum and the signless Laplacian spectrum of  $G$  are equal.*

Since the spectrum (the Laplacian spectrum or the signless Laplacian spectrum) of a graph  $G$  is the union of the spectra (the Laplacian spectra or the signless Laplacian spectra) of its components, from now on, all considered graphs in this thesis are simple, finite, connected and undirected unless stated otherwise.

### 1.3 Research background

The eigenvalues of graphs have been studied along with the development of graph theory since the 1960s (for instance, [1, 4, 15, 18, 20, 38]). Usually, we use the matrix analysis and linear algebra to study the adjacency matrix of graphs. In all the eigenvalues of a graph  $G$ , researchers are most likely to study the property of its spectral radius  $\lambda_1(G)$ .

There are many questions about  $\lambda_1(G)$  and people have got some results on some problems. For example, if a graph  $G$  is not regular, then how close to the maximum degree can the spectral radius be (see [16, 17, 50, 63, 77]); and which graphs have the maximum spectral radius with a given sequence of vertex degrees (see [3, 5, 49]). In addition, if graphs have some particular structures, like trees, planar graphs (see [10, 34, 37, 43, 45, 62]) and complete multipartite graphs (see [30, 36, 51, 57, 67]), how about their spectral radii.

With the development of computer science, we can find more results about the eigenvalues of graphs. A computer program called AutoGraphiX has been used to find extremal graphs with respect to some properties of eigenvalues. Through the experiments with AutoGraphiX, some conjectures related to the spectral radius of a graph have been formulated (see [2, 11]). There are other programs or software that people are relying on to test their ideas and conjectures, such as Graffiti [35], GrInvIn [56], newGRAPH [66] and so on. Of course, not all of these conjectures have been proved. There are still a lot of work needed to be done on these problems.

Sometimes, it is more convenient to use the signless Laplacian spectrum of a graph to characterize the structures of graphs. For example, a connected graph is bipartite if and only if its least signless Laplacian eigenvalue is zero (see Proposition 1.8), while there is no similar result for the adjacency matrix.

Another example follows from papers [29] and [40]. They provide spectral uncertainties with respect to the adjacency matrix, the Laplacian matrix and the signless Laplacian matrix of sets of all graphs of order  $n$  with  $n \leq 11$ . From those results,

we are sure that studying graphs by the signless Laplacian spectrum is more efficient than by the adjacency spectrum. By an idea in [29], we deeply believe that the signless Laplacian matrix is likely to be the most convenient when studying graph properties among some matrices associated with a graph.

However, researchers did not study the signless Laplacian matrix as early as study the adjacency matrix. The paper [31] seems to be almost the only one paper published before 2003. During the recent decades, researchers began to pay attention to it. And many results about the signless Laplacian matrix have been published. D. Cvetković and S.K. Simić have built the signless Laplacian spectral theory of graphs (see [25–27]). We can find many results related to the signless Laplacian matrix from these three papers. Papers [22] and [23] provide some basic properties about the signless Laplacian matrix.

Again, using the AutoGraphiX system, some conjectures related to the signless Laplacian spectral radius have been obtained (see [41]). Some of them have been proved while some are still open. And D. Stevanović has collected some open problems that were presented at the Aveiro Workshop on Graph Spectra (see [64]).

## 1.4 Outline of the thesis

The graph spectral theory has many applications and is used as another way to study the structure properties of graphs, which is a strong basis for our work on graph spectral theory. In this thesis, we mainly focus on the adjacency matrix and the signless Laplacian matrix of  $k$ -connected graphs. The structure of this thesis is as follows.

In Chapter 1, we mainly introduce some basic notation and terminologies of graphs and some useful theorems related to matrices. Then we give some information about three kinds of matrices associated with a graph as well as the research background.

In Chapter 2, we first give some definitions about a diameter critical graph and

study its properties. P. Hansen and D. Stevanović have determined the graphs with maximum spectral radius among all connected graphs of given order and diameter. We then generalize this result to  $k$ -connected graphs of given order and diameter. The main results are my work that have been published in *Linear Algebra and its Applications* (see [46]) during my studies.

In Chapter 3, we focus on the signless Laplacian spectral radius of a  $k$ -connected irregular graph. Since for any regular graph, the signless Laplacian spectral radius is two times of the maximum vertex degree. We study how close these two variables can be when a graph is not regular. The main results have been published in *Linear and Multilinear Algebra* (see [47]) during my studies.

In Chapter 4, we provide some other results for the signless Laplacian matrix when  $k = 1$ . Firstly, we obtain a relation between the numbers of walks and semi-edge walks. Using this relation, we give upper bounds on the signless Laplacian spectral radius of connected graphs and planar graphs. In addition, we obtain a combinatorial expression for the fifth coefficient of the Laplacian and the signless Laplacian characteristic polynomials of a graph.

In Chapter 5, we summarise this thesis and give some suggested future work.

# Chapter 2

## The spectral radius of $k$ -connected graphs with given diameter

In this chapter, we focus on investigating the spectral radii of  $k$ -connected graphs. Brualdi and Solheid [9] proposed the following problem concerning the spectral radius of graphs: Given a set  $\mathcal{G}$  of graphs, find an upper bound for the spectral radius of graphs in  $\mathcal{G}$  and characterize the graphs for which the maximal spectral radius is attained. For many different sets  $\mathcal{G}$ , this problem has been solved (see [6, 9, 20, 21]).

Let  $\mathcal{G}_n^d$  be the set of connected graphs of order  $n$  with diameter  $d$ . P. Hansen and D. Stevanović [42] and E.R. van Dam [28] solved the problem on  $\mathcal{G}_n^d$  using two different methods. The graph obtained from a complete graph  $K_p$  by deleting an edge  $uv$  and attaching paths  $P_{q_1}$  and  $P_{q_2}$  at  $u$  and  $v$  respectively is called a *bug*  $Bug_{p,q_1,q_2}$ . A bug is *balanced* if  $|q_1 - q_2| \leq 1$ . The following is their main result.

**Theorem 2.1** ([42]). *Among all connected graphs of order  $n$  with diameter  $d$ , the maximal spectral radius is attained by*

$$\begin{cases} a \text{ complete graph } K_n, & \text{when } d = 1, \\ a \text{ balanced bug } Bug_{n-d+2, \lfloor d/2 \rfloor, \lfloor d/2 \rfloor}, & \text{when } d \geq 2. \end{cases}$$

In this chapter, we generalize the result of Theorem 2.1 to  $k$ -connected graphs

since there are many graphs with high connectivity. Let  $\mathcal{G}_{n,k}^d$  be the set of all  $k$ -connected graphs of order  $n$  with diameter  $d$ . We solve the problem of [9] on the set  $\mathcal{G}_{n,k}^d$ . This chapter is from an article published in Linear Algebra and its Applications on January 1, 2016.

## 2.1 Preliminaries

The diameter  $d(G)$  of a graph  $G$  may decrease (or remain unchanged) when a new edge  $e$  is added to it. We say that  $G$  is *diameter critical* when the addition of any edge decreases the diameter. In this section, we will introduce the structure of a diameter critical graph which is obtained by O. Ore [55].

We denote a complete graph with vertex set  $U$  by  $K(U)$ . Let  $k$  be a positive integer. A graph

$$G = \bigcup_{i=0}^{k-1} K(U_i), \quad V(G) = \bigcup_{i=0}^{k-1} U_i \quad (2.1)$$

which is the union of complete graphs, is called a *simplex chain* if

$$\begin{cases} U_i \cap U_j = \emptyset, & \text{when } i \text{ and } j \text{ are not consecutive,} \\ U_i \cap U_j \neq \emptyset, & \text{when } i \text{ and } j \text{ are consecutive.} \end{cases}$$

Such a simplex chain is *tight* if each vertex in  $U_i$  belongs to either  $U_{i-1}$  or  $U_{i+1}$ .

Let

$$V_i = U_{i-1} \cap U_i, \quad i \in \{1, 2, \dots, k-1\}. \quad (2.2)$$

And we define the end sets by

$$V_0 = U_0 - U_0 \cap U_1, \quad V_k = U_{k-1} - U_{k-1} \cap U_{k-2}. \quad (2.3)$$

In some articles or books (for example, [59, 61]), a tight simplex chain is called a sequential join of some graphs.

The *sequential join*  $G_1 \vee \cdots \vee G_k$  of graphs  $G_1, \dots, G_k$  is the graph formed by taking one copy of each graph and adding additional edges from each vertex of  $G_i$  to all vertices of  $G_{i+1}$ , for  $i \in \{1, 2, \dots, k\}$ .

We can now introduce the result about diameter critical graphs.

**Lemma 2.1** ([55]). *A graph  $G$  with diameter  $d$  is diameter critical if and only if  $G$  is isomorphic to  $K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$ .*

This lemma can be extended to a  $k$ -connected graph as follows.

**Lemma 2.2** ([55]). *A  $k$ -connected graph with diameter  $d$  is diameter critical if and only if it is isomorphic to  $K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$  with  $n_i \geq k$ ,  $i \in \{1, 2, \dots, d-1\}$ .*

Fig. 2.1 illustrates an example of a 4-connected graph with diameter 5 that is diameter critical. In the later figures, we omit some edges for convenience.

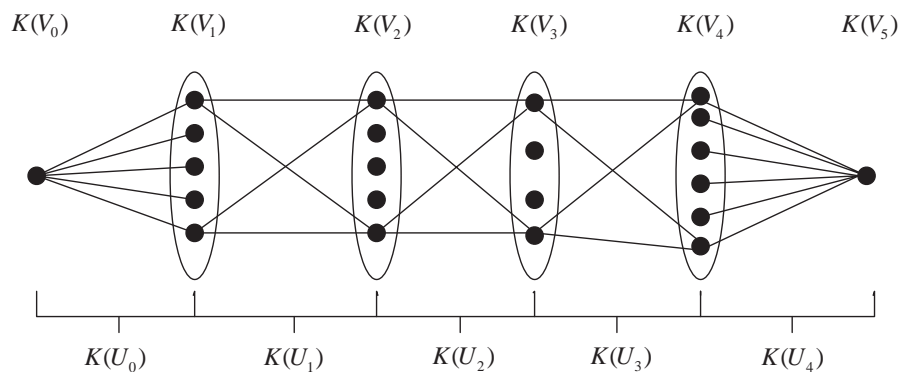


Figure 2.1: A diameter critical graph  $K_1 \vee K_5 \vee K_5 \vee K_4 \vee K_6 \vee K_1$ .

## 2.2 Graphs with maximum spectral radius

Let  $G^*$  be the graph which has the maximal spectral radius in  $\mathcal{G}_{n,k}^d$ . We call such a graph the *maximal graph* in  $\mathcal{G}_{n,k}^d$ . For  $k = 1$ , the problem has been solved by P. Hansen and D. Stevanović [42] (or E.R. van Dam [28]). If  $d = 1$ , then  $G^*$  must be the complete graph  $K_n$  since  $K_n$  is the only graph with diameter 1. Thus we may

suppose  $k \geq 2$  and  $d \geq 2$ . The following lemma is a well-known result about the spectral radius.

**Lemma 2.3** ([24]). *If  $G - uv$  is the graph obtained from a connected graph  $G$  by deleting the edge  $uv$ , then  $\lambda_1(G - uv) < \lambda_1(G)$ .*

By this lemma, we know that  $G^*$  must be a diameter critical graph since we can increase the spectral radius by adding edges. Thus  $G^*$  has the structure presented by Lemma 2.2. Let  $V_0, V_1, \dots, V_d$  be defined as in Section 2.1 and  $|V_i| = n_i$ . By Lemma 2.2 we have  $n_0 = n_d = 1$  and  $n_i \geq k$  for  $i \in \{1, 2, \dots, d-1\}$ . Suppose  $\mathbf{x}(G^*)$  is the Perron vector corresponding to  $\lambda_1(G^*)$ . If vertices  $u$  and  $v$  belong to the same  $V_i$ ,  $i \in \{1, 2, \dots, d-1\}$ , then the components of  $\mathbf{x}(G^*)$  corresponding to  $u$  and  $v$  are equal. Therefore we can denote  $x_i$  the components of  $\mathbf{x}(G^*)$  corresponding to the vertices in  $V_i$ ,  $i \in \{0, 1, \dots, d\}$ . Now we can prove the following lemma.

**Lemma 2.4** ([46]). *Let  $G^* = K_1 \vee K_{n_1} \vee \dots \vee K_{n_{d-1}} \vee K_1$  be the maximal graph of  $\mathcal{G}_{n,k}^d$ , where  $n_i \geq k$  for  $i \in \{1, 2, \dots, d-1\}$ . Suppose  $n_j \geq k+1$  for some  $j \in \{1, 2, \dots, d-1\}$ . Then  $x_j > x_i$  for all  $i \in \{1, 2, \dots, d-1\} \setminus \{j\}$ .*

*Proof.* When  $d = 2$ , the statement is logically true. Hence we assume that  $d \geq 3$ . Suppose there is an  $i \in \{1, 2, \dots, d-1\} \setminus \{j\}$  such that  $x_i \geq x_j$ . By symmetry, we may assume that  $i < j$ .

**Case 1:**  $j - i = 1$ . We consider the graph  $G'$  obtained from  $G^*$  by moving one vertex, say  $v$ , from  $V_j$  to  $V_i$ , and deleting the edges between  $v$  and all vertices in  $V_{j+1}$  as well as adding the edges between  $v$  and all vertices in  $V_{i-1}$ . Obviously, the new graph  $G' \in \mathcal{G}_{n,k}^d$  and  $G' \neq G^*$ . Fig. 2.2 shows the process of constructing  $G'$  in which the unchanged edges are omitted. The dash lines represent the edges that are deleted from  $G^*$  and the solid lines stand for the edges that are added to  $G^*$ . We use these two kinds of lines in the remaining figures.



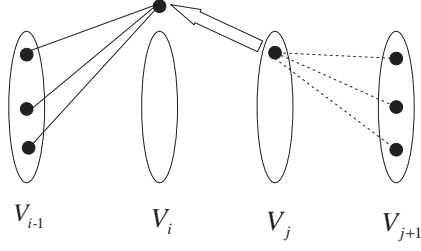


Figure 2.2: From  $G^*$  to  $G'$ .

Let  $\mathbf{x}(G')$  be the Perron vector of  $G'$  corresponding to  $\lambda_1(G')$ . By (1.3) and (1.4) we have

$$\begin{aligned}
\lambda_1(G') - \lambda_1(G^*) &= \mathbf{x}^T(G')A(G')\mathbf{x}(G') - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&\geq \mathbf{x}^T(G^*)A(G')\mathbf{x}(G^*) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&= 2n_{i-1}x_jx_{i-1} - 2n_{j+1}x_jx_{j+1} \\
&= 2x_j(n_{i-1}x_{i-1} - n_{j+1}x_{j+1}). \tag{2.4}
\end{aligned}$$

On the other hand, consider one vertex from  $V_i$  and  $V_j$  respectively. By the eigenvalue equation, we obtain

$$\lambda_1(G^*)x_i = n_{i-1}x_{i-1} + (n_i - 1)x_i + n_jx_j$$

and

$$\lambda_1(G^*)x_j = n_ix_i + (n_j - 1)x_j + n_{j+1}x_{j+1}.$$

Substituting these two equations into (2.4), we have

$$\lambda_1(G') - \lambda_1(G^*) \geq 2x_j(\lambda_1(G^*) + 1)(x_i - x_j) \geq 0$$

as  $x_i \geq x_j$ .

Next we prove that the equality does not hold. Otherwise,  $x_i = x_j$  and  $\mathbf{x}(G^*)$  is an eigenvector of  $G'$  corresponding to  $\lambda_1(G')$ . Set  $n_{-1} = x_{-1} = 0$ . Consider one vertex of  $V_{i-1}$ . In  $G^*$  we have

$$\lambda_1(G^*)x_{i-1} = n_{i-2}x_{i-2} + (n_{i-1} - 1)x_{i-1} + n_ix_i.$$

And in  $G'$  we have

$$\lambda_1(G')x_{i-1} = n_{i-2}x_{i-2} + (n_{i-1} - 1)x_{i-1} + n_ix_i + x_j.$$

Since  $\lambda_1(G^*) = \lambda_1(G')$ , we obtain  $x_j = 0$  which is impossible as  $\mathbf{x}(G^*)$  is a positive eigenvector. Consequently,  $\lambda_1(G') > \lambda_1(G^*)$  which means we construct a new graph  $G''$  whose spectral radius is larger than that of  $G^*$ . This contradicts that  $G^*$  is the maximal graph in  $\mathcal{G}_{n,k}^d$ .

**Case 2:**  $j - i \geq 2$ . We construct a new graph  $G''$  from  $G^*$  by moving a vertex, say  $u$ , from  $V_j$  to  $V_i$ , and deleting the edges between  $u$  and all the remaining vertices in  $V_{j-1} \cup V_j \cup V_{j+1}$  as well as adding the edges between  $u$  and all vertices in  $V_{i-1} \cup V_i \cup V_{i+1}$ . It is obvious that  $G'' \in \mathcal{G}_{n,k}^d$  and  $G'' \neq G^*$ . Fig. 2.3 shows the new graph  $G''$ .

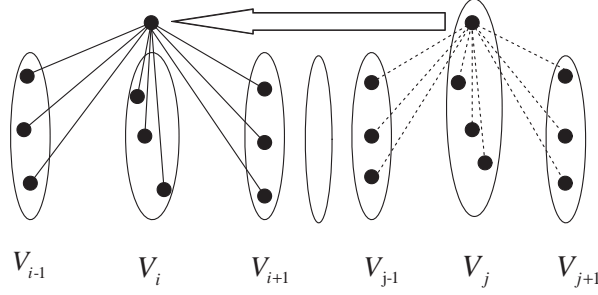


Figure 2.3: From  $G^*$  to  $G''$ .

Let  $\mathbf{x}(G'')$  be the Perron vector of  $G''$  corresponding to  $\lambda_1(G'')$ . Again by (1.3) and (1.4) we obtain

$$\begin{aligned} \lambda_1(G'') - \lambda_1(G^*) &= \mathbf{x}^T(G'')A(G'')\mathbf{x}(G'') - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\ &\geq \mathbf{x}^T(G^*)A(G'')\mathbf{x}(G^*) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\ &= 2n_{i-1}x_jx_{i-1} + 2n_ix_jx_i + 2n_{i+1}x_jx_{i+1} \\ &\quad - 2n_{j-1}x_jx_{j-1} - 2(n_j - 1)x_j^2 - 2n_{j+1}x_jx_{j+1} \\ &= 2x_j(n_{i-1}x_{i-1} + n_ix_i + n_{i+1}x_{i+1} - n_{j-1}x_{j-1} \\ &\quad - (n_j - 1)x_j - n_{j+1}x_{j+1}). \end{aligned}$$

In addition, consider one vertex from each of  $V_i$  and  $V_j$  respectively in  $G^*$ . We have the following two eigenvalue equations

$$\lambda_1(G^*)x_i = n_{i-1}x_{i-1} + (n_i - 1)x_i + n_{i+1}x_{i+1},$$

and

$$\lambda_1(G^*)x_j = n_{j-1}x_{j-1} + (n_j - 1)x_j + n_{j+1}x_{j+1}.$$

Combining these two equations, we obtain that

$$\lambda_1(G'') - \lambda_1(G^*) \geq 2x_j(x_i + \lambda_1(G^*)(x_i - x_j)) \geq 2x_i x_j > 0$$

since  $x_i \geq x_j > 0$ .

As a consequence, we find a new graph  $G''$  that has larger spectral radius than  $G^*$ , which is a contradiction.

Note that  $i - 1$  may be 0 and  $j + 1$  may be  $d$  in both cases. Also,  $i + 1$  may be  $j - 1$  in Case 2 and all these situations will not influence the previous discussion. This completes the proof.  $\square$

**Corollary 2.1** ([46]). *Let  $G^* = K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$  be the maximal graph of  $\mathcal{G}_{n,k}^d$ , where  $n_i \geq k$  for  $i \in \{1, 2, \dots, d-1\}$ . Then there exists at most one  $j$ ,  $j \in \{1, 2, \dots, d-1\}$ , such that  $n_j \geq k+1$ .*

*Proof.* This follows from Lemma 2.4 immediately.  $\square$

If there is no integer  $j$  such that  $n_j \geq k+1$ , then  $n_j = k$  for all  $j \in \{1, 2, \dots, d-1\}$  and the maximal graph  $G^*$  was determined. Hence by Corollary 2.1 we may assume that there exists exactly one  $s+1 \in \{1, 2, \dots, d-1\}$  such that  $n_{s+1} \geq k+1$ . When  $d = 2$  or  $3$ , the maximal graph  $G^*$  is fixed. Therefore we may assume that  $d \geq 4$ . Next, determine the value of  $s+1$  and then we have the structure of  $G^*$ . For convenience, we reassign the notation of vertex sets as showed in Fig. 2.4 in which  $V_0, V_1, \dots, V_d$  are the original notation and suppose  $|P_{s+1}| \geq k+1$ . Also we keep and

denote  $x_i$  and  $y_j$  as the components of  $\mathbf{x}(G^*)$  corresponding to the vertices in  $P_i$  and  $Q_j$ , with  $i \in \{1, 2, \dots, s+1\}$  and  $j \in \{1, 2, \dots, t\}$ , respectively.

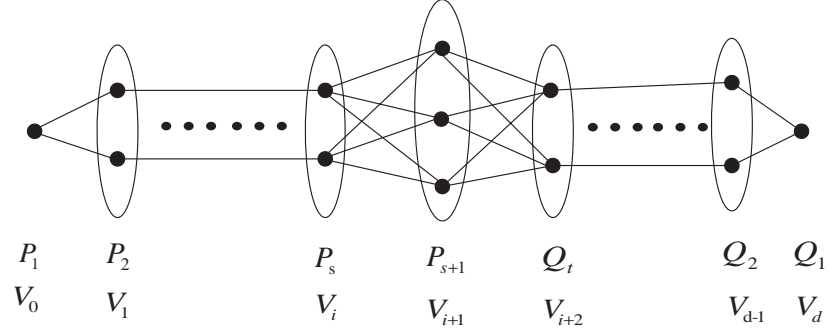


Figure 2.4:  $G^*$ .

Let  $|P_i| = p_i$ ,  $i \in \{1, 2, \dots, s+1\}$ , and  $|Q_j| = q_j$ ,  $j \in \{1, 2, \dots, t\}$ , where  $s+t = d$ .

So

$$G^* = K_{p_1} \vee K_{p_2} \vee \dots \vee K_{p_s} \vee K_{p_{s+1}} \vee K_{q_t} \vee \dots \vee K_{q_2} \vee K_{q_1}.$$

By Corollary 2.1, we know that  $p_1 = q_1 = 1$ ,  $p_{s+1} \geq k+1$  and  $p_2 = \dots = p_s = q_t = \dots = q_2 = k$ . We can prove the following result by a method similar to that in [71].

**Lemma 2.5** ([46]). *Let  $G^* = K_{p_1} \vee K_{p_2} \vee \dots \vee K_{p_s} \vee K_{p_{s+1}} \vee K_{q_t} \vee \dots \vee K_{q_2} \vee K_{q_1}$  with  $p_1 = q_1 = 1$ ,  $p_{s+1} \geq k+1$  and  $p_2 = \dots = p_s = q_t = \dots = q_2 = k$ , which is the maximal graph of  $\mathcal{G}_{n,k}^d$ . Let  $x_1, \dots, x_{s+1}, y_t, \dots, y_1$  be the components of Perron vector  $\mathbf{x}(G^*)$  corresponding to vertex sets of  $K_{p_1}, \dots, K_{p_{s+1}}, K_{q_t}, \dots, K_{q_1}$ . If  $t \geq s+1$ , then*

(a)  $x_i > y_i$ , for all  $i \in \{1, 2, \dots, s+1\}$ ,

(b)  $q_2 y_2 > x_1$ .

*Proof.* Let  $\lambda = \lambda_1(G^*)$ . By the eigenvalue equation, we have

$$\left\{ \begin{array}{l} \frac{p_2x_2}{p_1x_1} = \lambda \\ \frac{p_3x_3}{p_2x_2} = \frac{\lambda - p_2 + 1}{p_2} - \frac{p_1x_1}{p_2x_2} \\ \vdots \\ \frac{p_sx_s}{p_{s-1}x_{s-1}} = \frac{\lambda - p_{s-1} + 1}{p_{s-1}} - \frac{p_{s-2}x_{s-2}}{p_{s-1}x_{s-1}} \\ \frac{p_{s+1}x_{s+1}}{p_sx_s} = \frac{\lambda - p_s + 1}{p_s} - \frac{p_{s-1}x_{s-1}}{p_sx_s}, \end{array} \right. \left\{ \begin{array}{l} \frac{q_2y_2}{q_1y_1} = \lambda \\ \frac{q_3y_3}{q_2y_2} = \frac{\lambda - q_2 + 1}{q_2} - \frac{q_1y_1}{q_2y_2} \\ \vdots \\ \frac{q_t y_t}{q_{t-1}y_{t-1}} = \frac{\lambda - q_{t-1} + 1}{q_{t-1}} - \frac{q_{t-2}y_{t-2}}{q_{t-1}y_{t-1}} \\ \frac{p_{s+1}x_{s+1}}{q_t y_t} = \frac{\lambda - q_t + 1}{q_t} - \frac{q_{t-1}y_{t-1}}{q_t y_t}. \end{array} \right. \quad (2.5)$$

Note that when  $s = 1$ , only the first equation at the left hand side occurs.

When  $s = 1$ , we have  $kx_2 = \lambda x_1$  and  $ky_2 = \lambda y_1$ . From Lemma 2.4 we have  $x_2 > y_2$ , hence  $x_1 > y_1$ .

Now we assume  $s \geq 2$ . By mathematical induction, we obtain

$$\frac{p_{i+1}x_{i+1}}{p_i x_i} = \frac{q_{i+1}y_{i+1}}{q_i y_i}, \quad i \in \{1, 2, \dots, s\}.$$

Therefore,

$$\frac{p_{s+1}x_{s+1}}{p_i x_i} = \frac{q_{s+1}y_{s+1}}{q_i y_i}, \quad i \in \{1, 2, \dots, s\}. \quad (2.6)$$

From Lemma 2.4,  $x_{s+1} > x_i$  and  $x_{s+1} > y_j$  for  $i \in \{2, \dots, s\}$  and  $j \in \{2, \dots, t\}$ . In particular,  $x_{s+1} > y_{s+1}$ . From  $p_{s+1} \geq k + 1 > q_{s+1}$  and (2.6), we obtain  $x_i > y_i$  for  $i \in \{1, 2, \dots, s\}$ . Hence we obtain part (a) of the lemma.

Now we are going to prove part (b). When  $s = 1$  and  $t = s + 1$ , from (2.5) we have  $p_2x_2 = \lambda x_1$ ,  $q_2y_2 = \lambda y_1$  and  $p_2x_2 = (\lambda - q_2 + 1)y_2 - y_1$ . Combining these three identities, we have  $x_1 = \left(\frac{\lambda^2 + \lambda - \lambda k - k}{\lambda^2 k}\right)ky_2 = \left(\frac{\lambda^2 + \lambda - \lambda k - k}{\lambda^2 k}\right)q_2y_2$ . Clearly  $\lambda^2 k + \lambda k - \lambda^2 - \lambda + k > 0$  for  $k \geq 2$ . Hence  $q_2y_2 > x_1$ .

So we assume  $s \geq 2$  or  $t \geq s + 2 \geq 3$ . Suppose  $q_2y_2 \leq x_1$ . There are two cases that we need to consider as follows.

**Case 1:**  $p_2x_2 \geq q_3y_3$ . We construct  $G_1$  from  $G^*$  by the following steps. Firstly, we choose one vertex, say  $u$ , from  $Q_2$ . Then we delete all the edges between  $Q_3$  and

$Q_2 - u$  (this vertex set is not empty since  $k \geq 2$ ), the edges between  $u$  and  $Q_2 - u$  and the edge between  $u$  and  $Q_1$ . Finally, we add all the possible edges between  $P_2$  and  $Q_2 - u$ , the edges between  $P_1$  and  $Q_2 - u$  and the edge between  $P_1$  and  $Q_1$ . Obviously,  $G_1 \in \mathcal{G}_{n,k}^d$  and  $G_1 \neq G^*$ . Fig. 2.5 shows the process.

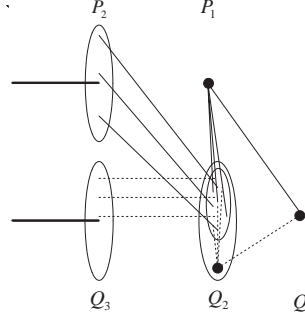


Figure 2.5: From  $G^*$  to  $G_1$

Let  $\mathbf{x}(G_1)$  be the Perron vector of  $G_1$  corresponding to  $\lambda_1(G_1)$ . Now from (1.3) and (1.4), we obtain

$$\begin{aligned}
\lambda_1(G_1) - \lambda_1(G^*) &= \mathbf{x}^T(G_1)A(G_1)\mathbf{x}(G_1) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&\geq \mathbf{x}^T(G^*)A(G_1)\mathbf{x}(G^*) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&= 2(p_2(q_2 - 1)x_2y_2 + (q_2 - 1)x_1y_2 + x_1y_1 \\
&\quad - q_3(q_2 - 1)y_3y_2 - (q_2 - 1)y_2^2 - y_1y_2) \\
&= 2((q_2 - 1)y_2(p_2x_2 - q_3y_3) + (q_2 - 1)y_2(x_1 - y_2) + y_1(x_1 - y_2)).
\end{aligned}$$

Note that  $p_2x_2 \geq q_3y_3$ ,  $x_1 \geq q_2y_2 > y_2$  and  $q_2 - 1 > 0$  as  $k \geq 2$ . We have  $\lambda_1(G_1) > \lambda_1(G^*)$ , which is a contradiction.

**Case 2:**  $p_2x_2 < q_3y_3$ . We construct  $G_2$  by deleting all the edges between  $P_1$  and  $P_2$  and the edges between  $Q_2$  and  $Q_3$  from  $G^*$ , then adding all the edges between  $P_2$  and  $Q_2$  and the edges between  $P_1$  and  $Q_3$ . It is evident that  $G_2 \in \mathcal{G}_{n,k}^d$  and  $G_2 \neq G^*$ . Fig. 2.6 shows the process.

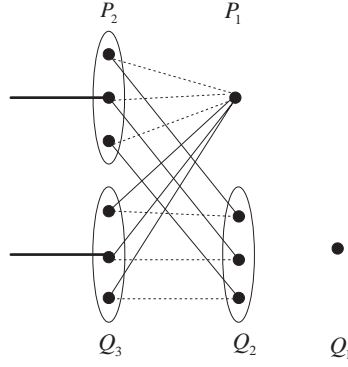


Figure 2.6: From  $G^*$  to  $G_2$

Let  $\mathbf{x}(G_2)$  be the Perron vector of  $G_2$  corresponding to  $\lambda_1(G_2)$ . Again, by (1.3) and (1.4), we have

$$\begin{aligned}
\lambda_1(G_2) - \lambda_1(G^*) &= \mathbf{x}^T(G_2)A(G_2)\mathbf{x}(G_2) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&\geq \mathbf{x}^T(G^*)A(G_2)\mathbf{x}(G^*) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&= 2(p_2q_2x_2y_2 + q_3x_1y_3 - q_2q_3y_2y_3 - p_2x_1x_2) \\
&= 2(q_2y_2(p_2x_2 - q_3y_3) + x_1(q_3y_3 - p_2x_2)) \\
&= 2(q_3y_3 - p_2x_2)(x_1 - q_2y_2) \geq 0
\end{aligned}$$

as  $q_3y_3 > p_2x_2$  and  $x_1 \geq q_2y_2$ .

If the equality holds, then  $\lambda_1(G_2) = \lambda_1(G^*)$  and  $\mathbf{x}(G^*)$  is also an eigenvector of  $G_2$  corresponding to  $\lambda_1(G_2)$ . We consider the vertex in  $P_1$ . In  $G^*$ , we have  $\lambda_1(G^*)x_1 = p_2x_2$ . And in  $G_2$ , we have  $\lambda_1(G_2)x_1 = q_3y_3$ . Since  $\lambda_1(G_2) = \lambda_1(G^*)$ ,  $p_2x_2 = q_3y_3$ , which contradicts our assumption. Thus  $\lambda_1(G_2) > \lambda_1(G^*)$ , which is impossible.

Consequently, we obtain  $q_2y_2 > x_1$ . □

**Lemma 2.6** ([46]). *Keeping the assumptions and notation in Lemma 2.5, we have*

$$p_{s+1}x_{s+1} > q_{s+1}y_{s+1} > p_sx_s > q_sy_s > \cdots > p_2x_2 > q_2y_2 > p_1x_1 > q_1y_1. \quad (2.7)$$

*Proof.* By Lemma 2.5, it suffices to show that  $q_{i+1}y_{i+1} > p_ix_i$  for all  $i \in \{1, \dots, s\}$ .

We prove this result by mathematical induction.

When  $i = 1$ , the statement is true from Lemma 2.5. Suppose the statement is true for  $i = l \geq 1$ . That is,  $q_{l+1}y_{l+1} > p_l x_l$ .

Suppose  $q_{l+2}y_{l+2} \leq p_{l+1}x_{l+1}$ . We construct  $G_3$  by deleting all the edges between  $P_l$  and  $P_{l+1}$  and the edges between  $Q_{l+1}$  and  $Q_{l+2}$  from  $G^*$ , then adding all the edges between  $P_{l+1}$  and  $Q_{l+1}$  and the edges between  $P_l$  and  $Q_{l+2}$ . Note that  $G_3 \in \mathcal{G}_{n,k}^d$  and  $G_3 \neq G^*$ . Fig. 2.7 shows the process.

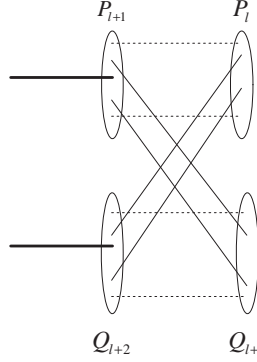


Figure 2.7: From  $G^*$  to  $G_3$

Let  $\mathbf{x}(G_3)$  be the Perron vector of  $G_3$  corresponding to  $\lambda_1(G_3)$ . As a consequence, we obtain

$$\begin{aligned}
\lambda_1(G_3) - \lambda_1(G^*) &= \mathbf{x}^T(G_3)A(G_3)\mathbf{x}(G_3) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&\geq \mathbf{x}^T(G^*)A(G_3)\mathbf{x}(G^*) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&= 2(p_{l+1}q_{l+1}x_{l+1}y_{l+1} + p_l q_{l+2}x_l y_{l+2} \\
&\quad - p_l p_{l+1}x_l x_{l+1} - q_{l+1}q_{l+2}y_{l+1}y_{l+2}) \\
&= 2(p_{l+1}x_{l+1} - q_{l+2}y_{l+2})(q_{l+1}y_{l+1} - p_l x_l) \geq 0
\end{aligned}$$

since  $q_{l+1}y_{l+1} > p_l x_l$  and  $q_{l+2}y_{l+2} \leq p_{l+1}x_{l+1}$ .

If  $\lambda_1(G_3) = \lambda_1(G^*)$ , then  $\mathbf{x}(G^*)$  is an eigenvector of  $G_3$  corresponding to  $\lambda_1(G_3)$ . Take one vertex of  $P_{l+1}$  into consideration. In  $G^*$ , we have

$$\lambda_1(G^*)x_{l+1} = p_l x_l + (p_{l+1} - 1)x_{l+1} + p_{l+2}x_{l+2} \text{ (or } q_l y_l).$$



And in  $G_3$ , we have

$$\lambda_1(G_3)x_{l+1} = q_{l+1}y_{l+1} + (p_{l+1} - 1)x_{l+1} + p_{l+2}x_{l+2} \text{ (or } q_ly_t).$$

Since  $\lambda_1(G_3) = \lambda_1(G^*)$ ,  $q_{l+1}y_{l+1} = p_lx_l$ . This contradicts  $q_{l+1}y_{l+1} > p_lx_l$ . Thus  $\lambda_1(G_3) > \lambda_1(G^*)$ , which is impossible. Therefore  $q_{l+2}y_{l+2} > p_{l+1}x_{l+1}$ . Consequently, we obtain the lemma.  $\square$

With the discussion above, we now present our main result.

**Theorem 2.2** ([46]). *Let  $\mathcal{G}_{n,k}^d$  be the set of  $k$ -connected graphs of order  $n$  with diameter  $d$ , where  $k \geq 2$  and  $d \geq 2$ . Then the maximal graph  $G^*$  of  $\mathcal{G}_{n,k}^d$  is isomorphic to  $K_1 \vee K_{n_1} \vee \cdots \vee K_{n_{d-1}} \vee K_1$  with  $n_i = k$  for  $i \in \{1, 2, \dots, d-1\} \setminus \{\lfloor d/2 \rfloor\}$  and  $n_{\lfloor d/2 \rfloor} \geq k$ .*

*Proof.* From Corollary 2.1, it is sufficient to prove that “if  $n_i \geq k+1$ , then  $i = \lfloor d/2 \rfloor$ ”.

When  $d = 2$  or  $3$ , there is nothing to prove. Hence we assume that  $d \geq 4$ .

We use the notation defined in Lemma 2.6. Thus  $i = \lfloor d/2 \rfloor$  if and only if  $|s-t| \leq 1$ , which means we need to prove  $|s-t| \leq 1$ .

Without loss of generality, we may assume  $t \geq s$ . Suppose  $t \geq s+2$  (this holds since  $d \geq 4$ ). In  $G^*$ , we have  $q_{s+1}y_{s+1} > p_sx_s$  by Lemma 2.6. In addition, from Lemma 2.4,  $p_{s+1}x_{s+1} > q_{s+2}y_{s+2}$  as  $p_{s+1} \geq k+1 > q_{s+2}$ . We construct  $G_4$  from  $G^*$  by deleting all the edges between  $P_{s+1}$  and  $P_s$  and the edges between  $Q_{s+2}$  and  $Q_{s+1}$ , then adding all the edges between  $P_{s+1}$  and  $Q_{s+1}$  and the edges between  $P_s$  and  $Q_{s+2}$ . Again,  $G_4 \in \mathcal{G}_{n,k}^d$  and  $G_4 \neq G^*$ . Fig. 2.8 shows the process.

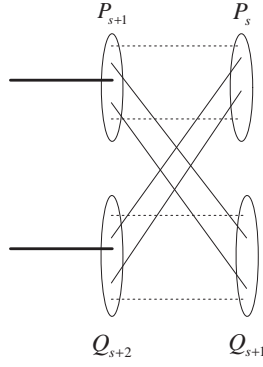


Figure 2.8: From  $G^*$  to  $G_4$

Let  $\mathbf{x}(G_4)$  be the Perron vector of  $G_4$  corresponding to  $\lambda_1(G_4)$ , as a result,

$$\begin{aligned}
\lambda_1(G_4) - \lambda_1(G^*) &= \mathbf{x}^T(G_4)A(G_4)\mathbf{x}(G_4) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&\geq \mathbf{x}^T(G^*)A(G_4)\mathbf{x}(G^*) - \mathbf{x}^T(G^*)A(G^*)\mathbf{x}(G^*) \\
&= 2(p_{s+1}q_{s+1}x_{s+1}y_{s+1} + p_sq_{s+2}x_sy_{s+2} \\
&\quad - p_sp_{s+1}x_sx_{s+1} - q_{s+1}q_{s+2}y_{s+1}y_{s+2}) \\
&= 2(p_{s+1}x_{s+1} - q_{s+2}y_{s+2})(q_{s+1}y_{s+1} - p_sx_s) > 0
\end{aligned}$$

since  $q_{s+1}y_{s+1} > p_sx_s$  and  $p_{s+1}x_{s+1} > q_{s+2}y_{s+2}$ .

Hence  $\lambda_1(G_4) > \lambda_1(G^*)$  which is impossible as  $G^*$  is the maximal graph in  $\mathcal{G}_{n,k}^d$ . Therefore  $t - s \leq 1$  and so  $i = \lfloor \frac{d}{2} \rfloor$ . This completes the proof.  $\square$

## 2.3 Concluding remarks

When  $d \geq 2$ , and  $k$  and  $n$  are fixed,  $\lambda_1(G^*)$  is a decreasing function of the diameter  $d$ .

Indeed, let  $G_{d_1}^*$  and  $G_{d_2}^*$  be the maximal graphs in  $\mathcal{G}_{n,k}^{d_1}$  and  $\mathcal{G}_{n,k}^{d_2}$ , respectively. Suppose  $d_2 = d_1 + 1 \geq 3$ . Then according to Theorem 2.2, we can obtain  $G_{d_1}^*$  from  $G_{d_2}^*$  by moving all the vertices in some vertex set  $V_{i_0}$ ,  $i_0 \in \{1, 2, \dots, d_2 - 1\} \setminus \{\lfloor d_2/2 \rfloor\}$ , to  $V_{\lfloor d_2/2 \rfloor}$  and changing some edges accordingly.

From Lemma 2.4, we know that  $x_{\lfloor d_2/2 \rfloor} > x_{i_0}$  in  $G_{d_2}^*$ . Thus with a similar discussion in Lemma 2.4, we can obtain  $\lambda_1(G_{d_1}^*) > \lambda_1(G_{d_2}^*)$  while  $d_2 > d_1$ .

# Chapter 3

## The signless Laplacian spectral radii of $k$ -connected graphs

In this chapter, we mainly study the signless Laplacian spectral radii of  $k$ -connected graphs. We give an upper bound on the signless Laplacian spectral radii for the irregular graphs. And similarly, we give an upper bound on the Laplacian spectral radii for the irregular graphs which is better than some known results on the Laplacian spectral radius. This chapter is an accepted manuscript of an article published by Taylor & Francis in Linear and Multilinear Algebra on July 18, 2016, available on line: <http://dx.doi.org/10.1080/03081087.2016.1209731>.

### 3.1 Some known results

Given a connected graph  $G$  of order  $n$  and size  $m$ , it is known that  $q_1(G) \leq 2\Delta$  and the equality holds if and only if  $G$  is a regular graph. We want to determine the gap between  $2\Delta$  and  $q_1(G)$  if  $G$  is irregular. In 2012, Ning (see [53]) proved that

$$2\Delta - q_1(G) > \frac{1}{n(d - \frac{1}{4})}. \quad (3.1)$$

There are several results involving  $\Delta - \lambda_1(G)$  (see [16, 17, 50, 60, 63, 77]). Recently, Chen and Hou considered the  $k$ -connected irregular graphs and gave a new lower

bound on  $\Delta - \lambda_1(G)$  (see [12]):

$$\Delta - \lambda_1(G) > \frac{(n\Delta - 2m)k^2}{(n\Delta - 2m)(n^2 - 2(n - k)) + nk^2}. \quad (3.2)$$

They also considered the signless Laplacian spectral radius of a  $k$ -connected graph and provided a lower bound on  $2\Delta - q_1(G)$  (see [13]):

$$2\Delta - q_1(G) > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - 2(n - k)) + nk^2}. \quad (3.3)$$

In their paper, they mainly proposed the following bound on the Laplacian spectral radius:

$$2\Delta - \mu_1(G) > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - 2(n - k)) + nk^2}. \quad (3.4)$$

In this chapter, we take the vertex connectivity into account and establish a lower bound on  $2\Delta - q_1(G)$ , which will be proved in next section. When  $k \geq \sqrt{n}$ , our lower bound on  $2\Delta - q_1(G)$  is better than the bound in (3.1). With the same arguments in this chapter, we can improve the bound in (3.2), which are presented in the remarks. Moreover, we give a similar result on the Laplacian spectral radius which improves the bound in (3.4).

## 3.2 Bounds on the signless Laplacian spectral radius of irregular graphs

In this section, we obtain a lower bound on  $2\Delta - q_1(G)$  as follows.

**Theorem 3.1** ([47]). *Let  $G$  be a  $k$ -connected irregular graph ( $k \geq 1$ ) of order  $n$  ( $\geq 3$ ), size  $m$  and maximum degree  $\Delta$ . We have*

$$2\Delta - q_1(G) > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2}. \quad (3.5)$$

*Proof.* Let  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  be the Perron vector corresponding to  $q_1(G)$ . Thus  $Q(G)\mathbf{x} = q_1(G)\mathbf{x}$ ,  $x_i > 0$  and  $\sum_{i=1}^n x_i^2 = 1$ . Let  $s$  and  $u$  be vertices of  $G$  such that

$x_s = \max_{1 \leq i \leq n} \{x_i\}$  and  $x_u = \min_{1 \leq i \leq n} \{x_i\}$ . Since  $\sum_{i=1}^n x_i^2 = 1$  and  $G$  is irregular, we have  $x_s > \frac{1}{\sqrt{n}} > x_u$ . Consider the following two cases:

**Case 1:** Suppose  $d_s \leq \Delta - 1$ . Since  $Q(G)\mathbf{x} = q_1(G)\mathbf{x}$ , we have

$$q_1(G)x_s = d_s x_s + \sum_{j \in N(s)} x_j \leq (\Delta - 1)x_s + (\Delta - 1)x_s = 2(\Delta - 1)x_s.$$

Thus  $q_1(G) \leq 2\Delta - 2$  as  $x_s > 0$ . Note that  $1 \leq k \leq \delta \leq \Delta - 1 \leq n - 2$  as  $G$  is irregular. We obtain  $n^2 - (\Delta - k + 2)(n - k) \geq n^2 - (n - 1 - 1 + 2)(n - k) = nk > 0$ .

Therefore,

$$\begin{aligned} & \frac{(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2} \\ & \leq \frac{(n\Delta - 2m)k^2}{2(n\Delta - 2m)nk + nk^2} < \frac{(n\Delta - 2m)k^2}{2(n\Delta - 2m)k^2 + nk^2} \\ & = \frac{n\Delta - 2m}{2(n\Delta - 2m) + n} < 1. \end{aligned}$$

Consequently,

$$2\Delta - q_1(G) \geq 2 > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2}.$$

**Case 2:** Suppose  $d_s = \Delta$ . For the vertex  $u$ , we have

$$q_1(G)x_u = d_u x_u + \sum_{j \in N(u)} x_j \geq d_u x_u + d_u x_u = 2d_u x_u.$$

Moreover,  $G$  is irregular implies that  $q_1(G)x_u < 2\Delta x_u$ . Hence  $d_u < \Delta$  since  $x_u > 0$ .

Next, we state a property about the length of the paths between  $s$  and  $u$ . As  $G$  is  $k$ -connected, by Menger's Theorem (Theorem 1.2), there are at least  $k$  vertex-disjoint paths between  $s$  and  $u$ . We choose  $k$  paths from them such that the sum of the lengths of these  $k$  paths is as small as possible. Let  $P_1, P_2, \dots, P_k$  be such  $k$  paths. Obviously, each of these path  $P_i$  can only contain one vertex of  $N_G(s)$ . Otherwise, we can find another  $k$  paths that have a smaller sum of lengths. Hence there exist at least  $\Delta - k$  vertices  $v_i$ , where  $i \in \{1, 2, \dots, \Delta - k\}$ , such that  $v_i \in N_G(s)$  but  $v_i \notin \bigcup_{i=1}^k V(P_i)$ . As a result,

$$\sum_{i=1}^k |V(P_i)| \leq n - (\Delta - k) + 2(k - 1).$$

Following the argument of Chen [12] and Ning [53], we obtain

$$\begin{aligned}
2\Delta - q_1(G) &= 2\Delta - \mathbf{x}^T Q(G) \mathbf{x} \\
&= 2\Delta \sum_{i=1}^n x_i^2 - \sum_{v_i v_j \in E(G)} (x_i + x_j)^2 \\
&= 2\Delta \sum_{i=1}^n x_i^2 - (2 \sum_{i=1}^n d_i x_i^2 - \sum_{v_i v_j \in E(G)} (x_i - x_j)^2) \\
&= 2 \sum_{i=1}^n (\Delta - d_i) x_i^2 + \sum_{v_i v_j \in E(G)} (x_i - x_j)^2 \tag{3.6}
\end{aligned}$$

$$\geq 2(n\Delta - 2m)x_u^2 + \sum_{v_i v_j \in E(G)} (x_i - x_j)^2. \tag{3.7}$$

Note that  $\sum_{i=1}^k |V(P_i)| \leq n - (\Delta - k) + 2(k - 1)$ . In addition, by Cauchy-Schwarz inequality, we have

$$\sum_{v_i v_j \in E(P_t)} (x_i - x_j)^2 \geq \frac{1}{|V(P_t)| - 1} \left( \sum_{v_i v_j \in E(P_t)} (x_i - x_j) \right)^2.$$

And using Arithmetic Mean-Geometric Mean inequality, we have

$$\sum_{t=1}^k \frac{1}{|V(P_t)| - 1} \geq \frac{k^2}{\sum_{t=1}^k (|V(P_t)| - 1)}.$$

Therefore, from these two inequalities, we obtain

$$\begin{aligned}
\sum_{v_i v_j \in E(G)} (x_i - x_j)^2 &\geq \sum_{t=1}^k \sum_{v_i v_j \in E(P_t)} (x_i - x_j)^2 \\
&\geq \sum_{t=1}^k \frac{1}{|V(P_t)| - 1} \left( \sum_{v_i v_j \in E(P_t)} (x_i - x_j) \right)^2 \\
&= \sum_{t=1}^k \frac{1}{|V(P_t)| - 1} (x_s - x_u)^2 \\
&\geq \frac{k^2}{\sum_{t=1}^k (|V(P_t)| - 1)} (x_s - x_u)^2 \\
&\geq \frac{k^2}{n - \Delta(G) + 2k - 2} (x_s - x_u)^2. \tag{3.8}
\end{aligned}$$

Combining (3.7) and (3.8), we have

$$\begin{aligned}
2\Delta - q_1(G) &\geq 2(n\Delta - 2m)x_u^2 + \frac{k^2}{n - \Delta + 2k - 2}(x_s - x_u)^2 \\
&= \left(2(n\Delta - 2m) + \frac{k^2}{n - \Delta + 2k - 2}\right)x_u^2 \\
&\quad - \frac{2k^2}{n - \Delta + 2k - 2}x_sx_u + \frac{k^2}{n - \Delta + 2k - 2}x_s^2.
\end{aligned} \tag{3.9}$$

Let  $f(x_u) = \left(2(n\Delta - 2m) + \frac{k^2}{n - \Delta + 2k - 2}\right)x_u^2 - \frac{2k^2}{n - \Delta + 2k - 2}x_sx_u + \frac{k^2}{n - \Delta + 2k - 2}x_s^2$ . If we regard  $f(x_u)$  as a quadratic function, then we have

$$2\Delta - q_1(G) \geq \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n - \Delta + 2k - 2) + k^2}x_s^2. \tag{3.10}$$

Let

$$C = \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2}$$

and consider the following two subcases:

**Subcase 1:** Suppose  $k = 1$ . We have

$$2\Delta - q_1(G) \geq \frac{2(n\Delta - 2m)}{2(n\Delta - 2m)(n - \Delta) + 1}x_s^2 \tag{3.11}$$

and

$$C = \frac{2(n\Delta - 2m)}{2(n\Delta - 2m)(n^2 - (\Delta + 1)(n - 1)) + n}.$$

If  $x_u^2 \geq \frac{C}{2(n\Delta - 2m)}$ , then from (3.9), we obtain

$$2\Delta - q_1(G) \geq 2(n\Delta - 2m) \cdot \frac{C}{2(n\Delta - 2m)} + \frac{k^2}{n - \Delta + 2k - 2}(x_s - x_u)^2 > C,$$

since  $x_s > x_u$  as  $G$  is irregular.

If  $x_u^2 < \frac{C}{2(n\Delta - 2m)}$ , then since  $\sum_{i=1}^n x_i^2 = 1$ , we have

$$x_s^2 \geq \frac{1 - x_u^2}{n - 1} > \frac{1}{n - 1} \cdot \left(1 - \frac{C}{2(n\Delta - 2m)}\right).$$

Hence from (3.11) and  $n^2 - (\Delta + 1)(n - 1) = (n - \Delta)(n - 1) + 1 > (n - \Delta)(n - 1)$ ,

we have

$$\begin{aligned}
2\Delta - q_1(G) &\geq \frac{2(n\Delta - 2m)}{2(n\Delta - 2m)(n - \Delta) + 1} x_s^2 \\
&> \frac{2(n\Delta - 2m)}{2(n\Delta - 2m)(n - \Delta) + 1} \times \frac{1}{n - 1} \\
&\quad \times \left( 1 - \frac{1}{2(n\Delta - 2m)(n^2 - (\Delta + 1)(n - 1)) + n} \right) \\
&= \frac{2(n\Delta - 2m)}{2(n\Delta - 2m)(n^2 - (\Delta + 1)(n - 1)) + n} \\
&\quad \times \frac{2(n\Delta - 2m)(n^2 - (\Delta + 1)(n - 1)) + n - 1}{2(n\Delta - 2m)(n - \Delta)(n - 1) + n - 1} \\
&> C \times 1 \\
&= C.
\end{aligned}$$

**Subcase 2:** Suppose  $k \geq 2$ .

If  $x_u^2 \geq \frac{C}{2(n\Delta - 2m)}$ , then the result can be obtained by using a similar argument of Subcase 1.

Since  $d_u \geq k$ , we can choose  $k-1$  vertices from  $N_G(u)$ , denoted by  $u_1, u_2, \dots, u_{k-1}$ , such that  $s \notin \{u_1, u_2, \dots, u_{k-1}\}$ . If  $\sum_{t=1}^{k-1} x_{u_t}^2 > C(1 + \frac{k-1}{2(n\Delta - 2m)})$ , then by (3.7) and the method to derive (3.10), we obtain

$$\begin{aligned}
2\Delta - q_1(G) &\geq 2(n\Delta - 2m)x_u^2 + \sum_{t=1}^{k-1} (x_{u_t} - x_u)^2 \\
&= \sum_{t=1}^{k-1} \left( \frac{2(n\Delta - 2m)}{k-1} x_u^2 + (x_{u_t} - x_u)^2 \right) \\
&\geq \sum_{t=1}^{k-1} \frac{2(n\Delta - 2m)}{2(n\Delta - 2m) + k - 1} x_{u_t}^2 \\
&= \frac{2(n\Delta - 2m)}{2(n\Delta - 2m) + k - 1} \cdot \sum_{t=1}^{k-1} x_{u_t}^2 \\
&> \frac{2(n\Delta - 2m)}{2(n\Delta - 2m) + k - 1} \cdot \frac{2(n\Delta - 2m) + k - 1}{2(n\Delta - 2m)} \cdot C \\
&= C.
\end{aligned}$$

It remains to show that our result is valid when  $x_u^2 < \frac{C}{2(n\Delta - 2m)}$  and  $\sum_{t=1}^{k-1} x_{u_t}^2 \leq$



$C(1 + \frac{k-1}{2(n\Delta-2m)})$ . Using  $\sum_{i=1}^n x_i^2 = 1$  again, we have

$$x_s^2 \geq \frac{1}{n-k} \left( 1 - x_u^2 - \sum_{t=1}^{k-1} x_{u_t}^2 \right) > \frac{1}{n-k} \left( 1 - \frac{2(n\Delta-2m)+k}{2(n\Delta-2m)} \cdot C \right).$$

Therefore, from (3.10) again,

$$\begin{aligned} 2\Delta - q_1(G) &> \frac{2(n\Delta-2m)k^2}{2(n\Delta-2m)(n-\Delta+2k-2)+k^2} \cdot \frac{1}{n-k} \cdot \left( 1 - \frac{2(n\Delta-2m)+k}{2(n\Delta-2m)} \cdot C \right) \\ &= \frac{2(n\Delta-2m)k^2}{2(n\Delta-2m)(n^2 - (\Delta-k+2)(n-k)) + nk^2} \\ &= C. \end{aligned}$$

This completes the proof.  $\square$

From Proposition 1.12, we know that  $\mu_1(G) \leq q_1(G)$ . Thus every upper bound on  $q_1(G)$  is an upper bound on  $\mu_1(G)$ . Therefore

**Corollary 3.1.** *Let  $G$  be a  $k$ -connected irregular graph ( $k \geq 1$ ) of order  $n$  ( $\geq 3$ ), size  $m$  and maximum degree  $\Delta$ . We have*

$$2\Delta - \mu_1(G) > \frac{2(n\Delta-2m)k^2}{2(n\Delta-2m)(n^2 - (\Delta-k+2)(n-k)) + nk^2}. \quad (3.12)$$

**Remark 3.1.** Obviously, the bound in (3.5) is better than the bound in (3.3) and the bound in (3.12) is better than the bound in (3.4) since  $\Delta - k > 0$ .

**Remark 3.2.** Note that the bound in (3.5) increases when  $n\Delta - 2m$  increases. It is obvious that  $n\Delta - 2m \geq 1$  as  $G$  is irregular. Hence from Theorem 3.1 we can easily find that

$$2\Delta - q_1(G) > \frac{2k^2}{2(n^2 - (\Delta-k+2)(n-k)) + nk^2}.$$

Let

$$f(k) = \frac{2k^2}{2(n^2 - (\Delta-k+2)(n-k)) + nk^2}.$$

We have

$$\begin{aligned} f(k) &\geq \frac{2k^2}{2(n^2 - 3(n-k)) + nk^2} \\ &= \frac{1}{n/2 + (n^2 - 3n)/k^2 + 3/k}. \end{aligned}$$

Note that  $\frac{1}{n/2+(n^2-3n)/k^2+3/k}$  is also an increasing function of  $k$ . Thus when  $k \geq \sqrt{n}$ , we have

$$f(k) \geq \frac{1}{(3n)/2 + 3/\sqrt{n} - 3} > \frac{1}{(7n)/4} \geq \frac{1}{n(d-1/4)}.$$

The second inequality holds as  $n \geq 3$  and the third holds since  $G$  is irregular, which implies  $d \geq 2$ . Therefore, when  $k \geq \sqrt{n}$ , the bound in (3.5) is better than the bound in (3.1).

**Remark 3.3.** In the proof of Theorem 3.1, we use the fact that there are at least  $\Delta - k$  vertices of  $G$  that do not belong to the subgraph  $H = G[\bigcup_{t=1}^k V(P_t)]$ . The lower bound on  $2\Delta - q_1(G)$  can be improved when the vertices outside the subgraph  $H$  are increased. In fact, one can show that if there are  $l$  vertices outside the subgraph  $H$ , then

$$2\Delta - q_1(G) > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (l+2)(n-k)) + nk^2}. \quad (3.13)$$

The bound in (3.5) is a particular case ( $l = \Delta - k$ ) of the bound in (3.13).

**Remark 3.4.** Using the same arguments, we can find that

$$\Delta - \lambda_1(G) > \frac{(n\Delta - 2m)k^2}{(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2}.$$

This result improves the bound in (3.2). Similar to (3.13), if there are  $l$  vertices outside the subgraph  $H$ , then

$$\Delta - \lambda_1(G) > \frac{(n\Delta - 2m)k^2}{(n\Delta - 2m)(n^2 - (l+2)(n-k)) + nk^2}.$$

### 3.3 Bounds on the signless Laplacian spectral radius of subgraphs

To consider the signless Laplacian spectral radius of a subgraph, we begin with the following lemma.

**Lemma 3.1** ([22]). *Let  $G$  be a graph on  $n$  vertices and  $m$  edges and let  $e$  be an edge of  $G$ . Let  $q_1, q_2, \dots, q_n$  ( $q_1 \geq q_2 \geq \dots \geq q_n$ ) and  $s_1, s_2, \dots, s_n$  ( $s_1 \geq s_2 \geq \dots \geq s_n$ ) be the signless Laplacian spectra of  $G$  and of  $G - e$ , respectively. Then*

$$0 \leq s_n \leq q_n \leq \dots \leq s_2 \leq q_2 \leq s_1 \leq q_1.$$

Let  $G$  be an irregular connected graph with maximum degree  $\Delta$  and order  $n$ . We cannot always find a  $\Delta$ -regular graph  $G'$  such that  $G$  is a proper spanning subgraph of  $G'$ . In fact, if  $n\Delta$  is an odd number, then the  $\Delta$ -regular graph  $G'$  cannot be found as  $n\Delta = 2m \equiv 0 \pmod{2}$  for  $G'$ . Thus if  $G$  is a proper spanning subgraph of  $\Delta$ -regular graph  $G'$ , then we can prove the following theorem.

**Theorem 3.2** ([47]). *Let  $G$  be a proper spanning subgraph of a  $\Delta$ -regular  $k$ -connected graph  $G'$  of order  $n$ . If  $k \geq 2$ , then*

$$2\Delta - q_1(G) > \frac{2(k-1)^2}{2(n-\Delta)(n-\Delta+2k-4) + (n+1)(k-1)^2}.$$

*Proof.* Lemma 3.1 implies that the signless Laplacian spectral radius cannot be increased by deleting an edge. Thus we may assume that  $G = G' - e$  for some edge  $e$  of  $G'$ . Let  $e = uv$ . We have  $d_G(u) = d_G(v) = \Delta - 1$  and  $d_G(w) = \Delta$  for other vertices  $w$ . Since  $G$  is connected when  $k \geq 2$ , there exists a Perron vector,  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  with  $x_i > 0$ , corresponding to  $q_1(G)$ . Let  $s$  be a vertex of  $G$  such that  $x_s = \max_{1 \leq i \leq n} \{x_i\}$ . Hence

$$q_1(G)x_s = d_G(s)x_s + \sum_{j \in N_G(s)} x_j \leq d_G(s)x_s + d_G(s)x_s = 2d_G(s)x_s$$

which means that  $q_1(G) \leq 2d_G(s)$ . Moreover, using the fact that

$$\lambda_1(G) > \frac{2|E(G)|}{n} = \frac{n\Delta - 2}{n}$$

(see [24]) together with  $2 \leq k \leq n - 1$ , we have

$$q_1(G) \geq 2\lambda_1(G) > 2 \frac{2|E(G)|}{n} = 2 \frac{n\Delta - 2}{n} = 2\Delta - \frac{4}{n} \geq 2\Delta - \frac{4}{3} > 2\Delta - 2.$$

Combining this with  $q_1(G) \leq 2d_G(s)$ , we obtain  $d_G(s) > \Delta - 1$ . Therefore,  $d_G(s) = \Delta$  and so  $s \neq u$  and  $s \neq v$ .

In addition, formula (3.6) gives

$$\begin{aligned} 2\Delta - q_1(G) &= 2 \sum_{i=1}^n (\Delta - d_G(v_i))x_i^2 + \sum_{v_i v_j \in E(G)} (x_i - x_j)^2 \\ &= 2(x_u^2 + x_v^2) + \sum_{v_i v_j \in E(G)} (x_i - x_j)^2. \end{aligned} \quad (3.14)$$

With the same arguments as Chen in [12], we know that

$$\sum_{v_i v_j \in E(G)} (x_i - x_j)^2 \geq \frac{(k-1)^2}{n - \Delta + 2k - 4} (x_s - x_u)^2.$$

Hence, similar to the proof of (3.10), we have

$$\begin{aligned} 2\Delta - q_1(G) &\geq 2(x_u^2 + x_v^2) + \frac{(k-1)^2}{n - \Delta + 2k - 4} (x_s - x_u)^2 \\ &> 2x_u^2 + \frac{(k-1)^2}{n - \Delta + 2k - 4} (x_s - x_u)^2 \\ &\geq \frac{2(k-1)^2}{2(n - \Delta + 2k - 4) + (k-1)^2} x_s^2. \end{aligned} \quad (3.15)$$

Define

$$C' = \frac{2(k-1)^2}{2(n - \Delta)(n - \Delta + 2k - 4) + (n+1)(k-1)^2}.$$

If  $x_u^2 + x_v^2 > \frac{C'}{2}$ , then from (3.14),

$$2\Delta - q_1(G) = 2(x_u^2 + x_v^2) + \sum_{v_i v_j \in E(G)} (x_i - x_j)^2 > 2 \frac{C'}{2} + \sum_{v_i v_j \in E(G)} (x_i - x_j)^2 \geq C'.$$

Since  $d_G(u) = \Delta - 1$ , it is possible to choose  $\Delta - 2$  vertices  $\{u_1, u_2, \dots, u_{\Delta-2}\}$  from  $N_G(u)$  such that  $s \notin \{u_1, u_2, \dots, u_{\Delta-2}\}$ . Hence if  $\sum_{t=1}^{\Delta-2} x_{u_t}^2 \geq \frac{\Delta}{2} C'$  and using (3.14) again,

$$\begin{aligned} 2\Delta - q_1(G) &> 2x_u^2 + \sum_{t=1}^{\Delta-2} (x_{u_t} - x_u)^2 \\ &= \sum_{t=1}^{\Delta-2} \left( \frac{2}{\Delta-2} x_u^2 + (x_{u_t} - x_u)^2 \right) \\ &\geq \sum_{t=1}^{\Delta-2} \frac{\frac{2}{\Delta-2}}{1 + \frac{2}{\Delta-2}} x_{u_t}^2 \geq \frac{2}{\Delta} \frac{\Delta}{2} C' = C'. \end{aligned}$$

The remaining case is  $x_u^2 + x_v^2 \leq \frac{C'}{2}$  and  $\sum_{t=1}^{\Delta-2} x_{u_t}^2 < \frac{\Delta}{2}C'$ . Obviously,

$$x_s^2 \geq \frac{1 - x_u^2 - x_v^2 - \sum_{t=1}^{\Delta-2} x_{u_t}^2}{n - \Delta} > \frac{1}{n - \Delta} \left(1 - \frac{C'}{2} - \frac{\Delta}{2}C'\right) = \frac{1}{n - \Delta} \left(1 - \frac{\Delta + 1}{2}C'\right)$$

and from (3.15) we obtain

$$\begin{aligned} 2\Delta - q_1(G) &> \frac{2(k-1)^2}{2(n-\Delta+2k-4) + (k-1)^2} \times \frac{1}{n-\Delta} \times \left(1 - \frac{\Delta+1}{2}C'\right) \\ &= \frac{2(k-1)^2}{2(n-\Delta)(n-\Delta+2k-4) + (n+1)(k-1)^2} \\ &= C'. \end{aligned}$$

This completes the proof. □

The most critical condition in estimating the value of  $\sum_{v_i v_j \in E(G)} (x_i - x_j)^2$  in the proof of Theorem 3.1 and Theorem 3.2 is that we can use each edge of  $G$  at most one time. As a consequence, if a graph  $G$  is  $k$ -edge-connected, then this condition would be satisfied because we can find pairwise edge-disjoint paths by Menger's Theorem (Theorem 1.2). Therefore we have the theorem below.

**Theorem 3.3** ([47]). *Let  $G$  be a  $k$ -edge-connected irregular graph ( $k \geq 1$ ) of order  $n$  ( $n \geq 3$ ), size  $m$  and maximum degree  $\Delta$ . Then we have*

$$2\Delta - q_1(G) > \frac{2(n\Delta - 2m)k^2}{2(n\Delta - 2m)(n^2 - (\Delta - k + 2)(n - k)) + nk^2}.$$

**Remark 3.5.** It can be shown that Theorem 3.2 holds for any proper subgraphs no matter the proper subgraph is spanning or not. Indeed, if  $G$  is a proper subgraph but not a spanning subgraph of  $G'$ , then we can construct a new graph  $G''$  by adding some isolated vertices such that the order of  $G''$  is the same as the order of  $G'$ . For  $G''$ , we know that  $q_1(G'') = q_1(G)$  and  $G''$  is a proper spanning subgraph of  $G'$ . Hence Theorem 3.2 holds for any proper subgraph  $G$ .

# Chapter 4

## Other results related to the signless Laplacian matrix of a graph

In this chapter, firstly, we establish a relation between the number of semi-edge walks of a connected graph and the number of walks of two auxiliary graphs. We then give upper bounds on the signless Laplacian spectral radius of connected graphs and planar graphs using this relationship. Finally, we obtain a combinatorial expression for the fifth coefficients of the Laplacian and the signless Laplacian characteristic polynomials of graphs.

### 4.1 A relationship between the walks and the semi-edge walks of graphs

Given a graph  $G$ , it is known that the number of walks of length  $k$  from vertex  $v_i$  to vertex  $v_j$  is the  $(i, j)$ -entry of the matrix  $A^k(G)$  (see Theorem 1.8). Based on this property, the number of walks has been widely used to study spectral radius, energy, the  $k$ -th spectral moment and other parameters (see [14, 52, 68, 69] for details).

Also, we have a similar result on the number of semi-edge walks of a graph, that is, the number of semi-edge walks of length  $k$  from vertex  $v_i$  to vertex  $v_j$  is the  $(i, j)$ -entry of the matrix  $Q^k(G)$  (see Theorem 1.9). From this result, we can study some algebraic properties of a graph, such as signless Laplacian spectral radius, by counting its number of semi-edge walks. In this section, we obtain a relation between the numbers of walks and semi-edge walks. Using this relation, we can study the number of semi-edge walks by the number of walks since the latter has been well studied.

### 4.1.1 The relation between these two walks

Before stating our main result, we need to construct two new graphs.

Let  $G$  be a connected graph. For each edge  $uv$ , we add two loops  $l_u(v)$  and  $l_v(u)$  incident with  $u$  and  $v$ , respectively. We denote the resulting graph by  $G_1$ .

**Remark 4.1.** For each edge  $uv$  in  $G$ , the semi-edges  $u^v u$  and  $v^u v$  are corresponding to loops  $l_u(v)$  and  $l_v(u)$  in  $G_1$ , respectively. Clearly, this corresponding is a bijection between the set of all semi-edges of  $G$  and the set of all loops in  $G_1$ .

Let  $V(G) = \{v_1, v_2, \dots, v_n\}$ . We duplicate  $G$  to get  $G'$ . The vertex in  $G'$  corresponding to  $v_i$  is denoted by  $v'_i$ . Consider the disjoint union graph  $G + G'$ . For each  $i \in \{1, 2, \dots, n\}$ , let  $N_G(v_i) = \{u_1, u_2, \dots, u_{d_i}\}$  where  $d_i = d_G(v_i)$ . We link  $v_i$  and  $v'_i$  with  $d_i$  parallel edges in  $G + G'$  and denote these edges by  $\varepsilon_{v_i}(u_j)$ , for  $j \in \{1, 2, \dots, d_i\}$ , respectively. The resulting graph is denoted by  $G_2$ .

**Remark 4.2.** Suppose  $v_i u_j \in E(G)$ . It associates a loop  $l_{v_i}(u_j)$  incident to  $v_i$  in  $G_1$ . Then the corresponding  $l_{v_i}(u_j) \mapsto \varepsilon_{v_i}(u_j)$  is a bijection from  $E(G_1) \setminus E(G)$  onto  $E(G_2) \setminus E(G + G')$ .

**Remark 4.3.** There are no edges in  $G_2$  incident with  $v_i$  and  $v'_j$  except  $i = j$ .

Note that  $G_1$  and  $G_2$  are not simple, where  $G_1$  has loops and  $G_2$  has parallel edges. The following figure shows the graphs that we have defined.

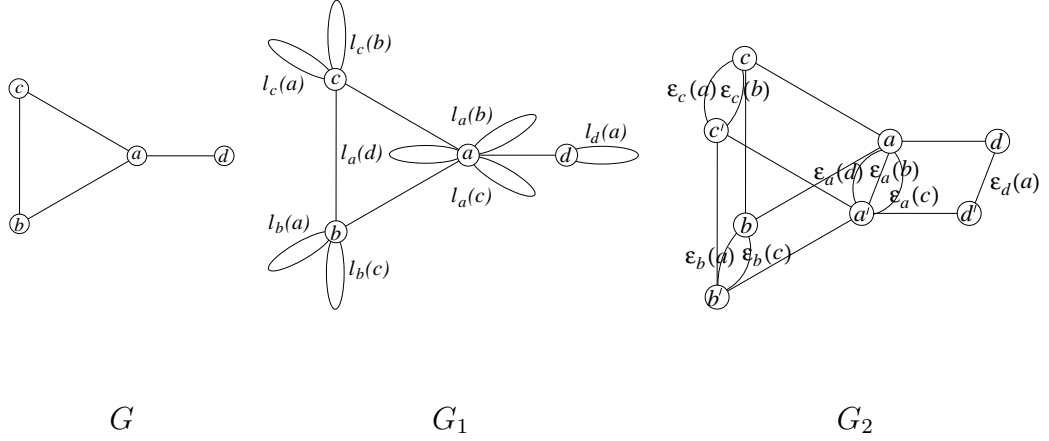


Figure 4.1: Two constructions.

The following theorem gives a relation between the semi-edge walks in  $G$  and the walks in  $G_1$  and  $G_2$ .

**Theorem 4.1.** *Let  $G$  be a graph and let  $G_1$  and  $G_2$  be graphs constructed from  $G$  as above. If we ignore the direction of all loops, then the number of semi-edge walks in  $G$  is equal to the number of walks in  $G_1$  and is equal to half of the number of walks in  $G_2$ .*

*Proof.* The first part of the theorem follows from Remark 4.1.

Let  $S_i$  be the set of walks in  $G_i$ ,  $i = 1, 2$ . Let  $W_2 = x_1 e_1 x_2 \cdots e_k x_{k+1}$  be a walk of length  $k$  in  $G_2$ . According to the definition,  $x_j$  is either  $v_j$  or  $v'_j$  for some  $v_j \in V(G)$ ,  $j \in \{1, 2, \dots, k+1\}$ . Define  $\phi(W_2) = v_1 g_1 v_2 \cdots g_k v_{k+1}$ , where

$$g_j = \begin{cases} v_j v_{j+1} & \text{if } e_j = v_j v_{j+1} \text{ or } e_j = v'_j v'_{j+1} \text{ is a link;} \\ l_{v_j}(v) & \text{if } e_j = \varepsilon_{v_j}(v) \text{ for some } v \in V(G). \end{cases}$$

So  $\phi(W_2) \in S_1$ . Clearly,  $\phi : S_2 \rightarrow S_1$  is a mapping. We will show by induction on the length of a walk that  $\phi$  is a 2-to-1 surjection and hence we prove the second part of the theorem.

From the definition of  $\phi$ , we have  $\phi(WU) = \phi(W)\phi(U)$  if the end vertex of  $W$  is the initial vertex of  $U$ .



Suppose  $W_1 = v_1 g_1 v_2 \in S_1$ . Let  $W_2 = x_1 e_1 x_2 \in \phi^{-1}[W_1]$  be the pre-image of  $W_1$ . According to the definition of  $\phi$ ,  $x_i \in \{v_i, v'_i\}$  for  $i = 1, 2$ . Suppose  $x_1 = v_1$ . If  $g_1$  is a link, then  $v_1 \neq v_2$  and hence  $g_1 = v_1 v_2$  and  $x_2 = v_2$  (by Remark 4.3). If  $g_1$  is a loop, then  $g_1 = l_{v_1}(v)$  for some  $v \in N(v_1)$ . Thus  $e_1 = \varepsilon_{v_1}(v)$  and  $x_2 = v'_1$ . Suppose  $x_1 = v'_1$ . If  $g_1$  is a link, then  $v_1 \neq v_2$  and hence  $g_1 = v_1 v_2$  and  $x_2 = v'_2$ . If  $g_1$  is a loop, then  $g_1 = l_{v_1}(v)$  for some  $v \in N(v_1)$ . Thus  $e_1 = \varepsilon_{v_1}(v)$  and  $x_2 = v_1$  and hence  $|\phi^{-1}[W_1]| = 2$ .

Suppose  $|\phi^{-1}[W]| = 2$  for any walk  $W$  of length  $k-1$  in  $S_1$ , where  $k \geq 2$ . Now suppose  $W_1 = v_1 g_1 v_2 \cdots g_{k-1} v_k g_k v_{k+1} \in S_1$ . Let  $W_2 = x_1 e_1 x_2 \cdots e_{k-1} x_k e_k x_{k+1} \in \phi^{-1}[W_1]$ . Let  $U_1 = v_1 g_1 v_2 \cdots g_{k-1} v_k$  and  $U_2 = x_1 e_1 x_2 \cdots e_{k-1} x_k$ . Then  $\phi(U_2) = U_1$ . That means,  $U_2 \in \phi^{-1}[U_1]$ . Now  $x_k \in \{v_k, v'_k\}$  and  $x_{k+1} \in \{v_{k+1}, v'_{k+1}\}$ . Similar to the case when the walk of length 1,  $x_{k+1}$  is determined uniquely. Therefore, according to the two choices of  $U_1$  we obtain  $|\phi^{-1}[W_1]| = 2$ .  $\square$

#### 4.1.2 Some applications about this relation

In this section, we provide some applications of Theorem 4.1. Let  $\rho(M)$  be the spectral radius of matrix  $M \in \mathbf{M}_n(\mathbb{C})$ , then  $\rho(M)$  can be represented as a limit of a matrix norm, that is,  $\rho(M) = \lim_{k \rightarrow \infty} |||M^k|||^{1/k}$  (see Theorem 1.6).

This result holds for any matrix norm. Thus we can choose some particular norms to study the signless Laplacian matrix of a graph. Here we use the  $l_1$ -norm which is defined as

$$|||M|||_1 = \sum_{i,j=1}^n |m_{ij}|,$$

where  $m_{ij}$  is the  $(i, j)$ -entry of  $M$ .

Note that the signless Laplacian matrix of a graph is a nonnegative matrix. Hence, taking the matrix norm with  $l_1$ -norm in Theorem 1.6, we have

**Corollary 4.1.** *Let  $G$  be a graph of order  $n$ ,  $Q(G)$  be the signless Laplacian matrix*

of  $G$  and  $\mathbf{u}$  be the  $n$ -vector with all entries equal to 1, then

$$q_1(G) = \lim_{k \rightarrow \infty} \sqrt[k]{\mathbf{u}^T Q^k(G) \mathbf{u}}.$$

Obviously,  $\mathbf{u}^T Q^k(G) \mathbf{u}$  stands for the sum of all entries of  $Q^k(G)$ , which is the number of semi-edges walks of length  $k$  in  $G$  by Theorem 1.9. Therefore, we obtain some bounds on  $q_1(G)$  by estimating the number of semi-edges walks of length  $k$  in  $G$ . We can use Theorem 4.1 to estimate the number of semi-edges walks since the walks of a graph have been well studied.

T.P. Hayer gave an upper bound on the spectral radius by estimating the number of walks as follows.

**Lemma 4.1** ([43]). *Let  $G$  be a graph with maximum degree  $\Delta$ . If there is an orientation of  $G$  such that the maximum out-degree  $\Delta^+ \leq \Delta/2$ , then  $\lambda_1 \leq 2\sqrt{\Delta^+(\Delta - \Delta^+)}$ .*

In his proof, he used the following result on the number of walks.

**Lemma 4.2** ([43]). *Let  $G$  be a graph of order  $n$  with maximum degree  $\Delta$ . If there is an orientation of  $G$  such that the maximum out-degree  $\Delta^+ \leq \Delta/2$ , then the number of walks of length  $k$  in  $G$  is at most  $n2^k(\sqrt{\Delta^+(\Delta - \Delta^+)})^k$ .*

Note that Lemma 4.2 holds for graphs with parallel edges but without loop. A similar result about semi-edge walks can be obtained by Theorem 4.1.

**Lemma 4.3.** *Let  $G$  be a (simple) graph of order  $n$  with maximum degree  $\Delta$ . If there is an orientation of  $G$  such that the maximum out-degree  $\Delta^+ \leq \Delta/2$ , then the number of semi-edge walks of length  $k$  is at most  $n2^k(\Delta^+ + \lceil \frac{\Delta}{2} \rceil)^{\frac{k}{2}}(\Delta + \lfloor \frac{\Delta}{2} \rfloor - \Delta^+)^{\frac{k}{2}}$ .*

*Proof.* Let  $G_2$  be the graph constructed in Section 4.1.1 by adding some parallel edges to the disjoint union of two copies of  $G$ . Suppose there is an orientation of  $G$  such that  $\Delta^+ \leq \Delta/2$ . Define an orientation on  $G_2$  from the orientation on  $G$ : For any edge  $e = v_i v_j$  in  $G$ , if its direction is from  $v_i$  to  $v_j$ , then orient the edge  $v_i v_j$  from  $v_i$  to  $v_j$  and the edge  $v'_i v'_j$  from  $v'_i$  to  $v'_j$  in  $G_2$ . For the  $d_G(v_i)$  parallel edges between  $v_i$

and  $v'_i$  in  $G_2$ , we choose  $\lceil d_G(v_i)/2 \rceil$  parallel edges arbitrarily and orient them from  $v_i$  to  $v'_i$  while the other parallel edges from  $v'_i$  to  $v_i$ .

Under the above orientation of  $G_2$ , it is easy to see that its maximum out-degree and maximum degree are  $\Delta^+ + \lceil \frac{\Delta}{2} \rceil$  and  $2\Delta$ , respectively. When  $\Delta$  is even,

$$\Delta^+ + \lceil \frac{\Delta}{2} \rceil \leq \frac{\Delta}{2} + \frac{\Delta}{2} = \Delta = \frac{1}{2} \times 2\Delta.$$

And when  $\Delta$  is odd,  $\Delta^+ \leq \frac{\Delta-1}{2}$  as  $\Delta^+$  is an integer. Hence

$$\Delta^+ + \lceil \frac{\Delta}{2} \rceil \leq \frac{\Delta-1}{2} + \frac{\Delta+1}{2} = \Delta = \frac{1}{2} \times 2\Delta.$$

Therefore, by Lemma 4.2, the number of walks of length  $k$  in  $G_2$  is at most

$$\begin{aligned} & 2n \cdot 2^k (\lceil \frac{\Delta}{2} \rceil + \Delta^+)^{\frac{k}{2}} (2\Delta - (\lceil \frac{\Delta}{2} \rceil + \Delta^+))^{\frac{k}{2}} \\ &= 2n \cdot 2^k (\lceil \frac{\Delta}{2} \rceil + \Delta^+)^{\frac{k}{2}} (\Delta + \lfloor \frac{\Delta}{2} \rfloor - \Delta^+)^{\frac{k}{2}}. \end{aligned}$$

As a result, by Theorem 4.1, the number of semi-edge walks of length  $k$  in  $G$  is at most

$$n2^k (\lceil \frac{\Delta}{2} \rceil + \Delta^+)^{\frac{k}{2}} (\Delta + \lfloor \frac{\Delta}{2} \rfloor - \Delta^+)^{\frac{k}{2}}.$$

□

From Corollary 4.1, we know that  $\mathbf{u}^T Q^k(G) \mathbf{u}$  equals the number of semi-edge walks of length  $k$  in  $G$ . Combining with Lemma 4.3, we have

**Theorem 4.2.** *Let  $G$  be a graph with maximum degree  $\Delta$ . If there is an orientation such that the maximum out-degree  $\Delta^+ \leq \frac{\Delta}{2}$ , then*

$$q_1(G) \leq 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + \Delta^+)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - \Delta^+)}. \quad (4.1)$$

**Remark 4.4.** The bound in (4.1) is sharp. It is easy to show, by induction, that  $K_{2n+1}$  admits an orientation such that  $\Delta^+ = n$ . Then  $q_1(G) = 2\sqrt{2n \cdot 2n} = 4n = 2\Delta$ .

**Remark 4.5.** Not every graph can admit an orientation such that  $\Delta^+ \leq \frac{\Delta}{2}$ : Consider the complete graph  $K_{2n}$ , then, by Theorem 1.3,

$$n(2n - 1) = |E(K_{2n})| = \sum_{i=1}^{2n} d_i^+ \leq 2n\Delta^+.$$

Since  $\Delta^+$  is an integer,  $\Delta^+ \geq \lceil \frac{2n-1}{2} \rceil = n > \Delta/2$ .

**Remark 4.6.** We know that matrix  $L(G) = D(G) - A(G)$  is the Laplacian matrix of  $G$ . Let  $\mathbf{I}_n$  and  $\mathbf{O}_n$  be the identity matrix and zero matrix of order  $n$ , respectively. Given a graph  $G$  of order  $n$ , we construct  $G_2$  as in Section 4.1.1. Consider its adjacency matrix  $A(G_2)$  and we have

$$\begin{aligned} \det(\lambda\mathbf{I}_{2n} - A(G_2)) &= \det \begin{pmatrix} \lambda\mathbf{I}_n - A(G) & -D(G) \\ -D(G) & \lambda\mathbf{I}_n - A(G) \end{pmatrix} \\ &= \det \begin{pmatrix} \lambda\mathbf{I}_n - (A(G) + D(G)) & \lambda\mathbf{I}_n - (A(G) + D(G)) \\ -D(G) & \lambda\mathbf{I}_n - A(G) \end{pmatrix} \\ &= \det(\lambda\mathbf{I}_n - Q(G)) \det \begin{pmatrix} \mathbf{I}_n & \mathbf{I}_n \\ -D(G) & \lambda\mathbf{I}_n - A(G) \end{pmatrix} \\ &= \det(\lambda\mathbf{I}_n - Q(G)) \det \begin{pmatrix} \mathbf{I}_n & \mathbf{I}_n \\ \mathbf{O}_n & \lambda\mathbf{I}_n - (A(G) - D(G)) \end{pmatrix} \\ &= \det(\lambda\mathbf{I}_n - Q(G)) \det(\lambda\mathbf{I}_n - (-L(G))). \end{aligned}$$

As a result, the spectrum of  $G_2$  is exactly the union of the signless Laplacian spectrum and the minus of the Laplacian spectrum of  $G$ . In particular,  $q_1(G) = \lambda_1(G_2)$  and  $\mu_1(G) = -\lambda_{2n}(G_2)$ , where  $\mu_1(G)$  is the Laplacian spectral radius of  $G$  and  $\lambda_{2n}(G_2)$  is the least eigenvalue of  $G_2$ .

If  $G$  is a tree, then it admits an orientation with maximum out-degree 1 by using the depth-first tree search and orienting each edge from child to parent. Hence we have

**Corollary 4.2.** *Let  $T$  be a tree with maximum degree  $\Delta \geq 2$ , then*

$$q_1(G) \leq 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + 1)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - 1)}.$$

For planar graphs, D. Gonalves proved the following decomposition result.

**Lemma 4.4** ([39]). *If  $G$  is a planar graph, then  $E(G) = E(T_1) \cup E(T_2) \cup E(T_3)$ , where  $T_1, T_2$  and  $T_3$  are forests and  $\Delta(T_3) \leq 4$ .*

**Theorem 4.3.** *If  $G$  is a planar graph with the maximum degree  $\Delta \geq 2$ , then*

$$q_1(G) \leq 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + 2)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - 2)} + 2\sqrt{15}.$$

*Proof.* If  $\Delta \leq 3$ , then

$$q_1 \leq 2\Delta \leq 6 < 2\sqrt{15} < 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + 2)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - 2)} + 2\sqrt{15}.$$

So we may assume  $\Delta \geq 4$ . Let  $E(G) = E(T_1) \cup E(T_2) \cup E(T_3)$  be the edge decomposition of  $G$  by Lemma 4.4. Since  $T_1$  and  $T_2$  are forests, they admit an orientation with maximum out-degree 1, respectively. Hence  $T_1 \cup T_2$  has an orientation with maximum out-degree at most 2. By Theorem 4.2, each component  $C$  of  $T_1 \cup T_2$  has

$$q_1(C) \leq 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + 2)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - 2)}.$$

Therefore,

$$q_1(T_1 \cup T_2) \leq 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + 2)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - 2)}.$$

Note that each component  $T$  of  $T_3$  is a tree with maximum degree at most 4. From Corollary 4.2, we have  $q_1(T) \leq 2\sqrt{15}$  and thus  $q_1(T_3) \leq 2\sqrt{15}$ .

Obviously,  $Q(G) = Q(T_1 \cup T_2) + Q(T_3)$ . Hence, by Weyl inequality (see Theorem 1.5), we have

$$q_1(G) \leq 2\sqrt{(\lceil \frac{\Delta}{2} \rceil + 2)(\Delta + \lfloor \frac{\Delta}{2} \rfloor - 2)} + 2\sqrt{15}.$$

□

We now use the linear 2-arboricity to determine the signless Laplacian spectral radius of a planar graph.

**Lemma 4.5.** *Let  $G$  be a graph and  $la_2(G)$  be its linear 2-arboricity. Then*

$$q_1(G) \leq 3 \cdot la_2(G).$$

*Proof.* Let  $E(G) = E(T_1) \cup \cdots \cup E(T_{la_2(G)})$  be its edge decomposition, where  $T_i$  is a forest whose components are paths of length at most 2 for  $i \in \{1, 2, \dots, la_2(G)\}$ . And for each component  $P$  of  $T_i$ , we can easily obtain  $q_1(P) \leq 3$  as  $P$  is a path of length at most 2. Hence  $q_1(T_i) \leq 3$  for  $i \in \{1, 2, \dots, la_2(G)\}$ .

On the other hand,  $Q(G) = Q(T_1) + \cdots + Q(T_{la_2(G)})$ . Then by Weyl inequality, we have

$$q_1(G) \leq q_1(T_1) + \cdots + q_1(T_{la_2(G)}) \leq 3 \cdot la_2(G).$$

□

Recently, Y.Q. Wang studied  $la_2(G)$  for a planar graph and got the following upper bound on  $la_2(G)$ .

**Lemma 4.6** ( [70]). *If  $G$  is a planar graph with maximum degree  $\Delta$ , then*

$$la_2(G) \leq \lceil \frac{\Delta+1}{2} \rceil + 6.$$

Combining these two lemmas, we have

**Theorem 4.4.** *If  $G$  is a planar graph with maximum degree  $\Delta$ , then*

$$q_1(G) \leq 3 \lceil \frac{\Delta+1}{2} \rceil + 18. \tag{4.2}$$

Now we give an improvement of the above results.

**Lemma 4.7** ( [34]). *If  $G$  is a planar graph with maximum degree  $\Delta \geq 2$ , then*

$$\lambda_1(G) \leq \sqrt{8(\Delta - 2)} + 2\sqrt{3}.$$

**Lemma 4.8** ([41]). *If  $G$  is a graph with maximum degree  $\Delta$ , then  $q_1(G) \leq \Delta + \lambda_1(G)$ .*

One can deduce the following result directly from the above two lemmas.

**Corollary 4.3.** *If  $G$  is a planar graph with maximum degree  $\Delta \geq 2$ , then*

$$q_1(G) \leq \Delta + \sqrt{8(\Delta - 2)} + 2\sqrt{3}. \quad (4.3)$$

Simple deduction shows that the bound in (4.3) is better than that in (4.2) and the bound in (4.2) is better than that in (4.1) when  $\Delta$  is large enough.

## 4.2 The Laplacian and signless Laplacian coefficient of a graph

In this section, we provide a combinatorial expression for the fifth coefficients of the Laplacian and the signless Laplacian characteristic polynomial of a graph. As in Chapter 1, for a graph  $G$ , let the Laplacian and the signless Laplacian characteristic polynomial of  $G$  be

$$\Phi_{L(G)}(x) = \det(x\mathbf{I} - L(G)) = \sum_{i=0}^n \alpha_i x^{n-i}$$

and

$$\Phi_{Q(G)}(x) = \det(x\mathbf{I} - Q(G)) = \sum_{i=0}^n \beta_i x^{n-i},$$

respectively.

In 2002, C.S. Oliveira gave the formulas for the first four coefficients of the Laplacian characteristic polynomial of a graph (see [54]). And D. Cvetković gave the first three coefficients of the signless Laplacian characteristic polynomial of a graph (see [23]). In [72], J.F. Wang provided the fourth coefficient of the signless Laplacian characteristic polynomial of a graph. Furthermore, these coefficients were used to discuss the Laplacian and signless Laplacian characterizations of two kinds of graphs,  $\infty$ -graphs and 3-rose graphs (see [73, 74]). In this section, we study the fifth coefficients of these two characteristic polynomials.

### 4.2.1 The Laplacian coefficient

Given a graph  $G$ , Laplacian coefficients  $\alpha_i$  can be expressed in terms of subtree structures of  $G$  using the following result by A.K. Kelmans.

**Theorem 4.5** ([48]). *Let  $F$  be a spanning forest of a graph  $G$  with components  $T_i$ ,  $i \in \{1, 2, \dots, k\}$ , having  $n_i$  vertices each, and let  $\gamma(F) = \prod_{i=1}^k n_i$ . Then the Laplacian coefficient  $\alpha_{n-k}$  of  $G$  is given by*

$$(-1)^{n-k} \alpha_{n-k} = \sum_{F \in \mathcal{F}_k} \gamma(F),$$

where  $\mathcal{F}_k$  is the set of all spanning forests of  $G$  with exactly  $k$  components.

Using Theorem 4.5, it is easy to see that  $\alpha_0 = 1$  and  $\alpha_1 = -2m$ . In addition, C.S. Oliveira gave the third and the fourth Laplacian coefficients as follows.

**Theorem 4.6** ([54]). *Let  $G$  be a simple graph of order  $n$  and size  $m$  and  $(d_1, d_2, \dots, d_n)$  be its degree sequence. Then*

$$\alpha_2 = 2m^2 - m - \frac{1}{2} \sum_{i=1}^n d_i^2,$$

and

$$\alpha_3 = \frac{1}{3} \left( -4m^3 + 6m^2 + 3(m-1) \sum_{i=1}^n d_i^2 - \sum_{i=1}^n d_i^3 + \text{Tr}(A^3(G)) \right).$$

By Theorem 1.8, we have  $\text{Tr}(A^3(G)) = 6n_3(G)$ , where  $n_3(G)$  is the number of  $C_3$  in  $G$ . Thus from Theorem 4.6, we also have

$$\alpha_3 = \frac{1}{3} \left( -4m^3 + 6m^2 + 3(m-1) \sum_{i=1}^n d_i^2 - \sum_{i=1}^n d_i^3 + 6n_3(G) \right). \quad (4.4)$$

Just as C.S. Oliveira pointed that in order to find the third Laplacian coefficient, all one needs to do is to count the number of  $H_2$ -spanning trees which is a spanning graph with only one component isomorphic to  $P_3$  and  $n-3$  components isomorphic to  $K_1$ . However, determining  $\alpha_4$  is not that easy. In order to find the fifth Laplacian coefficient, we need the following result.



**Lemma 4.9** ([78]). Let  $M \in \mathbf{M}_n(\mathbb{C})$  be a matrix with characteristic polynomial

$$\Phi_M(x) = \det(x\mathbf{I} - M) = x^n + \sum_{i=1}^n a_i x^{n-i},$$

and  $s_k = \text{Tr}(M^k)$ . Then the coefficients of  $\Phi_M(x)$  satisfy

$$ka_k = -s_k - a_1 s_{k-1} - a_2 s_{k-2} - \cdots - a_{k-1} s_1, \quad k \in \{1, 2, \dots, n\}.$$

In the following, we will give a simpler proof of Theorem 4.6. Furthermore, we will provide the fifth Laplacian coefficient.

**Theorem 4.7.** Let  $G$  be a simple graph of order  $n$  and size  $m$  and  $(d_1, d_2, \dots, d_n)$  be its degree sequence. Then the fifth Laplacian coefficient

$$\begin{aligned} \alpha_4 = & -\frac{1}{4} \sum_{i=1}^n d_i^4 + \left(\frac{2m}{3} - 1\right) \sum_{i=1}^n d_i^3 + \frac{1}{8} \left(\sum_{i=1}^n d_i^2\right)^2 - \frac{1}{2} (2m^2 - 5m + 1) \sum_{i=1}^n d_i^2 \\ & - \sum_{v_i v_j \in E(G)} d_i d_j + 2 \sum_{i=1}^n d_i t_3(v_i) - 2n_4 - 4mn_3 \\ & + \frac{2}{3} m^4 - 2m^3 + \frac{1}{2} m^2 + \frac{1}{2} m, \end{aligned} \quad (4.5)$$

where  $t_3(v_i)$  denotes the number of  $C_3$  in  $G$  through the vertex  $v_i$ , and  $n_3$  and  $n_4$  denote the numbers of  $C_3$  and  $C_4$  in  $G$ , respectively.

*Proof.* Let  $s_k = \text{Tr}(L^k(G))$  in Lemma 4.9. It is easy to see that  $s_1 = 2m$ . Thus from Lemma 4.9 we have  $\alpha_1 = -2m$ . In the following, we simply denote  $D(G)$  and  $A(G)$  as  $D$  and  $A$ , respectively. By direct calculation, we obtain

$$(D - A)^2 = D^2 - DA - AD + A^2, \quad (4.6)$$

$$(D - A)^3 = D^3 - D^2A - DAD - AD^2 + DA^2 + ADA + A^2D - A^3, \quad (4.7)$$

$$\begin{aligned} (D - A)^4 = & D^4 - D^3A - D^2AD - DAD^2 + D^2A^2 + DA^2D \\ & + DADA - DA^3 - AD^3 + AD^2A + ADAD - ADA^2 \\ & + A^2D^2 - A^2DA - A^3D + A^4. \end{aligned} \quad (4.8)$$

Since

$$\text{Tr}(D^2) = \sum_{i=1}^n d_i^2, \quad \text{Tr}(DA) = \text{Tr}(AD) = 0, \quad \text{Tr}(A^2) = \sum_{i=1}^n d_i = 2m,$$

from (4.6), we have

$$s_2 = \sum_{i=1}^n d_i^2 + 2m.$$

By Lemma 4.9, we obtain

$$\alpha_2 = 2m^2 - m - \frac{1}{2} \sum_{i=1}^n d_i^2.$$

Note that

$$\begin{aligned} \text{Tr}(D^3) &= \sum_{i=1}^n d_i^3, \\ \text{Tr}(D^2A) &= \text{Tr}(DAD) = \text{Tr}(AD^2) = 0, \\ \text{Tr}(DA^2) &= \text{Tr}(ADA) = \text{Tr}(A^2D) = \sum_{i=1}^n d_i^2, \\ \text{Tr}(A^3) &= 6n_3. \end{aligned}$$

From (4.7), we have

$$s_3 = \sum_{i=1}^n d_i^3 + 3 \sum_{i=1}^n d_i^2 - 6n_3.$$

By Lemma 4.9 again, we can get

$$\alpha_3 = \frac{1}{3} \left( -4m^3 + 6m^2 + 3(m-1) \sum_{i=1}^n d_i^2 - \sum_{i=1}^n d_i^3 + 6n_3(G) \right).$$

By some calculations, we have

$$\begin{aligned} \text{Tr}(D^4) &= \sum_{i=1}^n d_i^4, \\ \text{Tr}(D^3A) &= \text{Tr}(D^2AD) = \text{Tr}(DAD^2) = \text{Tr}(AD^3) = 0, \\ \text{Tr}(D^2A^2) &= \text{Tr}(DA^2D) = \text{Tr}(AD^2A) = \text{Tr}(A^2D^2) = \sum_{i=1}^n d_i^3, \\ \text{Tr}(DADA) &= \text{Tr}(ADAD) = 2 \sum_{v_i v_j \in E(G)} d_i d_j, \\ \text{Tr}(DA^3) &= \text{Tr}(ADA^2) = \text{Tr}(A^2DA) = \text{Tr}(A^3D) = 2 \sum_{i=1}^n d_i t_3(v_i), \\ \text{Tr}(A^4) &= 8n_4 + 2 \sum_{i=1}^n d_i^2 - 2m. \end{aligned}$$

Combining with (4.8), we have

$$s_4 = \sum_{i=1}^n d_i^4 + 4 \sum_{i=1}^n d_i^3 + 4 \sum_{v_i v_j \in E(G)} d_i d_j - 8 \sum_{i=1}^n d_i t_3(v_i) + 8n_4 + 2 \sum_{i=1}^n d_i^2 - 2m.$$

Therefore, by Lemma 4.9, (4.5) holds.  $\square$

## 4.2.2 The signless Laplacian coefficient

Given a graph  $G$ , a spanning subgraph of  $G$  whose components are trees or odd-unicyclic graphs is called a *TU-subgraph* of  $G$ . If  $H$  is a *TU-subgraph* of  $G$  consisting of  $c$  unicyclic graphs and trees  $T_1, T_2, \dots, T_s$ , then we define the quantity

$$W(H) = 4^c \prod_{i=1}^s (1 + |E(T_i)|)$$

as the weight of  $H$ . In ([23]), D. Cvetković expressed the signless Laplacian coefficients by the weight of *TU-subgraphs* of  $G$ , and they proved the following result.

**Theorem 4.8** ([23]). *Let  $\mathcal{H}_i$  be the set of all *TU-subgraphs* of  $G$  with  $i$  edges. We have  $\beta_0 = 1$  and, for each  $i \in \{1, 2, \dots, n\}$ ,*

$$\beta_i = \sum_{H \in \mathcal{H}_i} (-1)^i W(H).$$

By using the above result, D. Cvetković and J.F. Wang obtained the first three and the fourth signless Laplacian coefficients of a graph, respectively.

**Theorem 4.9** ([23]). *Let  $G$  be a simple graph of order  $n$  and size  $m$  and  $(d_1, d_2, \dots, d_n)$  be its degree sequence. Then*

$$\beta_0 = 1, \quad \beta_1 = -2m, \quad \beta_2 = 2m^2 - m - \frac{1}{2} \sum_{i=1}^n d_i^2.$$

**Theorem 4.10** ([72]). *Let  $G$  be a simple graph of order  $n$  and size  $m$  and  $(d_1, d_2, \dots, d_n)$  be its degree sequence. Then*

$$\beta_3 = \frac{1}{3} \left( -4m^3 + 6m^2 + 3(m-1) \sum_{i=1}^n d_i^2 - \sum_{i=1}^n d_i^3 - 6n_3 \right).$$

Now we can give a simpler proof of Theorem 4.9 and 4.10. In addition, we find the fifth signless Laplacian coefficient.

**Theorem 4.11.** *Let  $G$  be a simple graph of order  $n$  and size  $m$  and  $(d_1, d_2, \dots, d_n)$  be its degree sequence. Then the fifth signless Laplacian coefficient*

$$\begin{aligned} \beta_4 = & -\frac{1}{4} \sum_{i=1}^n d_i^4 + \left(\frac{2m}{3} - 1\right) \sum_{i=1}^n d_i^3 + \frac{1}{8} \left(\sum_{i=1}^n d_i^2\right)^2 - \frac{1}{2} (2m^2 - 5m + 1) \sum_{i=1}^n d_i^2 \\ & - \sum_{v_i v_j \in E(G)} d_i d_j - 2 \sum_{i=1}^n d_i t_3(v_i) - 2n_4 + 4mn_3 \\ & + \frac{2}{3} m^4 - 2m^3 + \frac{1}{2} m^2 + \frac{1}{2} m. \end{aligned} \quad (4.9)$$

*Proof.* Let  $s_k = \text{Tr}(Q^k(G))$  in Lemma 4.9. It is easy to have

$$\begin{aligned} (D + A)^2 &= D^2 + DA + AD + A^2, \\ (D + A)^3 &= D^3 + D^2A + DAD + AD^2 + DA^2 + ADA + A^2D + A^3, \\ (D + A)^4 &= D^4 + D^3A + D^2AD + DAD^2 + D^2A^2 + DA^2D \\ &\quad + DADA + DA^3 + AD^3 + AD^2A + ADAD + ADA^2 \\ &\quad + A^2D^2 + A^2DA + A^3D + A^4. \end{aligned}$$

From the proof of Theorem 4.7, we have

$$s_1 = 2m, \quad s_2 = \sum_{i=1}^n d_i^2 + 2m, \quad s_3 = \sum_{i=1}^n d_i^3 + 3 \sum_{i=1}^n d_i^2 + 6n_3,$$

and

$$s_4 = \sum_{i=1}^n d_i^4 + 4 \sum_{i=1}^n d_i^3 + 4 \sum_{v_i v_j \in E(G)} d_i d_j + 8 \sum_{i=1}^n d_i t_3(v_i) + 8n_4 + 2 \sum_{i=1}^n d_i^2 + 2m.$$

Using Lemma 4.9, we obtain

$$\begin{aligned} \beta_1 &= -2m, \quad \beta_2 = 2m^2 - m - \frac{1}{2} \sum_{i=1}^n d_i^2, \\ \beta_3 &= \frac{1}{3} \left( -4m^3 + 6m^2 + 3(m-1) \sum_{i=1}^n d_i^2 - \sum_{i=1}^n d_i^3 - 6n_3 \right), \end{aligned}$$

and our result (4.9). □

# Chapter 5

## Conclusion and future work

In this thesis, we mainly study the structural properties of the graphs whose spectral radius is maximum. Also, we obtain some upper bounds on the signless Laplacian spectral radii of graphs. We summarize the details about the results obtained in this thesis and introduce the direction of the future research.

### 5.1 Summary of the thesis

In Chapter 2, we focused on the  $k$ -connected graphs with given diameter. When  $k = 1$ , P. Hansen and D. Stevanović [42] and E.R. van Dam [28] determined the graphs with given diameter whose spectral radius is maximum, independently. We generalized their results to  $k$ -connected graphs using the properties of diameter critical graphs and graph transformation.

In Chapter 3, we mainly studied how close  $q_1(G)$  and  $2\Delta(G)$  can be when  $G$  is an irregular graph (they are the same when  $G$  is regular). We gave a new lower bound on  $2\Delta(G) - q_1(G)$  when  $G$  is a  $k$ -connected irregular graph. Since  $\mu_1(G) \leq q_1(G)$ , this lower bound can also be a lower bound on  $2\Delta(G) - \mu_1(G)$ . Moreover, we studied the signless Laplacian spectral radius of a subgraph and improved some known results.

In Chapter 4, we provided some other results. Firstly, we obtained a relationship between the number of semi-edge walks of a connected graph and the number of walks

of two auxiliary graphs. Using this relationship and combining the decomposition of a planar graph, we gave upper bounds on the signless Laplacian spectral radii of connected graphs and planar graphs, respectively. For each planar graph, we also used the linear 2-arboricity to determine its signless Laplacian spectral radius. In addition, we also studied the Laplacian and the signless Laplacian coefficients of a graph and provided a combinatorial expression for the fifth coefficients of the Laplacian and the signless Laplacian characteristic polynomial of a graph.

## 5.2 Future research

Besides the results mentioned in this thesis, there are still a lot of problems needed to be solved.

The problem concerning the spectral radii of graphs that Brualdi and Solheid [9] proposed belongs to the extremal graph theory which deals with problems of determining extremal values or extremal graphs for a given graph invariant in a given set of graphs  $\mathcal{G}$ . In Chapter 2, we solved the problem in one given set of graphs. There are still many sets of graphs in which the problems have not been solved. For instance, which graphs have the maximum or the minimum spectral radius when  $\mathcal{G}$  is the set of connected graphs of order  $n$  with the independence number  $\alpha$  (see [33]). And which graphs have the maximum or the minimum spectral radius when  $\mathcal{G}$  is the set of connected graphs of order  $n$  with the domination number  $\gamma$  (see [65]). Also, what is the solution of this problem when  $\mathcal{G}$  is the set of connected graphs of order  $n$  and size  $m$ .

For the signless Laplacian spectral radius, there are also a lot of problems. In Chapter 3, we gave a lower bound on  $2\Delta(G) - q_1(G)$ . But this bound is not tight which means we can improve the result by some new methods. Besides, not all the conjectures for the signless Laplacian matrix proposed by P. Hansen have been solved (see [41]). From [42] (or [28]) and [71], we know that there is a graph attaining

the maximum spectral radius and the maximum signless Laplacian spectral radius simultaneously. By some known results, we propose the following conjecture.

**Conjecture 5.1.** Let  $G_1$  and  $G_2$  be connected graphs. Then  $\lambda_1(G_1) \geq \lambda_1(G_2)$  if and only if  $q_1(G_1) \geq q_1(G_2)$ .

If this conjecture is proved, then we can generalize the result for the signless Laplacian spectral radius in [71] as in Chapter 2. Hence, we can solve the problem proposed by Brualdi and Solheid for the spectral radius and the signless Laplacian spectral radius simultaneously.

In the future, we will focus on the following aspects of graph spectral theory:

- (a) Keep studying the the problem proposed by Brualdi and Solheid for other graphs.
- (b) Find a new lower bound on  $2\Delta(G) - q_1(G)$  which can improve the results in Chapter 3.
- (c) Prove or disprove Conjecture 5.1.

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