CERTAIN ASPECTS OF SPECTRA OF GRAPHS

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CERTIFICATE

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This is to certify that the thesis entitled " **CERTAIN ASPECTS OF SPECTRA OF GRAPHS** " embodies the results of independent research works carried out by Mr. Kumud Chandra Nath, M.Sc., under my supervision and guidance. Neither the thesis nor any part thereof was previously submitted to this University or any other University / Institution for any research degree.

Mr. Nath fulfils the requirements of the regulations relating to the nature and prescribed period of research work for the award of Doctor of Philosophy of the Gauhati University. He has also published a number of research papers in different standard journals.

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DECLARATION

I do hereby declare that this thesis is the result of my own research work which has been carried out under the guidance and supervision of Dr. T. K. Dutta, Professor, Department of Mathematics, G.U. Also, I would like to declare that neither the thesis nor any part thereof has been submitted in this university or any other university / Institution for a research degree.

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Date : 04/05/2012

Place : Guwahati

DEDICATED

To

My Parents

&

All my respected

Teachers

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ABSTRACT

Keywords. Adjacency matrix, Singularity, Spectrum of a graph, Spectral radius of a graph, Energy of a graph, Distance matrix, Distance spectral radius.

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Algebraic graph theory deals with the interrelation between Graph Theory and Algebra. Results of Algebra are used to solve problems in Graph Theory and vice-versa. Some of the important problems in algebraic graph theory are Matrix completion problems, minimum rank problems and problems in spectra of graphs. Spectral graph theory is the study of relations between the structure of a graph and the spectra of certain matrices associated to the graph. The associated matrices include the adjacency matrix, the distance matrix and their normalized forms. During our literature survey, we noticed some conspicuous gaps between known results on spectra of graphs. For example, the complete classification of all singular graphs was not known. We have tried to fill up certain gaps.

This thesis is the outcome of our study of the spectrum of the adjacency matrix and the distance matrix of a graph and its relation to the structure of the graph. It contains seven chapters. Overview of the thesis is as given below:

In the first chapter, we have tried to introduce Graph terminologies. This chapter is an introduction to our investigation and subsequent findings.

In the second chapter, we derive a sufficient condition for a graph to be singular in terms of its graph properties. Moreover, we also derived some important results in this direction.

In the third chapter, we establish a necessary and sufficient condition for a graph G to be singular. Further, we characterize the nullity of a class of graphs.

In the fourth chapter, we have found the graph with maximal adjacency spectral radius in a class of polycyclic graphs.

In the fifth chapter, we established ordering of graphs in terms of their energies in the class of unicyclic graphs with independence number $2, 3$, respectively.

In the sixth chapter, we study the distance matrix of a graph and obtained a graph transformations which effects in the distance spectral radius for a special class of simple graphs. Also, we have determined the graphs with extremal distance spectral radius in the class of tree like graphs.

In the seventh chapter, we have proposed some open problems for future investigation.

Contents

Chapter 1

Introduction

Algebraic graph theory studies the interrelations between graph theory and algebra. Results of algebra are used to solve problems in graph theory and that of graph theory are used to solve problems in algebra. Some of the important problem in algebraic graph theory are Matrix completion problems, minimum rank problems and problems in spectra of graphs. Spectral Graph Theory is the study of relations between the structure of a graph and the spectra of certain matrices associated to the graph. The associated matrices include the adjacency matrix, the Laplacian matrix, the distance matrix and their normalized forms.

This thesis is the outcome of our study of the spectrum of the adjacency matrix and the distance matrix of a graph and its relation to the structure of the graph. During our literature survey, we noticed some conspicuous gaps between the known results on spectra of graphs. For example, the complete classification of all singular graphs was not known. This thesis is intended to fill up some of these gaps. We also try to answer certain recent questions on the distance matrix of a graph.

1.1 Graph terminologies

By a graph G we mean a finite set of vertices $V(G)$ and a set of edges $E(G)$ consisting of distinct, unordered pairs of vertices of $V(G)$. We only consider simple undirected graph, i.e., graphs without loops and parallel edges. By $|G|$ (i.e., the order of G) we mean the number of vertices in $V(G)$, and $d(v)$ denotes the degree of a vertex v in G. For two vertices u and v in G, d_{uv} denotes the distance (the length of a shortest path between u and v) between u and v. We use the standard notations C_n, K_n, P_n and S_n to denote the cycle, the complete graph, the path and the star, respectively, on n vertices. For some n, the complement of K_n (i.e., a graph having no edge) is called an *empty* graph.

If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two graphs on disjoint sets of m and n vertices, respectively, then their union is the graph $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. A *$k$-matching* M in G is a disjoint union of k paths of length one. If $e_1, e_2, \ldots, e_k$ are the edges (components) of a k-matching M, then we write $M = \{e_1, e_2, \ldots, e_k\}$. If the order of G is $2k$, then a k-matching of G is called a *perfect matching* of G.

A tree is a connected graph without a cycle, and a unicyclic graph is connected and has exactly one cycle. The cycle of a unicyclic graph G will always be denoted by C. Then, the number of vertices on C is called the *girth* of G. A tree (resp. a unicyclic graph) on n vertices has exactly $n - 1$ (resp. n) edges in it.

If S is a set of vertices and edges in a graph G, then by $G - S$ we mean the graph obtained from G by deleting all the elements of S. It is understood that when a vertex is deleted, all edges incident with it are deleted as well, but when an edge is deleted, the vertices incident with it are not. If H is an induced subgraph of G and v is a vertex not in $V(H)$, then by $H+v$ we mean the subgraph induced by the vertices in $V(H) \cup \{v\}$.

We say that a graph γ is *attached* at a vertex v of G to mean that a new graph is obtained by joining v and a vertex of γ by an edge. With this notion, a unicyclic graph is seen as a graph obtained by attaching a finite number of trees at vertices of cycle. Moreover, if we attach any tree at any vertex of a unicyclic graph, the resultant graph will be unicyclic.

If G is a graph and $v \in V(G)$, then a component of $G-v$ not containing any vertex of C is called a *tree-branch* of G at v. In particular, the tree-branches at a vertex on C are the trees attached to it. We say that a tree-branch is *odd (even)* if its order is odd (even).

1.2 The adjacency matrix of a graph

If $V(G) = \{v_1, v_2, \ldots, v_n\}$, then the *adjacency matrix* of G, is defined to be $A(G) = [a_{ij}]_n$, where

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

Clearly, $A(G)$ is a non-negative real symmetric matrix.

Example 1.2.1. *Consider the graph G_1 of Figure 1.1. Then*

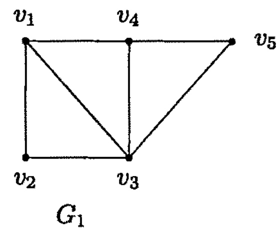


Figure 1.1:

$$A(G_1) = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

The characteristic polynomial of $A(G)$,

$$P(A(G);x) = \det(xI - A(G))$$

where I is the unit matrix of order n, is called the *characteristic polynomial* of G and is denoted by $P(G;x)$. Since $A(G)$ is a real symmetric matrix, all its eigenvalues are real and their algebraic multiplicities equal their geometric multiplicities. The *spectrum of* G is defined as

$$\sigma(G) = (\lambda_1(G), \lambda_2(G), \cdots, \lambda_n(G)),$$

where $\lambda_i(G)$ are the eigenvalues of $A(G)$. Throughout this thesis we will be using that $\lambda_i(G)$ are written in descending order, that is,

$$\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G).$$

The algebraic multiplicity of the eigenvalue 0 in $\sigma(G)$ is called the *nullity* of G and is denoted by $\eta(G)$. A graph G is said to be *singular* (resp. *nonsingular*) if $A(G)$ is singular (resp. nonsingular). It is clear that G is singular if and only if G has a connected component which is singular. In particular, if G has an isolated vertex, then G is singular.

1.3 Singularity of a graph

The problem of characterizing a singular graph by its graph theoretic properties is a classical problem which was first posed by Collatz and Sinogowitz [13] almost fifty years back. The search for such a characterization was important in many disciplines of science which use spectra of graphs. For example, the occurrence of a zero eigenvalue in the spectrum of a graph (especially a bipartite graph) associated to the structure of a molecule (like that of a hydrocarbon) indicates chemical instability of the molecule. Several partial answers to this central question are known for long, but a complete characterization of a general singular graph by its graph properties is still not known.

Theorem 1.3.1. [16] *If v is a pendent vertex of a graph G and u is the vertex in G adjacent to v, then, $\eta(G) = \eta(G - u - v)$.*

Theorem 1.3.2. [17] *Let G_1 and G_2 be bipartite graphs with $\eta(G_1) = 0$. If G is obtained by joining an arbitrary vertex of G_1 by an edge with an arbitrary vertex of G_2, then $\eta(G) = \eta(G_2)$.*

Theorem 1.3.3. [16] *If q is the maximum number of mutually nonadjacent edges in a tree T having n vertices, then $\eta(T) = n - 2q$. In particular, a tree is nonsingular if and only if it has a perfect matching.*

Theorem 1.3.3 was generalized to the case of bipartite graphs not containing cycles of lengths $4s$ $(s = 1, 2, \ldots)$ by Cvetković *et al.* [17] in 1972. However, there has not been much development on the problem in this line for last several decades, though the problem is still relevant. For some recent developments on singularity of graphs in very specific situations, see [52, 55, 49, 50].

In Chapter 2, we derive a sufficient condition for a graph to be singular in terms of its graph properties. Moreover, we also derived some important result in this direction.

In Chapter 3, we give a necessary and sufficient condition for graph to be singular. Using our results we completely determined the nullity of θ-graphs.

1.4 Adjacency spectral radius

The largest eigenvalue $\lambda_1(G)$ is known as the *spectral radius* of G. If G is connected, then $A(G)$ is irreducible, and by the Perron-Frobenius theory, $\lambda_1(G)$ is simple and is afforded by a positive eigenvector, called the *Perron vector.*

The spectrum of a graph arises in a variety of applications in organic chemistry, where the energy levels of certain molecules (such as polycyclic hydrocarbons) are essentially the eigenvalues of the graph of the molecule [53]. It is well known that the spectrum of a graph does provide a wealth of information about the graph.

The spectral radius of a graph is an important invariant related to structure. The investigation of spectral radii of graphs is an important topic in graph spectra, and it is directly related with several parameters (the chromatic number, the independence number and the clique number, etc.). For results on the spectral radius of graphs one may refer [8, 9, 7, 11, 12, 15, 30, 31, 33, 61, 62, 64] and the references therein. The problem concerning graphs with maximal or minimal spectral radii of a given class of graphs has been studied extensively. The spectral radii of trees, unicyclic graphs and bicyclic graphs have been studied by many authors [11, 12, 31, 33, 61, 62]. Guo [30] determined the graphs with the largest spectral radii among all the unicyclic and bicyclic graphs with n vertices and k-pendant vertices respectively. The cacti are a class of polycyclic graphs in which any two of its cycles have at most one common vertex and the spectral radius of cactus has been studied by many authors [7, 61]. Motivated by these facts we will study the spectral radius of a class of polycyclic graphs in Chapter 4.

1.5 Energy of a graph

Spectra of graphs has important applications to fields like quantum chemistry. Though the graphs which are of interest in chemistry belong to a rather restricted class of graphs, this class is sufficiently large and many relevant nontrivial questions can be posed which are even difficult in Graph Theory. The graphs that the chemists are interested in are all connected, planar and in most of the cases have restrictions on the vertex degrees. A cycle of length three seldom appear in chemical graphs, but cycles of higher length can do. Regular graphs also appear very rarely.

In 1931, Hückel [37] suggested a discrete linear model for the highly nonlinear analytic theory of energy of molecules in Quantum theory, whereby a connection between the energy of hydrocarbon molecules and spectra of the associated graphs was observed. The theory is known as *Hückel Molecular Orbital (HMO) Theory* in quantum Chemistry. In certain situations, the eigenvalues of the graph associated to the structure of a molecule can be interpreted as the energy levels of an electron in the molecule. In HMO, the connection between the so-called *total π-electron energy* is associated to the sum of the magnitudes of the eigenvalues of the associated molecular graph. A brief mathematical formulation of the theory can be seen in Section 8.1 of [15]. This prompted Gutman [23] in 1978 to define energy of a graph as follows: If G is a graph of order n with eigenvalues λ_i, where $i = 1, 2, \cdots, n$, then the *energy* of G is

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

In the literature, there is no standard algebraic expression (formula) readily available for the sum of the magnitudes of the roots of a polynomial in terms of its coefficients. Hence finding energy of a graph without actually obtaining the spectra is a non-trivial task. The best-known formula for energy of a graph G with characteristic polynomial $P(G; x)$ was obtained by Coulson in 1940, and is in the form of an integral:

$$\begin{aligned} E(G) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - \frac{ix\phi'(G, ix)}{\phi(G, ix)} \right] dx \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - x\frac{d}{dx} \ln \phi(G, ix) \right] dx. \end{aligned} \tag{1.5.1}$$

The formula (1.5.1) is known as the *Coulson's formula for energy.*

If

$$P(G;x) = \sum_{i=0}^{n} a_i x^{n-i},$$

then (1.5.1) gives

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{dx}{x^2} \ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j+1}x^{2j+1}\right)^2\right].$$

The above formula gives a way to compare energy of certain graphs.

Some experimental studies in Quantum Chemistry had pointed towards a simple regularity that the energy of a graph increases with the increase of the number of vertices (say n) and edges (say m). A famous approximation, quantifying the above regularity, is the McClelland formula [46]

$$E(G) \approx a\sqrt{2mn};\ a \approx 0.9,$$

which was found chemically highly satisfactory (see [23] for details). A naive extension of this rule to all graphs resulted in the conjecture by Gutman [23] in 1978 that among n-vertex graphs, the complete graph K_n has maximal energy. This conjecture was disproved first by Chris Godsil in the early 1980s, and there exist graphs whose energy exceeds $E(K_n)$. A graph G, such that $E(G) \geq E(K_n)$, is called *hyperenergetic*. There exist hyperenergetic graphs on n vertices, for every $n \geq 9$. Walikar et al. [60] proved in 1998 that the line graph of K_n is hyperenergetic, for $n \geq 5$.

Though several lower and upper bounds for $E(G)$ were known, a very simple and elegant bound has been observed only very recently. Gutman [24] has shown in 2000 that

$$2\sqrt{m} \leq E(G) \leq 2m,$$

and, if G has no isolated vertex, then

$$E(G) \leq 2\sqrt{n-1}. \tag{1.5.2}$$

Moreover, the bound (1.5.2) is sharp if and only if G is the n-vertex star S_n.

The following bounds for energy is known for long as *McCelland inequalities*, and was obtained by McCelland [46] in 1971.

$$\sqrt{2m + n(n-1)|\det A(G)|^{\frac{2}{n}}} \leq E(G) \leq \sqrt{2mn}.$$

In 1978, Gutman [23] had shown that

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} = B_1.$$

For a k-regular graph G, $k = \frac{2m}{n}$, and we get, as an immediate consequence of (1.5.3),

$$E(G) \leq k + \sqrt{k(n-1)(n-k)} = B_2.$$

There are regular graphs (all complete graphs for example) for which the equality in (1.5.2) holds. In other words, the bounds B_1 and B_2 are both sharp. Recently, using (1.5.2) Balakrishnan [2] has shown that given $\epsilon > 0$, there exists a k-regular graph G of order n with $k < n-1$ and $\frac{E(G)}{B_2} < \epsilon$, for infinitely many values of n.

Koolen *et al.* [40] has improved the upper bound (1.5.3) for bipartite graphs in 2003 and proved that for such graphs

$$E(G) \leq 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left[2m - 2\left(\frac{2m}{n}\right)^2\right]}. \tag{1.5.3}$$

Moreover, they found an upper bound without involving of m for the energy of bipartite graphs,

$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{2} + \sqrt{n}), \tag{1.5.4}$$

and characterized the graphs for which (1.5.3) and (1.5.4) are sharp.

Graphs with extremal energies in certain classes of graphs have been studied by several authors and we present below some of the known results.

Graphs with extremal energy have been determined for n-vertex trees [22, 41, 66] and n-vertex trees with perfect matchings [65]. For a given positive integer d, the tree with the minimal energy having diameter at least d is determined in [36]. In [63], trees with the smallest and the second smallest energies in the class of trees having matchings of a given size are characterized.

Let S_n^3 be the graph obtained from the star graph S_n by adding an edge. For $n \geq 6$, it is proved in [35] that S_n^3 is the unique graph having minimal energy among all unicyclic graphs of order n.

Caporossi et al. [10] conjectured in 1999 that among all n-vertex unicyclic graphs, C_n has the maximum energy for $n \leq 7$ and $n = 9, 10, 11, 13, 15$. For other values of n the graph P_n^6 is the unicyclic graph having the maximum energy, where P_n^6 is obtained by attaching P_{n-6} to one of the vertices of C_6. In [35], Hou et al. attempted in 2002 to solve the problem, but succeeded only partially.

In Chapter 5, we give ordering of graphs in terms of their energy among all unicyclic graphs with independence number $\beta = 2, 3$.

1.6 Distance spectra of graphs

The distance between two vertices $u, v \in V$ is denoted by d_{uv} and is defined as the length of the shortest path between u and v in G. The distance matrix $D = (d_{uv})_{u,v \in V}$ is a symmetric real matrix, with real eigenvalues [15]. The *distance* *spectral radius* $\rho(G) = \rho_G$ of G is the largest eigenvalue of the distance matrix D of the graph G.

Distance energy $DE(G)$ is a newly introduced molecular graph-based analog of the total π-electron energy, and it is defined as the sum of the absolute eigenvalues of the molecular distance matrix. The distance spectra of trees and unicyclic graphs have exactly one positive eigenvalue, and therefore the distance energy for trees and unicyclic graphs is equal to the double of distance spectral radius [6, 47].

The distance spectral radius is a useful molecular descriptor in QSPR modelling, as demonstrated by Consonni and Todeschini in [14]. For more details on distance matrices and distance energy one may refer to [39, 51, 57].

Balaban et al. [1] proposed the use of $\rho(G)$ as a molecular descriptor, while in [28] it was successfully used to infer the extent of branching and model boiling points of alkanes. Recently in [68] and [69], Zhou and Trinajstić provided upper and lower bounds for $\rho(G)$ in terms of the number of vertices, Wiener index and Zagreb index. Balasubramanian in [5, 4] pointed out that the spectra of the distance matrices of many graphs such as the polyacenes, honeycomb and square lattice have exactly one positive eigenvalue, and he computed the spectrum of fullerenes C_{60} and C_{70}.

Bapat et al. in [6] showed various connections between the distance matrix $D(G)$ and the Laplacian matrix $L(G)$ of a graph. Bapat in [5, 6] calculated the determinant and inverses of the distance matrices of weighted trees and unicyclic graphs. Merris in [47] obtained an interlacing inequality involving the distance and Laplacian eigenvalues of trees.

Let $e = uv$ be an edge of the connected graph G such that $G' = G - e$ is also connected, and let D' be the distance matrix of $G - e$. The removal of e does not create shorter paths than the ones in G, and therefore, $d_{ij} \leq d'_{ij}$ for all $i, j \in V$. Moreover, $1 = d_{uv} < d'_{uv}$ and by the Perron-Frobenius theorem, one can conclude that

$$\rho(G) < \rho(G - e). \tag{1.6.1}$$

In particular, for any spanning tree T of G, we have that

$$\rho(G) \leq \rho(T). \tag{1.6.2}$$

Similarly, adding a new edge $f = st$ to G does not increase distances, while it does decrease at least one distance; the distance between s and t is one in $G + f$ and at least two in G. Again by the Perron-Frobenius theorem,

$$\rho(G + f) < \rho(G). \tag{1.6.3}$$

Inequality (1.6.3) tells us immediately that the complete graph K_n has the minimum distance spectral radius among the connected graphs on n vertices, while the inequality (1.6.2) shows that the maximum distance spectral radius will be attained for a particular tree.

G. Indulal in [39] has found sharp bounds on the distance spectral radius and the distance energy of graphs. In [38] Ilić characterized n-vertex trees with given matching number m which minimize the distance spectral radius. Liu has characterized graphs with minimal distance spectral radius in three classes of simple connected graphs with n vertices: with fixed vertex connectivity, matching number and chromatic number, respectively in [45]. Subhi and Powers in [58] proved that for $n \geq 3$ the path P_n has the maximum distance spectral radius among trees on n vertices. Stevanović and Ilić in [57] generalized this result, and proved that among trees with fixed maximum degree Δ, the broom graph has maximum distance spectral radius and proved that the star S_n is the unique graph with minimal distance spectral radius among trees on n vertices. The investigation on the spectral radius of graphs is an important topic in the theory of graph spectra. Recently, the problem of finding all graphs with maximal or minimal distance spectral radius among a class of graphs has been studied extensively.

In Chapter 6, we study the distance matrix of a graph and obtained some graph transformations which effects the distance spectral radius of graphs. Applying our transformation, we determine the graphs having maximal and minimal distance spectral radius among the tree like graphs.

Lastly, in Chapter 7, we give some open problems for future research.

Chapter 2

Singularity of graphs

In this chapter we derive some results regarding the singularity of graphs.

2.1 Introduction

Let G be a simple graph. The multiplicity of 0 as an eigenvalue of $A(G)$ is the *nullity* of G and is denoted by $\eta(G)$. For a singular graph G, the eigenvectors of $A(G)$ corresponding to the eigenvalue 0 are the *null-eigenvectors* of G and the null-space of $A(G)$ is the *null-space* of G.

We will use the following well-known results in computing the nullity of a graph.

Theorem 2.1.1. [16] *Let v be a pendent vertex of a graph G and u be the vertex in G adjacent to v. Then $\eta(G) = \eta(G - u - v)$, where $G - u - v$ is the induced subgraph of G obtained by deleting u and v.*

Theorem 2.1.2. [52] *Let G be the graph obtained by joining the vertex x of a graph G_1 to the vertex y of a graph G_2 by an edge. Then*

$$\det A(G) = \det A(G_1) \det A(G_2) - \det A(G_1 - x) \det A(G_2 - y).$$

Theorem 2.1.3. [52] *Let $P_6[1,2,3,4,5,6]$ be an induced subgraph of G with* $\deg(2) = \deg(3) = \deg(4) = \deg(5) = 2$. *If H is the graph formed from $G - \{2,3,4,5\}$ by joining vertices 1 and 6 with an edge, then* $\det A(G) = \det A(H)$.

Corollary 2.1.4. [52] *Let $C_4[1,2,3,4,1]$ be a subgraph of G, where* $\deg(1) = 2$. *If G_0 is the graph obtained from G by removing the edges $[2,3]$ and $[3,4]$, then* $\det A(G_0) = \det A(G)$.

2.2 Some useful results regarding the singularity of a graph

Let $V(G)$ and $E(G)$ denote the vertex set $\{v_1, v_2, \dots, v_n\}$ and the edge set of a graph G, respectively. The *neighborhood* of a vertex $v \in V$ in G is defined to be $N(v) = \{u \in V(G) | \ uv \in E(G)\}$. A nonzero vector $(\alpha_1, \alpha_2, \dots, \alpha_n)^t$ is a null-eigenvector of G if and only if for each $v_i \in V(G)$ we have $\sum_{v_j \in N(v_i)} \alpha_j = 0$.

Definition 2.2.1. [49] A pair V_1, V_2 of subsets of $V(G)$ is said to satisfy *property (N)* if

(a) V_1 and V_2 are nonempty and disjoint, and

(b) $\bigcup_{v \in V_1} N(v) = \bigcup_{v \in V_1} N(v)$.

Further, such a pair is said to be *minimal satisfying the property (N)* if for any pair U_1, U_2 of subsets of $V(G)$ satisfying the property (N) with $U_1 \subseteq V_1$, $U_2 \subseteq V_2$, we have $U_1 = V_1,\ U_2 = V_2$.

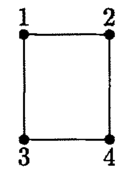


Figure 2.1: C_4

Example 2.2.2. *For the cycle C_4 in Figure 2.1, $V_1 = \{1, 2\}, V_2 = \{3, 4\}$ is a pair satisfying property (N). But V_1, V_2 is not a minimal pair as $U_1 = \{2\}$, $U_2 = \{4\}$ is a pair with property (N) and $U_1 \subset V_1$, $U_2 \subset V_2$.*

Theorem 2.2.3. [49] *Let G be a connected graph on $n \geq 2$ vertices. If G is singular, then $V(G)$ has a pair of subsets satisfying the property (N).*

Theorem 2.2.4. [49] *A unicyclic graph G is singular if and only if there is a pair of subsets V_1, V_2 of $V(G)$ satisfying the property (N).*

Definition 2.2.5. [49] A pair V_1, V_2 of subsets of $V(G)$ is said to satisfy *property (S)* if it satisfies the property (N) and for all pairs u, v in $V_i,\ i = 1, 2$, we have $N(u) \cap N(v) = \emptyset$.

Example 2.2.6. *In Figure 2.1, the cycle C_4 has $U_1 = \{2\}$, $U_2 = \{4\}$ as a pair satisfying property (S).*

Theorem 2.2.7. [49] *Let G be a graph and suppose that $V(G)$ has a pair of subsets V_1, V_2 satisfying the property (S). Then G is singular.*

Corollary 2.2.8. [49] *Let G be a graph with the pair V_1, V_2 of subsets of $V(G)$ satisfying the property (S). Let α_j be defined by*

$$\alpha_j = \begin{cases} 1 & \text{if } v_j \in V_1, \\ -1 & \text{if } v_j \in V_2, \\ 0 & \text{otherwise.} \end{cases} \tag{2.2.1}$$

Then $(\alpha_1, \alpha_2, \ldots, \alpha_n)^t$ is a null-eigenvector of G.

2.3 Singularity and determinant of a graph

The following Theorem is one of the main results of this chapter, which gives a sufficient condition for G to be singular.

Theorem 2.3.1. *Let G be a graph with a nonempty subset V_1 of $V(G)$, such that*

$$\left| \bigcup_{v \in V_1} N(v) \right| \leq |V_1| - 1.$$

Then G is singular.

Proof. Let G be a graph with a nonempty subset V_1 of $V(G)$, such that

$$\left| \bigcup_{v \in V_1} N(v) \right| \leq |V_1| - 1.$$

Let $V_1 = \{v_1, v_2, \ldots, v_p\}$. Consider the equation $\sum_{i=1}^{p} \alpha_i R_i = 0$, which is equivalent to the system of n equations

$$\sum_{i=1}^{p} \alpha_i R_{ij} = 0, \; j = 1, 2, \ldots, n. \tag{2.3.1}$$

Since at least $n - p + 1$ vertices are absent in $\bigcup_{v \in V_1} N(v)$, so at least that many equations in 2.3.1 take the form

$$\sum_{i=1}^{p} \alpha_i 0 = 0,$$

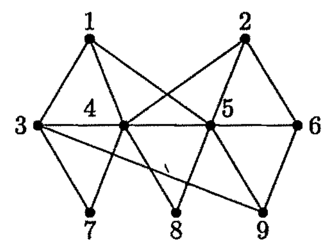
which can be omitted. Thus we are left with at most $p-1$ homogeneous equations in p variables, which have a nonzero solution. As a consequence, the rows of $A(G)$ are linearly dependent, implying that G is singular. ■

Example 2.3.2. *The graph $G_1(V_1, E_1)$ in the Figure 2.2, is singular. Since the subset $U = \{7, 8, 9, 1, 2\}$ of V_1 is such that $|U| = 5$ and*

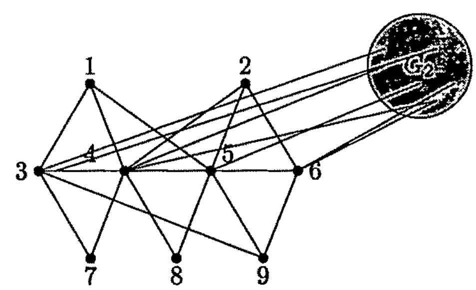
$$\left| \bigcup \{N(i) |\; i \in \{7, 8, 9, 1, 2\}\} \right| = 4.$$

We can see that G' is singular, where vertex of set G' is $V' = V_1 \cup V_2$ and edge set of G', $E' = E_1 \cup E_2 \cup E_3$ where $G_2(V_2, E_2)$ is any graph and $E_3 \subseteq \{uv |\; u \in \{3, 4, 5, 6\}, v \in V_2\}$.

Corollary 2.3.3. *Let G be a graph of order n. If there exists a subset U of V, the vertex set of G, such that U is a vertex independent set and $|U| > \frac{n}{2}$, then G is singular.*



G_1



G'

Figure 2.2: A singular graph which satisfies the condition of Theorem 2.3.1

Proof. Since U is vertex independent set, therefore

$$\begin{aligned} |\cup \{N(v)|\ v \in U\}| &\leq n - |U| \\ &< n - \frac{n}{2} \\ &= \frac{n}{2} \\ &= |U|. \end{aligned}$$

Hence G is singular. ■

Corollary 2.3.4. *Let G be a bipartite graph with bipartition V_1, V_2, such that $|V_1| \neq |V_2|$. Then G is singular.*

Corollary 2.3.5. *Let G be a bipartite graph with bipartition (Ω, Φ) and $A \subseteq \Omega$, if there exists no matching in G that covers the vertices in A then G is singular.*

Proof. By Hall's theorem, there exists at least one subset B of A such that $|N(B)| < |B|$, where $N(B)$ is the set of all vertices in Ω adjacent to a vertex in B. Therefore G is singular. ■

Corollary 2.3.6. *If in G there exists a subset V_1 of V such that*

$$\left|\bigcup_{v\in V_1} N(v)\right| = |V_1| - \lambda,$$

then $m(0) \geq \lambda$ where $m(0)$ denotes the multiplicity of zero as an eigenvalue of G.

Proof. Since $\left|\bigcup_{v\in V_1} N(v)\right| = |V_1| - \lambda$, by Theorem 2.3.1, G is singular. To get the highest order non vanishing minor of $A(G)$, we shall have to remove at least λ rows out of those represented by v in V_1. Therefore, $rank(G) \leq n - \lambda$ and so $m(0) \geq \lambda$. ■

Corollary 2.3.7. *If in G there exists an induced subgraph $X(m, f)$, such that there are no disjoint subsets V_1, V_2 of V with $\bigcup_{v\in V_1} N(v) = \bigcup_{v\in V_2} N(v)$, then $m(0) \leq n - m$.*

Proof. Let $V(X) = \{v_1, v_2, \ldots, v_m\}$. The given condition and Theorem 2.3.1 together imply that X is nonsingular. Now out of the rows of $A(G)$, at least m rows are linearly independent. Therefore $m(0) \leq n - m$. ■

Theorem 2.3.8. *If there exists a subset U of V_1 in G_1 such that*

$$|U| = \left|\bigcup_{v\in U} N(v)\right|,$$

then $\det G' = \det G_1 \det G_2$ *where G' is a graph obtained by joining a vertex x in*

$$\left(\bigcup_{v\in U} N(v)\right) - U$$

with any vertex y in any graph G_2.

Proof. By Theorem 2.1.2, we have

$$\det G' = \det G_1 \det G_2 - \det(G_1 - x) \det(G_2 - y).$$

Since $x \in \left(\bigcup_{v \in U} N(v)\right) - U$ we will have a nonempty subclass U' of V', the vertex set of $G_1 - x$, such that $|U'| > \left|\bigcup_{v \in U'} N(v)\right|$. Therefore $\det(G_1 - x) = 0$ and hence $\det G' = \det G_1 \det G_2$. ■

Theorem 2.3.9. *Let P_6 be an induced subgraph of G with* $\deg(2) = \deg(3) = \deg(4) = \deg(5) = 2$. *If there exists a subset U of V such that* $2, 3, 4, 5 \notin U$, $1 \in U$, $6 \in \bigcup_{i \in U} N(i)$ *and* $|U| = \left|\bigcup_{i \in U} N(i)\right|$, *then G is singular.*

Proof. Let H be a graph formed from $G - \{2, 3, 4, 5\}$ by joining 1 and 6 by an edge. By Theorem 2.1.3, $\det G = \det H$. Suppose $N(1) \in S$, $6 \in \bigcup_{i=1}^{p} N(i)$. Since $deg(2) = deg(3) = deg(4) = deg(5) = 2$ and $N(1) \in S$, therefore $2 \in \bigcup_{i=1}^{p} N(i)$ in G.

Again in H, $2 \notin \bigcup_{i=1}^{p} N(i)$ and 2 is replaced by 6. But, since 6 already exists in $\bigcup_{i=1}^{p} N(i)$ in G, so for H we get a nonempty subclass S' of $N(H)$ such that $|S'| > \left|\bigcup_{N(i) \in S'} N(i)\right|$.

Therefore $\det H = 0$ and so G is singular. ■

Example 2.3.10. *The graph in Figure 2.3 with $U = \{1, 7, 8, 9\}$, satisfies all the conditions of the Theorem 2.3.9 for any induced subgraph G_1, G_2 and G_3. Therefore the graph is singular.*

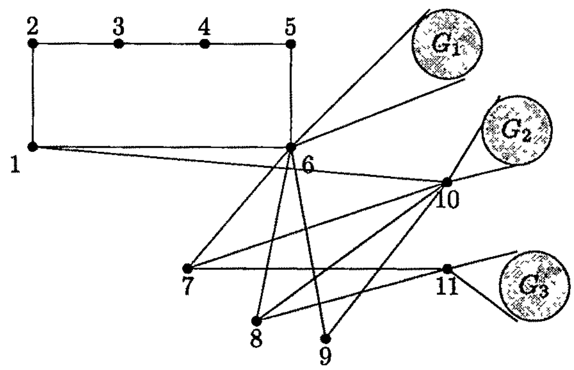
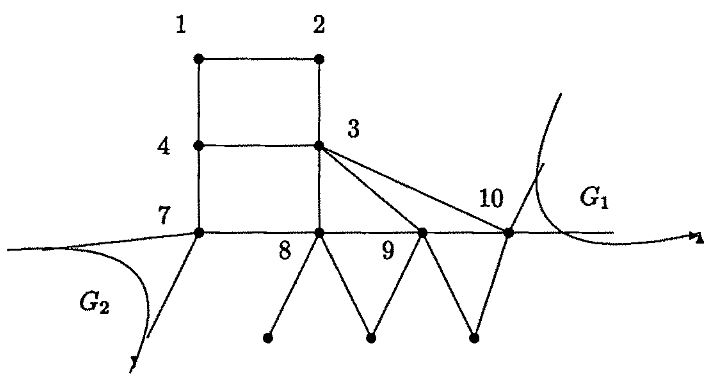


Figure 2.3: A singular graph which satisfies the condition of Theorem 2.3.9

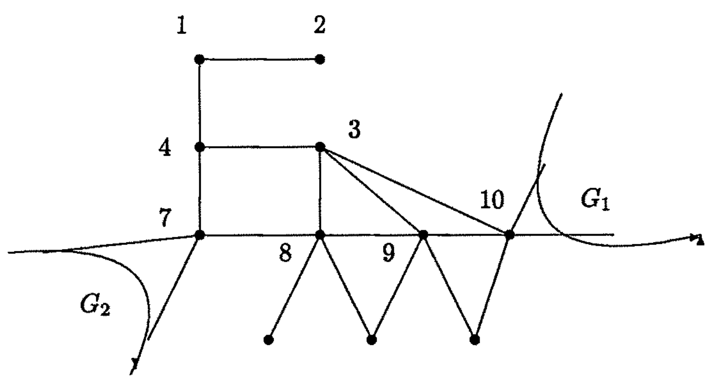
Theorem 2.3.11. *Let* $C_4 = [1,2,3,4,1]$ *be a subgraph of* G *where* $deg(1) = 2$. *If there exists a subclass* $S = \{N(1), N(2), \ldots, N(p)\}$ *of* N *such that* $3 \notin \bigcup_{i=1}^{p} N(i), i \neq 2,4; 2,4 \notin N(i), \forall\, i \neq 3$ *and* $N(1) \notin S$ *and either* $N(2), N(3) \in S$ *or* $N(3), N(4) \in S$ *and also* $|S| = \left|\bigcup_{N(i)\in S} N(i)\right| - 2$, *then* $\det G' = 0$, *where* G' *is a graph obtained from* G *by removing the edges* $[2,3]$ *and* $[3,4]$.

Proof. Let G' be the graph obtained from G by removing the edges $[2,3]$ and $[3,4]$. Therefore, by Corollary 2.1.4 $\det G = \det G'$. suppose $N(2), N(3) \in S$, since $3 \notin \bigcup_{i=1}^{p} N(i)$, $i \neq 2,4$; $2,4 \notin N(i)$, $\forall i \neq 3$ and $N(1) \notin S$ therefore $2,3,4 \in \bigcup_{N(i)\in S} N(i)$ in case of G but $2,3,4 \notin \bigcup_{N(i)\in S} N(i)$ in case of G'. Therefore we get a nonempty subclass S' of $N(G')$ in G' such that $|S'| > \left|\bigcup_{N(i)\in S'} N(i)\right|$. Therefore $\det G = 0$, $\det G' = 0$. Similarly considering $N(3), N(4) \in S$ we can show $\det G = \det G' = 0$. ∎

Example 2.3.12. *The graph* G *in Figure 2.4 satisfies the conditions of the The-*



G



G'

Figure 2.4: A graph which satisfies the conditions of the Theorem 2.3.11

orem 2.3.11 for any induced subgraph G_1 and G_2. Therefore G' is singular.

Corollary 2.3.13. *If* $\det G_1 = 0$ *or* $\det G_2 = 0$, *then* $\det G' = 0$.

Theorem 2.3.14. *If in a graph G there exist two disjoint subsets U, W of V, the vertex set of G such that $\bigcap_{v \in U} N(v) = \bigcap_{v \in W} N(v)$ and $N(v_1) \bigcup N(v_2) = V$ $\forall v_1, v_2 \in U$, $v_1 \neq v_2$ and $\forall v_1, v_2 \in W$, $v_1 \neq v_2$, then $\det \overline{G} = 0$, where $\overline{G}$ is the complement of G.*

Proof. Let us denote the neighborhood of any vertex v in $\overline{G}$ by $N'(v)$. Then

$N'(v) = \overline{N(v)}$, where $N(v)$ is the neighborhood of v in G. Now

$$\bigcap_{v\in U} N(v) = \bigcap_{v\in W} N(v)$$
$$\Rightarrow \bigcup_{v\in U} \overline{N(v)} = \bigcup_{v\in W} \overline{N(v)}$$
$$\Rightarrow \bigcup_{v\in U} N'(v) = \bigcup_{v\in W} N'(v).$$

Again

$$N(v_1)\bigcup N(v_2) = V$$

Which gives $\overline{N(v)}\bigcap\overline{N(v)} = \phi$ for all $v_1, v_2 \in U$, $v_1 \neq v_2$ and for all $v_1, v_2 \in W$, $v_1 \neq v_2$. Thus $det\overline{G} = 0$. ■

Theorem 2.3.15. *If in a graph G there exist p vertices $v_1, v_2, \ldots, v_p$ such that*

$$\left|\bigcap_{i=1}^{p} N(v_i)\right| \geq n - p + 1,$$

then $\det\overline{G} = 0$.

Proof. We have

$$\left|\bigcap_{i=1}^{p} N(v_i)\right| \geq n - p + 1$$
$$\Rightarrow \left|\overline{\bigcap_{i=1}^{p} N(v_i)}\right| \leq n - (n - p + 1)$$
$$\Rightarrow \left|\overline{\bigcup_{i=1}^{p} N(v_i)}\right| \leq (p - 1)$$
$$\Rightarrow \left|\bigcup_{i=1}^{p} N'(v_i)\right| \leq (p - 1).$$

Therefore $\det\overline{G} = 0$.

Definition 2.3.16. *The tensor product of two graphs G_1 and G_2, denoted by $G_1 \wedge G_2$, has the vertex set $V = V_1 \times V_2$ and $(u_1, v_1), (u_2, v_2) \in V$ are adjacent in $G_1 \wedge G_2$ if only if $[u_1, u_2] \in E_1$ and $[v_1, v_2] \in E_2$.*

Theorem 2.3.17. *If G is a graph such that there exists a subclass*

$$S = \{N(v_1), N(v_2), \ldots, N(v_p)\}$$

of N such that $|\bigcup_{i=1}^{p} N(v_i)| < p$, then $\det(G \wedge G_1 \wedge G_2 \wedge \ldots \wedge G_k) = 0$. For any graph G_i, $i = 1, 2, 3, \ldots, k$ the multiplicity of zero as an eigenvalue of $G' = G \wedge G_1 \wedge G_2 \wedge \ldots \wedge G_k$ is at least $\prod_{i=1}^{k} n_i$ where n_i is the number of vertices in G_i.

Proof. Let

$$S = \{N(u, u_1, u_2, \ldots, u_k) | N(u) \in S\}.$$

Then

$$|S| = p \times n_1 \times n_2 \times \ldots \times n_k.$$

Also

$$\cup_{N(x) \in S} N(x) \subseteq \{(u, u_1, \ldots, u_k), u \in \bigcup_{i=1}^{p} N(v_i)\}.$$

But

$$\left|\bigcup_{i=1}^{p} N(v_i)\right| \leq (p-1)$$

$$\Rightarrow \left|\bigcup_{N(x) \in S} N(x)\right| \leq (p-1) \times n_1 \times n_2 \ldots \times n_k = |S| - \prod_{i=1}^{k} n_i$$

Which gives

$$|S| \geq \left| \bigcup_{N(u)\in S} \right| + \prod_{i=1}^{k} n_i.$$

Therefore $\det(G \wedge G_1 \wedge G_2 \wedge \ldots \wedge G_k) = 0$ and $m(0) \geq \prod_{i=1}^{k} n_i$. ∎

Definition 2.3.18. *The total graph $T(G)$ of a graph G has the vertex set $V \cup E$ and two vertices of $T(G)$ are adjacent if one of the following holds*

(a) they are $v_i, v_j \in V$ and $[v_i, v_j] \in E$,

(b) one is $v \in V$ and the other $e \in E$ and e is incident with vertex v in G,

(c) they are $e_i, e_j \in E$ and the edges e_i, e_j are adjacent in G.

Theorem 2.3.19. *If G is singular, then there exist two disjoint subsets X and Y of the vertex set of $T(G)$ such that $\bigcup_{v\in X} N(v)$ and $\bigcup_{v\in Y} N(v)$ have some vertices in common and the remaining vertices in each of the unions are adjacent to at least one of the remaining vertices of the other union and are adjacent to exactly one of the common vertices.*

Proof. Let $\det G = 0$. Then there exist two disjoint subsets $U$and W of V, the vertex set of G such that

$$\bigcup_{v\in X} N(v) = \bigcup_{v\in Y} N(v) = \Omega(say).$$

Now consider X and Y as subsets of vertex set of $T(G)$ then $\bigcup_{v\in X} N(v) = \Omega \cup W_1$, $\bigcup_{v\in Y} N(v) = \Omega \cup W_2$ where W_1 and W_2 are the sets of edges from X to Ω and from Y to Ω respectively in G, $\left(\bigcup_{v\in X} N(v)\right) \cap \left(\bigcup_{v\in Y} N(v)\right) = V$ and obviously the vertices in W_1 and W_2 are adjacent to at least one vertex in each other and exactly one vertex in Ω. ■

Chapter 3

Singularity of θ-graphs

In this chapter we establish a necessary and sufficient condition for a graph G to be singular. Further, we have characterized the singularity of θ-graphs and have found the nullity of θ-graphs.

3.1 Introduction

In the following we list some fundamental concepts which are useful for our purpose.

Definition 3.1.1. *A* bicyclic graph *is a simple connected graph in which number edges equal the number of vertices plus one.*

The cycle and the path on n vertices are denoted by C_n and P_n, respectively. Let C_p and C_q be two vertex-disjoint cycles. Suppose that v_0 is a vertex of C_p and v_l is a vertex of C_q. Joining v_0 and v_l by a path $v_0v_1 \ldots v_l$ of length l, where $l \geq 0$ ($l = 0$ means identifying v_0 with v_l), the resulting graph is called an ∞-graph and is denoted by $\infty(p, l, q)$ [see Figure 3.1]. We denote by $\mathcal{B}_n{}^*$, the class of all bicyclic graphs that have an ∞-graph as an induced subgraph.

Let P_{l+1}, P_{p+1} and P_{q+1} be three vertex-disjoint paths, where $min\{p, l, q\} \geq 1$ and at most one of them is 1. Identifying the initial vertices and the terminal vertices of P_{l+1}, P_{p+1} and P_{q+1}, respectively, the resultant graph is called a θ-graph and is denoted by $\theta(p, l, q)$. By $\mathcal{B}_n^{**}$, we denote the class of all bicyclic graphs that have a θ-graph as an induced subgraph.

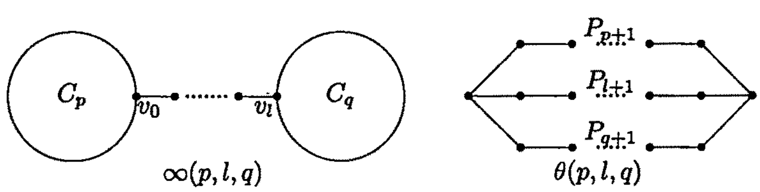


Figure 3.1: ∞-graph and θ-graph

Thus the class $\mathcal{B}_n$, of bicyclic graphs can be partitioned into two classes: the class of graphs which contain an ∞-graph as an induced subgraph and the class of graphs which contain a θ-graph as an induced subgraph i.e., $\mathcal{B}_n = \mathcal{B}_n^* \cup \mathcal{B}_n^{**}$.

Definition 3.1.2. A bicyclic graph G which is either a θ-graph or obtained by attaching some pendent vertices to a θ-graph is called an *elementary* θ-graph.

We will use the following well-known results in computing the nullity of a graph.

Theorem 3.1.3. [16] *Let v be a pendent vertex of a graph G and u be the vertex in G adjacent to v. Then, $\eta(G) = \eta(G - u - v)$, where $G - u - v$ is the induced subgraph of G obtained by deleting u and v.*

Theorem 3.1.4. [15] *A path with four vertices of valency* 2 *in a graph* G *can be replaced by an edge [see Figure 3.2] without changing the value of* $\eta(G)$.

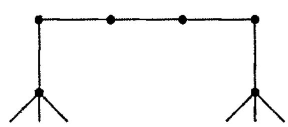


Figure 3.2:

Theorem 3.1.5. [15] *Let* G_1 *and* G_2 *be two bipartite graphs. If* $\eta(G_1) = 0$, *and if the graph* G *is obtained by joining an arbitrary vertex of* G_1 *by an edge with an arbitrary vertex of* G_2, *then the relation* $\eta(G) = \eta(G_2)$ *holds.*

Theorem 3.1.6. [15] *Let* G *be a bipartite graph in which there does not exist any cycle of length* $q \equiv 0 \pmod 4$, *then* $\eta(G) = n - 2q$, *where* q *is maximum number mutually nonadjacent edges in* G.

Definition 3.1.7. *[49] Let* $V(G)$ *and* $E(G)$ *denote the vertex set* $\{v_1, v_2, \dots, v_n\}$ *and the edge set of a graph* G, *respectively. The* neighborhood *of a vertex* $v \in V$ *in* G *is defined to be* $N(v) = \{u \in V(G) \mid uv \in E(G)\}$. *A nonzero vector* $(\alpha_1, \alpha_2, \dots, \alpha_n)^t$ *is a null-eigenvector of* G *if and only if for each* $v_i \in V(G)$ *we have* $\sum_{v_j \in N(v_i)} \alpha_j = 0$. *Let* $A(G) = [C_1, C_2, \dots, C_n]$, *where* C_j *is the* j*th column* *vector of $A(G)$. If G is singular and $(\alpha_1, \alpha_2, \ldots, \alpha_n)^t$ is a null-eigenvector of $A(G)$, then the relation*

$$\alpha_1 C_1 + \alpha_2 C_2 + \cdots + \alpha_n C_n = 0$$

is called a kernel relation of G.

Definition 3.1.8. *A subset A of a vector space is said to be minimal dependent set if*

(a) A is dependent

(b) any proper subset of A is linearly independent.

Definition 3.1.9. [49] A pair V_1, V_2 of subsets of $V(G)$ is said to satisfy the *property (N)* if (a) V_1 and V_2 are nonempty and disjoint, and (b) $\bigcup\{N(v) \mid v \in V_1\} = \bigcup\{N(v) \mid v \in V_2\}$. Further, such a pair is said to be *minimal satisfying the property (N)* if for any pair U_1, U_2 of $V(G)$ satisfying the property (N) with $U_1 \subseteq V_1,\ U_2 \subseteq V_2$, we have $U_1 = V_1,\ U_2 = V_2$.

Theorem 3.1.10. [49] *Let G be a connected graph on $n \geq 2$ vertices. If G is singular, then $V(G)$ has a pair of subsets satisfying the property (N).*

Definition 3.1.11. [49] A pair V_1, V_2 of subsets of $V(G)$ is said to satisfy the *property (S)* if it satisfies the property (N) and for all pairs u, v in $V_i,\ i = 1, 2$, we have $N(u) \cap N(v) = \emptyset$.

Theorem 3.1.12. [49]*If $V(G)$ has a pair of subsets V_1 and V_2 satisfying the property (S), then G is singular.*

Theorem 3.1.13. [49] *Let T be a nontrivial tree. Then, the following statements are equivalent.*

(a) T is singular.

(b) There exist subsets V_1 and V_2 of $V(T)$ satisfying the property (N).

(c) There exist subsets V_1 and V_2 of $V(T)$ satisfying the property (S).

Theorem 3.1.14. [49] *A unicyclic graph G is singular if and only if there is a pair of subsets V_1 and V_2 of $V(G)$ satisfying the property (N).*

Definition 3.1.15. [49] *An* elementary unicyclic graph *is a graph G which is either a cycle or is obtained by attaching some pendent vertices to a cycle. An* outer matching *of a unicyclic graph G which is not elementary is a matching M_0 in G such that $G - V(M_0)$ is the disjoint union of an elementary unicyclic graph and a set of isolated vertices (possibly empty).*

Proposition 3.1.16. [50] *Let G be an elementary unicyclic graph on n vertices having a pendant. Then $\eta(G) = n - 2q$, where q is the maximum number of mutually nonadjacent edges in G.*

Theorem 3.1.17. [50] *A unicyclic graph G is singular if and only if one of the following holds:*

(a) *G is singular elementary.*

(b) *G is obtained from a singular elementary unicyclic graph G_0 by attaching trees at vertices of G_0 such that the graph $G - V(G_0)$ has a perfect matching.*

(c) *There exists a tree T_v attached at a vertex u of the cycle with uv as the attaching edge such that none of T_v and $T_v - v$ has a perfect matching.*

Theorem 3.1.10 gives a necessary condition for G to be singular. Theorem 3.1.13 and Theorem 3.1.14 shows that this necessary condition is also sufficient for unicyclic and acyclic graphs. In general, this condition is not sufficient. For example, consider the graph $\infty(3,3,3)$ [see Figure 3.3] on the vertex set $\{1,2,3,4,5,6,7,8\}$. Then $V_1 = \{1,2,5,6\}$, $V_2 = \{3,4,7,8\}$ is a minimal pair in $\infty(3,3,3)$ satisfying the property (N), though $\infty(3,3,3)$ is nonsingular.

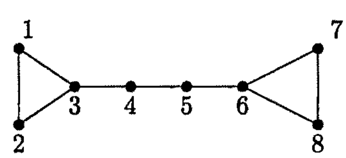


Figure 3.3: $\infty(3,3,3)$

In section 2 of this chapter, we derive a necessary and sufficient condition for a graph to be singular. We also prove two results which will be useful to find the nullity of a graph. In section 3, we show how this characterization can be used to find the nullity of a graph in $\mathcal{B}_n^{**}$.

3.2 Necessary and sufficient condition for a graph to be singular

By $A[n]$ we denote the multiset obtained by taking n copies of each element of the set A. By $A[n] \cup B[m]$ we mean the multiset obtained by taking n copies of each element of the set A and m copies of each element of the set B. Clearly $A[1] \cup B[1] = A \cup B$, if and only if A and B are disjoint.

Definition 3.2.1. *A pair of subsets $V_1 = \{v_i \mid i = 1, 2, \ldots, l\}$ and $V_2 = \{v_i \mid i = l+1, l+2, \ldots, k\}$ of $V(G)$ is said to satisfy the property (NS) if (a) V_1 and V_2 are nonempty and disjoint, (b) there exist positive itegers $\alpha_1, \alpha_2, \ldots, \alpha_l, \beta_{l+1}, \beta_{l+2}, \ldots \beta_k$ such that $\cup\{N(v_i)[\alpha_i] \mid v_i \in V_1\} = \cup\{N(v_i)[\beta_i] \mid v_i \in V_2\}$. Further, such a pair is said to be* minimal satisfying the property (NS) *if for any pair U_1, U_2 of $V(G)$ satisfying the property (NS) with $U_1 \subseteq V_1$, $U_2 \subseteq V_2$, we have $U_1 = V_1$, $U_2 = V_2$.*

Note that a pair V_1 and V_2 of $V(G)$ satisfying the property (NS) satisfy the property (N). Also a pair V_1 and V_2 of $V(G)$ satisfying the property (S) satisfy the property (NS).

Theorem 3.2.2. *A graph G is singular if and only if there exist a minimal pair satisfying the property (NS).*

Proof. **(Proof of the necessary part)** Let G be singular, therefore columns of $A(G)$ are linearly dependent. Let $\{C_1, C_2, \cdots, C_l\}$ be minimal dependent set of columns of $A(G)$. There exist non-zero integers $\alpha_1, \alpha_2, \ldots, \alpha_l$ with g.c.d. equal to 1 such that

$$\alpha_1 C_1 + \alpha_2 C_2 + \cdots + \alpha_l C_l = 0$$

Let $V_1 = \{v_j \mid \alpha_j > 0\}$ and $V_2 = \{v_j \mid \alpha_j < 0\}$. Since $A(G)$ is nonnegative and has no zero columns, V_1 and V_2 are nonempty. Clearly, $V_1 \cap V_2 = \emptyset$, and we have

$$\sum_{v_j \in V_1} \alpha_j C_j = \sum_{v_j \in V_2} \beta_j C_j, \tag{3.2.1}$$

where $\alpha_j = -\beta_j$.

Let

$$X = \cup\{N(v_j)[\alpha_j] \mid v_j \in V_1\}$$

and

$$Y = \cup\{N(v_j)[\beta_j] \mid v_j \in V_2\}.$$

Let $v_i \in X$ and it appears γ times in X. Therefore there exist

$$\alpha_i, \alpha_{i+1}, \ldots, \alpha_s \in \{\alpha_j \mid v_j \in V_1\}$$

such that $v_i \in N(v_p)$, where $p = i, i+1, \ldots, s$; $v_i \notin N(v_r)$ for $r \notin \{i, i+1, \ldots, s\}$ and $\alpha_i + \alpha_{i+1} + \ldots + \alpha_s = \gamma$ since G is without loops. Therefore $a_{ip} = 1$, where $p = i, i+1, \ldots, s$; and $a_{ir} = 0$ for $r \notin \{i, i+1, \ldots, s\}$. This implies that the ith entry of the vector $\sum_{v_j \in V_1} \alpha_j C_j$ is γ. In view of (3.2.1), the ith entry of the vector $\sum_{v_j \in V_2} \beta_j C_j$ must be γ. Consequently, there exist

$$\beta_j, \beta_{j+1}, \ldots, \beta_t \in \{\beta_j \mid v_j \in V_2\}$$

such that $a_{ip} = 1$, where $p = j, j+1, \ldots, t$; $a_{ir} = 0$ for $r \notin \{j, j+1, \ldots, t\}$ and $\beta_j + \beta_{j+1} + \ldots + \beta_t = \gamma$. Therefore $v_i \in N(v_p)$, where $p = j, j+1, \ldots, t$; $v_i \notin N(v_r)$ for $r \notin \{j, j+1, \ldots, t\}$, i.e., v_i appears γ times in $Y = \cup\{N(v_j)[\beta_j] \mid v_j \in V_2\}$.

Interchanging the role of X and Y, we can show that if v_i appears m times in Y, then it also appears m times in X. Therefore $X = Y$.

(Proof of the sufficient part) Suppose $V(G)$ has a minimal pair V_1, V_2 satisfying the property (NS). Let $V_1 = \{v_1, v_2, \ldots, v_l\}$ and $V_2 = \{v_{l+1}, v_{l+2}, \ldots, v_k\}$. Therefore there exist positive integers $\alpha_1, \alpha_2, \ldots, \alpha_l, \beta_{l+1}, \beta_{l+2}, \ldots \beta_k$ such that

$$\cup\{N(v_i)[\alpha_i] \mid v_i \in V_1\} = \cup\{N(v_i)[\beta_i] \mid v_i \in V_2\}.$$

Now v_i appears γ times in $\cup\{N(v_i)[\alpha_i] \mid v_i \in V_1\}$ if and only if it appears γ times in $\cup\{N(v_i)[\beta_i] \mid v_i \in V_2\}$. Therefore,

$$\sum_{v_j \in V_1} \alpha_j C_j = \sum_{v_j \in V_2} \beta_j C_j, \tag{3.2.2}$$

which shows that the columns of $A(G)$ are linearly dependent. ■

Corollary 3.2.3. *Let V_1, V_2 be a pair in $V(G)$ satisfying the property (NS). Let x_j be defined by*

$$x_j = \begin{cases} \alpha_j & \text{if } v_j \in V_1, \\ -\beta_j & \text{if } v_j \in V_2, \\ 0 & \text{otherwise.} \end{cases} \tag{3.2.3}$$

Then $(x_1, x_2, \ldots, x_n)^t$ is a null-eigenvector of G.

Example 3.2.4. *For the graph G, [see Figure 3.4] $V_1 = \{1, 5, 9, 13\}$ and $V_2 =$*

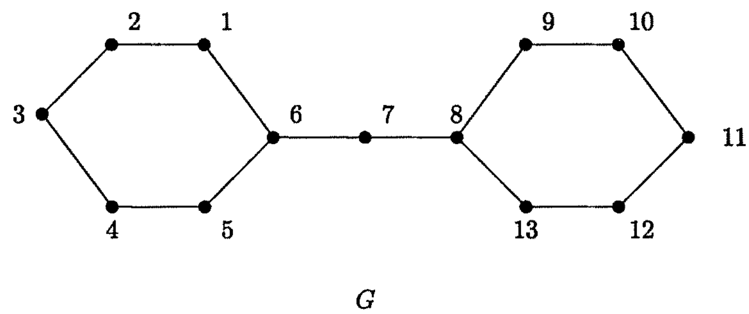


Figure 3.4:

$\{3, 7, 11\}$ is a pair satisfying property(NS). Since

$$N(1)[1] \cup N(5)[1] \cup N(9)[1] \cup N(13)[1] = N(3)[1] \cup N(7)[2] \cup N(11)[1],$$

therefore G is singular. Also, we see that

$$(1, 0, -1, 0, 1, 0, -2, 0, 1, 0, -1, 0, 1)^T$$

is a null eigenvector of G.

Before ending this section, we prove two results which will be useful for the next section.

Lemma 3.2.5. *Let G be a singular bipartite graph with bipartition V', V''. If V_1, V_2 is a minimal pair satisfying property (NS), then $V_1 \cup V_2 \subseteq V'$ or $V_1 \cup V_2 \subseteq V''$.*

Proof. The vertices of G can be labeled so that adjacency matrix takes the form

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}.$$

Let $\begin{pmatrix} x' \\ x'' \end{pmatrix}$ be the kernel eigenvector of G corresponding to the minimal pair V_1, V_2. If $x' \neq 0$ and $x'' \neq 0$, then $\begin{pmatrix} x' \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ x'' \end{pmatrix}$ are also kernel eigenvectors of G which are linearly independent of $\begin{pmatrix} x' \\ x'' \end{pmatrix}$. Therefore V_1, V_2 is not a minimal pair for G. Thus either $x' = 0$ or $x'' = 0$. Without loss of generality let $x'' = 0$, therefore $V_1, V_2 \subseteq V'$. ■

Theorem 3.2.6. *Let G be a singular graph with a minimal pair (V_1, V_2) satisfying property (NS). If $v_1 \in V_1 \cup V_2$ and $G - v_1$ is the induced subgraph of G obtained by deleting v_1, then $\eta(G) = \eta(G - v_1) + 1$.*

Proof. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$. Without loss of generality assume $V_1 = \{v_1, v_2, \ldots, v_k\}$ and $V_2 = \{v_{k+1}, v_{k+2}, \ldots, v_m\}$. Therefore there exist non zero real number α_i, where $i = 1, 2, 3, \ldots, m$ such that

$$\cup\{N(v_i)[\alpha_i] \mid v_i \in V_1\} = \cup\{N(v_i)[\alpha_j] \mid v_i \in V_2\}.$$

Also $A(G)$ has the following form

$$A(G) = \begin{pmatrix} 0 & a_{12} & a_{13} & \cdots & a_{1m} & \cdots & a_{1n} \\ a_{12} & 0 & a_{23} & \cdots & a_{2m} & \cdots & a_{2n} \\ a_{13} & a_{23} & 0 & \cdots & a_{3m} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{1m} & a_{2m} & a_{3m} & \cdots & 0 & \cdots & a_{mn} \\ \vdots & \vdots & \vdots & \vdots & \vdots & A(G - V_1 \cup V_2) & \\ a_{1n} & a_{2n} & a_{3n} & \cdots & a_{mn} & & \end{pmatrix}$$

where a_{ij} are either 0 or 1. Applying the elementary operations $R_1 \to \alpha_1 R_1 + \alpha_2 R_2 + \ldots + \alpha_m R_m$ and $C_1 \to \alpha_1 C_1 + \alpha_2 C_2 + \ldots + \alpha_m C_m$ to the matrix $A(G)$, we see that

$$A(G) \sim \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & a_{23} & \dots & a_{2m} & \dots & a_{2n} \\ 0 & a_{23} & 0 & \dots & a_{3m} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & a_{2m} & a_{3m} & \dots & 0 & \dots & a_{mn} \\ \vdots & \vdots & \vdots & \vdots & \vdots & A(G - V_1 \cup V_2) & \\ 0 & a_{2n} & a_{3n} & \dots & a_{mn} & & \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & & & & \\ 0 & & & & \\ \vdots & & A(G - v_1) & & \\ 0 & & & & \end{pmatrix}$$

Thus $\eta(G) = 1 + \eta(G - v_1)$. ■

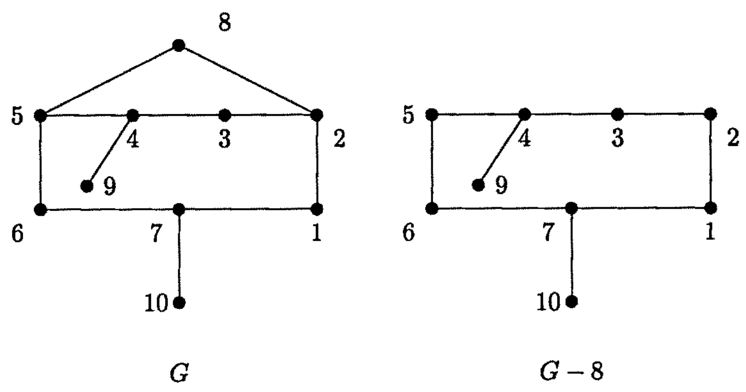


Figure 3.5:

Example 3.2.7. *The graph G in Figure 3.5 is singular. Note that $V_1 = \{8, 10\}$ and $V_2 = \{1, 6\}$ is a minimal pair satisfying property(NS). Thus $\eta(G) = 1 + \eta(G - 8)$. Also $U_1 = \{9, 1\}$ and $U_2 = \{3, 16\}$ is a minimal pair satisfying property(NS). Therefore $\eta(G - 8) \geq 1$. Since $\eta(G - 8 - 3) = 0$, therefore $\eta(G) = 2$.*

3.3 Singularity of a graph in $\mathcal{B}_n^{**}$

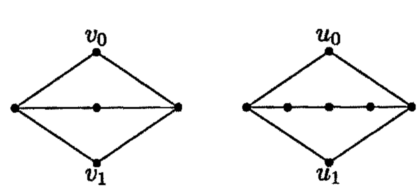
Proposition 3.3.1. *Let $\theta(p, l, q)$ be a θ-graph where $p = l = q \equiv 0 \pmod 2$, then*

$$\eta(\theta(p,l,q)) = \begin{cases} 3 & \textit{if } p = l = q \equiv 2 \pmod 4 \textit{ or } p = l = q \equiv 0 \pmod 4, \\ 1 & \textit{if } p = l \equiv 2 \pmod 4, q \equiv 0 \pmod 4 \\ & \textit{or } p = l \equiv 0 \pmod 4, q \equiv 2 \pmod 4. \end{cases}$$

.

Proof. By Theorem 3.1.4, we have

$$\eta(\theta(p,l,q)) = \begin{cases} \eta(\theta(2,2,2)) & \text{if } p = l = q \equiv 2 \pmod 4, \\ \eta(\theta(4,4,4)) & \text{if } p = l = q \equiv 4 \pmod 4, \\ \eta(\theta(2,2,4)) & \text{if } p = l \equiv 2 \pmod 4, q \equiv 4 \pmod 4, \\ \eta(\theta(4,4,2)) & \text{if } p = l \equiv 4 \pmod 4, q \equiv 2 \pmod 4. \end{cases}$$



$\theta(2,2,2)$ $\theta(2,2,4)$

Figure 3.6:

Now $(\{v_0\},\{v_1\})$ is a minimal pair in $\theta(2,2,2)$ [see Figure 3.6] satisfying property (S). Therefore $\theta(2,2,2)$ is singular. By Theorem 3.2.6, $\eta(\theta(2,2,2)) = 1 + \eta(\theta(2,2,2) - v_0) = 1 + \eta(C_4) = 3$. Similarly $\eta(\theta(4,4,4)) = 3$.
Again $(\{u_0\},\{u_1\})$ is a minimal pair in $\theta(2,2,4)$ [see Figure 3.6] satisfying property (S). Therefore $\theta(2,2,4)$ is singular. By Theorem 3.2.6, $\eta(\theta(2,2,4)) = 1 + \eta(\theta(2,2,4) - u_0 = 1 + \eta(C_6) = 1$. Similarly $\eta(\theta(4,4,2)) = 1$. Thus the result follows. ∎

Proposition 3.3.2. *Let $\theta(p,l,q)$ be a θ-graph where $p = l = q \equiv 1 \pmod 2$, then*

$$\eta(\theta(p,l,q)) = 0$$

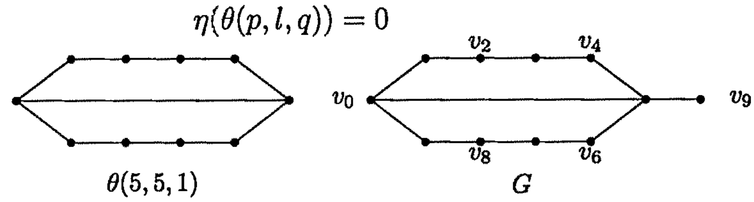


Figure 3.7:

Proof. By Theorem 3.1.4, we have

$$\eta(\theta(p,l,q)) = \begin{cases} \eta(\theta(5,5,1)) & \text{if } p = l = q \equiv 1 \pmod 4, \\ \eta(\theta(3,3,3)) & \text{if } p = l = q \equiv 3 \pmod 4, \\ \eta(\theta(5,1,3)) & \text{if } p = l \equiv 1 \pmod 4, q \equiv 3 \pmod 4, \\ \eta(\theta(3,3,1)) & \text{if } p = l \equiv 3 \pmod 4, q \equiv 1 \pmod 4. \end{cases}$$

Consider the graph G which is obtained from $\theta(5,5,1)$ by attaching a single pendent vertex [see Figure 3.7]. By Theorem 3.1.3, G is singular and $\eta(G) = 1$. Also $(\{v_0, v_4, v_6\}, \{v_2, v_8, v_9\})$ is a minimal pair satisfying property (S). By Theorem 3.2.6,

$$\eta(G) = 1 + \eta(G - v_9) = 1 + \eta(\theta(5,5,1))$$

and therefore, $\eta(\theta(5,5,1)) = 0$. Similarly we can show that

$$\eta(\theta(3,3,3)) = 0 = \eta(\theta(5,1,3)) = \eta(\theta(3,3,1)).$$

Thus the result follows. ∎

Proposition 3.3.3. *If $\theta(p,l,q)$ is a θ-graph where p, l are even and q is odd, then*

$$\eta(\theta(p,l,q)) = \begin{cases} 0 & \text{if } p+l \not\equiv 0 \pmod 4, \\ 1 & \text{if } p+l \equiv 0 \pmod 4. \end{cases}$$

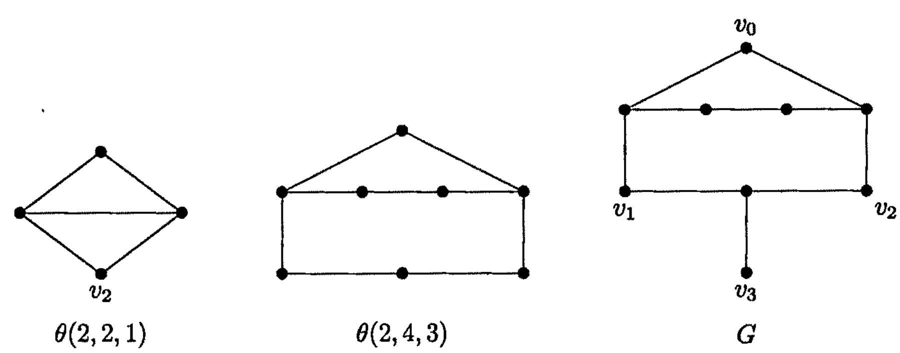


Figure 3.8:

Proof. Let $p = l \equiv 2 \pmod 4$ and $q \equiv 1 \pmod 4$. By Theorem 3.1.4, we have

$$\eta(\theta(p,l,q)) = \begin{cases} \eta(\theta(2,2,1)) & \text{if } q \equiv 1 \pmod 4, \\ \eta(\theta(2,2,3)) & \text{if } q \equiv 3 \pmod 4, \\ \eta(\theta(4,4,1)) & \text{if } q \equiv 1 \pmod 4, \\ \eta(\theta(4,4,3)) & \text{if } q \equiv 3 \pmod 4. \end{cases}$$

Also $(\{v_0\}, \{v_2\})$ is a minimal pair in $\theta(2,2,1)$ [see Figure 3.8] satisfying property (S). By Theorem 3.2.6, $\eta(\theta(2,2,1)) = 1 + \eta(\theta(2,2,1) - v_0) = 1$. Similarly considering other cases we can show that $\eta(\theta(p,l,q)) = 1$.

Again let, $p+l \not\equiv 0 \pmod 4$, therefore either $p \equiv 2 \pmod 4$, $l \equiv 0 \pmod 4$ or $p \equiv 0 \pmod 4$, $l \equiv 2 \pmod 4$. Suppose $p \equiv 2 \pmod 4$ and $l \equiv 0 \pmod 4$. By Theorem 3.1.4, we have

$$\eta(\theta(p,l,q)) = \begin{cases} \eta(\theta(2,4,3)) & \text{if } q \equiv 3 \pmod 4, \\ \eta(\theta(2,4,1)) & \text{if } q \equiv 1 \pmod 4. \end{cases}$$

Consider the graph G of Figure 3.8. Then $(\{v_0, v_3\}, \{v_1, v_2\})$ is minimal pair satisfying property (NS). Therefore G is singular. By Theorem 3.2.6,

$$\eta(G) = 1 + \eta(G - v_3) = 1 + \eta(\theta(2,4,3)).$$

Also $\eta(G) = 1+\eta(G-v_2) = 1$, therefore, $\eta(\theta(2,4,3)) = 0$. Similarly we can show that $\eta(\theta(2,4,1) = 0$. Thus the result follows. ∎

Proposition 3.3.4. *If $\theta(p,l,q)$ is a θ-graph where p,l are odd and q is even, then*

$$\eta(\theta(p,l,q)) = \begin{cases} 0 & \text{if } p+l \not\equiv 0 \pmod 4, \\ 1 & \text{if } p+l \equiv 0 \pmod 4. \end{cases}$$

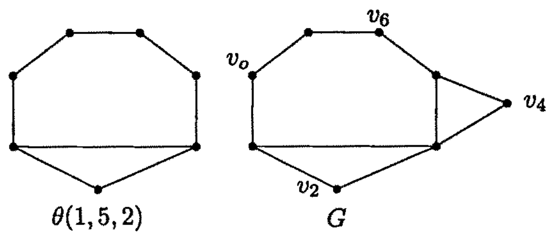


Figure 3.9:

Proof. Let $p+l \not\equiv 0 \pmod 4$. Therefore either $p = l \equiv 1 \pmod 4$ or $p = l \equiv 3 \pmod 4$. Let $p = l \equiv 1 \pmod 4$. By Theorem 3.1.4, we have

$$\eta(\theta(p,l,q)) = \begin{cases} \eta(\theta(1,5,2)) & \text{if } q \equiv 2 \pmod 4, \\ \eta(\theta(1,5,4)) & \text{if } q \equiv 0 \pmod 4. \end{cases}$$

Consider the graph G of Figure 3.9. Then $G - v_4 = \theta(1,5,2)$. Now $(\{v_0, v_4\}, \{v_2, v_6\})$ is a minimal pair satisfying property (NS). Therefore G is singular. By Theorem 3.2.6,

$$\eta(G) = 1 + \eta(G - v_4) = 1 + \eta(\theta(1,5,2)).$$

Also by Theorem 3.2.6, $\eta(G) = 1 + \eta(\infty(3,0,3))$. Since $\infty(3,0,3)$ is nonsingular, therefore $\eta(\theta(1,5,2)) = 0$. Thus $\eta(\theta(p,l,q)) = 0$ if $p = l \equiv 1 \pmod 4$. Similarly, we can show that, $\eta(\theta(p,l,q)) = 0$ if $p = l \equiv 3 \pmod 4$.

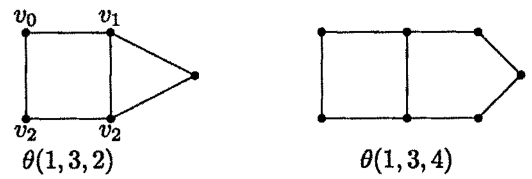


Figure 3.10:

Let $p+l \equiv 0 \pmod 4$. So let $p \equiv 1 \pmod 4$, $l \equiv 3 \pmod 4$. By Theorem 3.1.4, we have

$$\eta(\theta(p,l,q)) = \begin{cases} \eta(\theta(1,3,2)) & \text{if } q \equiv 2 \pmod 4, \\ \eta(\theta(1,3,4)) & \text{if } q \equiv 0 \pmod 4. \end{cases}$$

Now $(\{v_0, v_1\}, \{v_2, v_3\})$ is a minimal pair in $\theta(1,3,2)$ [see Figure 3.10] satisfying property (NS). Therefore $\theta(1,3,2)$ is singular. Also by Theorem 3.2.6, $\eta(\theta(1,3,2)) = \eta(\theta(1,3,2) - v_0) = 1$. Similarly, we can show that $\eta(\theta(1,3,4) = 1$. Thus $\eta(\theta(p,l,q)) = 1$, if $p+l \equiv 0 \pmod 4$ and q is even . ∎

Singularity of elementary θ-graph: Let G_0 be an elementary θ-graph with pendent vertices. Let v be a pendent vertex in G attached at u of G_0. Then by Theorem 3.1.3, $\eta(G_0) = \eta(G_0 - uv)$. Since $G_0 - uv$ is disjoint union of a tree or a unicyclic graph and a set of isolated vertices (possibly empty), we can find the nullity of $G_0 - uv$.

Definition 3.3.5. A matching M_0 in a graph G in $\mathcal{B}_n^{**}$ is called an *outer matching* in G if $G - V(M_0)$ is the disjoint union of an elementary θ-graph and a set of isolated vertices (possibly empty). (Note that $M_0 = \emptyset$, if G is elementary.)

Remark 3.3.6. If G is a graph in $\mathcal{B}_n^{**}$ which is not elementary, then we construct an outer matching M_0 as follows. Let u_1 be a (pendent) vertex which is at a maximum distance from $\theta(p,l,q)$ in G and v_1 the vertex adjacent to u_1. Then v_1 is not on $\theta(p,l,q)$, since G is not elementary. We choose the edge $e_1 = u_1v_1$ as an edge in M_0. Clearly, $G - u_1 - v_1$ is a disjoint union of a elementary θ-graph G_1 and a set of isolated vertices (possibly empty). If G_1 is not elementary, we can choose another edge for M_0 by the same process, and then proceed recursively. The process must terminate and an outer matching M_0 of G is obtained.

Example 3.3.7. *Consider the graph G given in Figure 3.11. Here the set M_0 of edges in bold face in the figure is an outer matching of G. The corresponding elementary θ-graph is G_0(depicted in the figure)and the set of isolated vertices of $G - M_0$ is $\{17, 21\}$.*

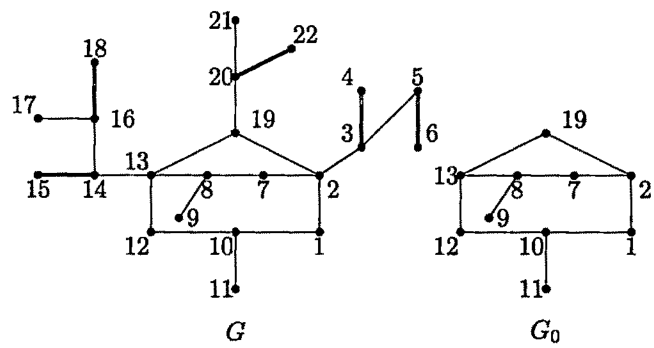


Figure 3.11: An outer matching and the resulting elementary θ-graph

We denote the set of isolated vertices and the elementary component of $G - V(M_0)$ by Λ_0 and G_0, respectively.

Theorem 3.3.8. *A graph G in $\mathcal{B}_n^{**}$ is singular if and only if one of the following holds:*

(a) *G is singular elementary θ-graph.*

(b) *G is obtained from a singular elementary θ-graph G_0 by attaching trees at vertices of G_0 such that the graph $G - V(G_0)$ has a perfect matching.*

(c) *There exists a tree T_v attached at a vertex u of the θ-graph with uv as the attaching edge such that none of T_v and $T_v - v$ has a perfect matching.*

Proof. Suppose G is not elementary and choose an outer matching M_0 of G. Let $G - V(M_0)$ be the disjoint union of the elementary θ-graph G_0 and a set Λ_0 of isolated vertices (possibly empty). We note that G is obtained by attaching trees at the vertices of G_0. In view of Theorem 3.1.3, we have $\eta(G) = \eta(G_0) + |\Lambda_0|$. Therefore, G is singular if and only if either $\Lambda_0 \neq \emptyset$ or G_0 is singular. If $\Lambda_0 = \emptyset$, then $G - V(G_0)$ has a perfect matching, and therefore G is singular if and only if (b) holds. Suppose $\Lambda_0 \neq \emptyset$ and $w \in \Lambda_0$. Let T_v be a tree in G, attached at a vertex u of the θ-graph with uv as the attaching edge, of which w is a vertex. Since $w \in \Lambda_0$, T_v does not have a perfect matching. Moreover, if $T_v - v$ has a perfect matching, then v is a vertex of G_0. In that case, w is a vertex of $T_v - v$ and therefore is in $V(M_0)$. Since this is not the case, therefore (c) holds. ∎

Corollary 3.3.9. *If G is a graph in $\mathcal{B}_n^{**}$ which is not a θ-graph then*

$$\eta(G) = \eta(G_0) + |\Lambda_0|$$

Example 3.3.10. *The graph G in Figure 3.11 has nullity, $\eta(G) = 2+\eta(G_0) = 4$, since $\eta(G_0) = 2$.*

Chapter 5

On the energy of unicyclic graphs

In this chapter, we study the energy of a unicyclic graph. Our main tool for this study will be " Coulson integral formula " for energy of a graph.

5.1 Introduction

Let G be a simple graph on n vertices and let $A(G)$ be its adjacency matrix. The characteristic polynomial of $A(G)$,

$$\phi(G;\lambda) = \det(\lambda I - A(G)) = \sum_{i=0}^{n} a_i x^{n-i}, \tag{5.1.1}$$

where I is the unit matrix of order n, is the *characteristic polynomial* of G. The eigenvalues of $A(G)$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are the *eigenvalues* of G. Since $A(G)$ is symmetric, λ_i are all real.

The *energy* of a graph G is defined to be

$$E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{5.1.2}$$

If the characteristic polynomial of G is as in (5.1.1), then the energy of G is given by the Coulson integral formula (see [26, 29]):

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j+1}x^{2j+1}\right)^2\right]. \tag{5.1.3}$$

For an n-vertex graph G let $b_i = b_i(G) = |a_i(G)|$, $i = 0, 1, \ldots, n$, where a_i are the coefficients of the characteristic polynomial of G, as in (5.1.1). Note that $b_0(G) = 1$, $b_1(G) = 0$ and $b_2(G)$ is the number of edges of G. If G is bipartite, then for $k \geq 0$, $b_{2k+1} = 0$. Let $m(G, k)$ denote the number of k-matchings of G. If G is acyclic, then for $k \geq 0$, $b_{2k} = m(G, k) = (-1)^k a_{2k}$. It is both convenient and consistent to define $m(G, k) = 0$ and $b_k(G) = 0$ for $k < 0$.

Lemma 5.1.1. [27] *If G is a unicyclic graph with a circuit of size l, then for all $k \geq 0$, $(-1)^k a_{2k} \geq 0$. Further, $(-1)^k a_{2k+1} \geq$ (resp. $\leq$) 0 if $l = 2r + 1$ and r is odd (resp. even).*

If G is a unicyclic graph, then by means of Lemma 5.1.1, formula (5.1.3) reduces to

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil} b_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil} b_{2j+1}x^{2j+1}\right)^2\right]. \tag{5.1.4}$$

Thus, in case of unicyclic graphs $E(G)$ is a monotonically increasing function of $b_i(G), i = 1, 2, \ldots, n$. Consequently, if G and H are graphs with at most one circuit such that

$$b_i(G) \geq b_i(H) \tag{5.1.5}$$

holds for all $i \geq 0$, then

$$E(G) \geq E(H). \tag{5.1.6}$$

Equality in (5.1.6) is attained only if (5.1.5) is an equality for all $i \geq 0$. This fact provides us a way of comparing the energies of graphs in the class of unicyclic graph order n and the *quasiordering* is thus introduced. If relations (5.1.5) holds for all i, then we write $G \succeq H$ or $H \preceq G$. If $G \succeq H$ but not $H \succeq G$, then we write $G \succ H$. With this quasiordering, the above result can be restated as follows:

Lemma 5.1.2. *Let G and H be unicyclic graphs. Then $G \succeq H$ implies $E(G) \geq E(H)$, and $G \succ H$ implies $E(G) > E(H)$.*

5.2 Energy of unicyclic graphs with $\beta_1 = 2$

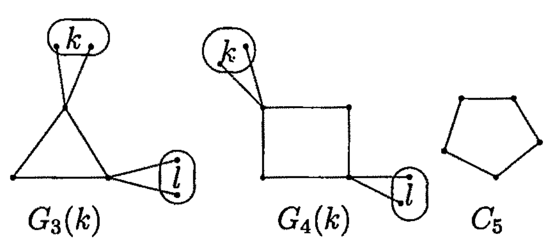


Figure 5.1: The graphs when $\beta_1 = 2$

Theorem 5.2.1. $G_3(1) \prec G_3(2) \prec \ldots \prec G_3\left(\left[\frac{n-3}{2}\right]\right)$.

Proof. We have

$$a_2(G_3(k)) = -n,$$

$$a_3(G_3(k)) = -2,$$

$$a_4(G_3(k)) = k(n-k-2) + n - k - 3.$$

and

$$a_i(G_3(k)) = 0, \text{ for all } i \geq 5$$

$$f(k) = a_4(G_3(k)) = k(n-k-2) + n - k - 3,$$

$$\begin{aligned} f'(k) &= n - k - 2 - k - 1 \\ &= n - 2k - 3 > 0, \text{ for all } k < \frac{n-3}{3}. \end{aligned}$$

Thus $f(k)$ is an increasing function of k and takes maximum value when $k = \frac{n-3}{2}$. Therefore by Lemma 5.1.2, the result follows. ∎

Theorem 5.2.2. $G_4(1) \prec G_4(2) \prec \ldots \prec G_4\left(\left[\frac{n-4}{2}\right]\right).$

Proof. We have

$$a_2(G_4(k)) = -n,$$

$$\begin{aligned} a_4(G_4(k)) &= -2 + k(n-k-2) + 2(n-k-3) \\ &= k(n-k-2) + 2(n-k-4). \end{aligned}$$

and $a_i(G_4(k)) = 0$, for other value of i. Now

$$\begin{aligned} f(k) &= b_4(G_4(k)) \\ &= |a_4(G_4(k))| \\ &= k(n-k-2) + 2(n-k-4), \end{aligned}$$

$$
\begin{aligned}
f'(k) &= -k + n - k - 2 - 2 \\
&= n - 2k - 4 > 0, \text{for all } k < \frac{n-4}{2}.
\end{aligned}
$$

Thus $f(k)$ is an increasing function of k and takes maximum value when $k = \frac{n-4}{2}$. Thus by Lemma 5.1.2, the result follows. ∎

5.3 Energy of unicyclic graphs with $\beta_1 = 3$

If $\beta_1(G) = 3$, then G is one of the form as shown in Figure 5.2.

Theorem 5.3.1. *$G_3(1, n-5, 1) \preceq G_3(k, l, m)$ for all $k, l, m \geq 1$ and $k + l + m + 3 = n$.*

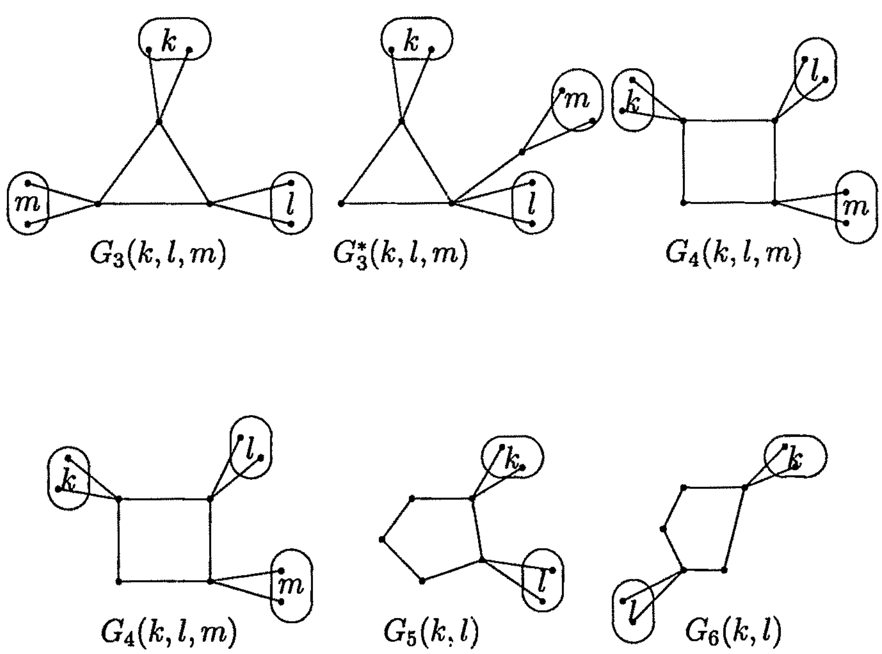


Figure 5.2:

Proof. We have

$$\begin{aligned} b_2(G_3(k,l,m)) &= n, \\ b_3(G_3(k)) &= 2, \\ b_4(G_3(k,l,m)) &= |a_4(G_3(k,l,m))| \\ &= k(l+m+1)+(l+m)+lm, \\ b_6(G_3(k,l,m)) &= |a_6(G_3(k,l,m))| \\ &= klm. \end{aligned}$$

Let k,l,m and n be positive integers with $k, l, m \leq n-5$ and $k+l+m = n-3$ and at least one of k and l is greater than or equal to 2 without loss generality assume that $k = 1$ and $l \geq 2$ and $k+l+m = n-3$ $l+m = n-4$. Now we show that $a_4(G_3(1, n-5, 1)) \leq a_4(G_3(k, l, m))$ and $a_6(G_3(1, n-5, 1)) \leq a_6(G_3(k, l, m))$. If possible let

$$a_4(G_3(1, n-5, 1)) \leq a_4(G_3(k, l, m))$$

$$\Rightarrow (m+2)+(m+1)+m > (l+m+1)+(m+l)+lm$$

$$\Rightarrow m+2 > 2l+lm$$

$$\Rightarrow 1 > l$$

Which is a contradiction to $l \geq 2$. ■

Similarly we can prove that $a_6(G_3(1, n-5, 1)) \leq a_6(G_3(k, l, m))$.

Theorem 5.3.2. $G_3(1, n-5, 1) \prec G_3(2, n-7, 2) \prec \ldots \prec G_3(p, n-2p-3, p)$, *where* $p = [\frac{n-3}{3}]$.

Proof. We have

$$\begin{aligned} a_4(G_3(k, n-2k-3, k)) &= k(n-k-2)+n-k-3+k(n-2k-3), \\ a_6(G_3(k, n-2k-3, k)) &= k^2(n-2k-3). \end{aligned}$$

Both these integer valued functions are increasing in $1 \leq k \leq [\frac{n-3}{3}]$ and have maximum value if $k = \left[\frac{n-3}{3}\right]$. Thus the result follows. ■

Theorem 5.3.3. *Let $G^*(k, l, l)$ be the unicyclic graph as shown in Figure 5.2, then*

$$G_3^*(1, l, l) \prec G_3^*(2, l, l) \prec \ldots \prec G_3^*\left(\left[\frac{n-5}{3}\right], l, l\right).$$

Prof: We have

$$\begin{aligned} b_2(G_3^*(k, l, m)) &= n, \\ b_3(G_3^*(k)) &= 2, \\ b_4(G_3^*(k, l, m)) &= |a_4(G_3^*(k, l, m))| \\ &= k(n-k-2)+2(m+1)+(l+m+1)+l(m+1)+m, \\ b_6(G_3^*(k, l, m)) &= |a_6(G_3^*(k, l, m))| \\ &= k(l+1)(m+1)+km+l(m+1)+m. \end{aligned}$$

Therefore,

$$\begin{aligned} b_4(G_3^*(k, l, l)) &= k(n-k-2)+2+n-k-5+n-k-4+n-k-5 \\ &\quad +\frac{1}{4}(n-k-5)^2. \end{aligned}$$

And hence

$$\begin{aligned} b_4'(G_3^*(k,l,l)) &= (n-k-2)-k-1-1-1-\frac{1}{2}(n-k-5) \\ &= n-2k-5-1-\frac{1}{2}(n-k-5) \\ &= \frac{1}{2}n-\frac{3}{2}k-\frac{7}{2} \\ &> 0, \text{ for all } k<\frac{n-7}{3}. \end{aligned}$$

Thus $b_4(G_3^*(k,l,l))$ is an increasing function of k and attains maximum value at $k=[\frac{n-5}{3}]$.

$$\begin{aligned} b_6(G_3^*(k,l,l)) &= k(l+1)^2+kl+l(l+1)+l \\ &= k[\frac{1}{2}(n-k-5)+1]^2+2k[\frac{1}{2}(n-k-5)]+ \\ &\quad \frac{1}{2}(n-k-5)(\frac{1}{2}(n-k-5)+1)+\frac{1}{2}(n-k-5), \end{aligned}$$

$$\begin{aligned} b_6'(G_3^*(k,l,l)) &= [\frac{1}{2}(n-k-5)+1]^2+2k[\frac{1}{2}(n-k-5)+1](-\frac{1}{2})+ \\ &\quad \frac{1}{2}(n-k-5)-\frac{1}{2}k+(-\frac{1}{2})[\frac{1}{2}(n-k-5)+1]+ \\ &\quad (-\frac{1}{2})\frac{1}{2}(n-k-5)-\frac{1}{2} \\ &= \frac{1}{2}(n-k-3)+2k(-\frac{1}{4})(nk-3)+\frac{1}{2}(n-k-5)- \\ &\quad \frac{1}{2}k-\frac{1}{4}(n-k-3)-\frac{1}{4}(n-k-5)-\frac{1}{2} \\ &= \frac{1}{4}(3k^2-k(4n-10)+n^2-6n+5) \\ &> 0 \text{ when } k<\frac{1}{3}(2n-5-\sqrt{n^2-2n+10}). \end{aligned}$$

Therefore b_6 is an increasing function of k for $1\le k\le[\frac{n-5}{3}]$. Thus the result follows. ■

Similarly we have the following theorems.

Theorem 5.3.4. $G_3(l,1,l) \prec G_3(l,1,l) \prec \ldots \prec G_3\left(l, \left[\frac{n-8}{3}\right], l\right)$.

Theorem 5.3.5. $G_4(0,l,l) \prec G_4(1,l,l) \prec \ldots \prec G_4\left(\left[\frac{n-6}{3}\right], l, l\right)$.

Proof. We have

$$\begin{aligned} b_2(G_4(k,l,m)) &= n, \\ b_4(G_4(k,l,m)) &= k(l+m+2) + (l+m+1) + (l+1) + lm + m, \\ b_6(G_4(k,l,m)) &= km(l+1) + lm. \end{aligned}$$

Now

$$\begin{aligned} b_4(G_4(k,l,l)) &= k(2l+2) + (2l+1) + (l+1) + l^2 + l, \\ b_6(G_4(k,l,l)) &= kl(l+1) + lk. \end{aligned}$$

Both are increasing function of k on $0 \le k \le [\frac{n-4}{3}]$. Thus the result follows. ∎

Similarly we have the following proposition.

Theorem 5.3.6. $G_4(l,0,l) \prec G_4(l,1,l) \prec \ldots \prec G_4\left(l, \left[\frac{n-4}{3}\right], l\right)$.

Theorem 5.3.7. $G_4(0,l,l) \prec G_4(1,l,l) \prec \ldots \prec G_4\left(\left[\frac{n-5}{3}\right], l, l\right)$.

Proof. We have

$$\begin{aligned}
b_2(G_4(k,l,m)) &= n,\\
b_4(G_4(k,l,m)) &= k(l+m+3)+2(l+m+2)+2m+lm,\\
b_6(G_4(k,l,m)) &= km(l+2)+2(l+1)m,\\
b_4(G_4(k,l,l)) &= k(2l+3)+2(2l+2)+2l+l^2\\
&= k(n-k-2)+2(n-k-3)+(n-k-5)+\frac{1}{4}(n-k-5)^2,\\
b_4'(G_4(k,l,l)) &= -k+n-k-2-2-1-\frac{1}{2}(n-k-5)\\
&= \frac{1}{2}(n-5-3k)>0,\ \text{for all } k\leq \frac{n-5}{3}.
\end{aligned}$$

Therefore $b_4(G_4(k,l,l))$ is an increasing function of k in $0 \leq k \leq [\frac{n-5}{3}]$.

$$\begin{aligned}
b_6(G_4(k,l,l)) &= kl(l+2)+2(l+1)l\\
&= k[\frac{1}{2}(n-k-1)][\frac{1}{2}(n-k-5)]+2[\frac{1}{2}(n-k-3)][\frac{1}{2}(n-k-5)]\\
&= \frac{1}{4}(k(n-k-1)(n-k-5)+2(n-k-3)(n-k-5)),
\end{aligned}$$

$$\begin{aligned}
b_6'(G_4(k,l,l)) &= \frac{1}{4}(3k^2-4kn+11k+n^2-5n+21)\\
&> 0,\ \text{for all } k<\frac{1}{6}(4n-11-\sqrt{4n^2-28n-108}).
\end{aligned}$$

Therefore $b_6(G_4(k,l,l))$ is an increasing function of k in $0 \leq k \leq [\frac{n-5}{3}]$. ∎

Similarly we have the following theorems.

Theorem 5.3.8. $G_4(l,0,l) \prec G_4(l,1,l) \prec \ldots \prec G_4\left(l, \left[\frac{n-8}{3}\right], l\right)$.

Theorem 5.3.9. $G_4(l,l,0) \prec G_4(l,l,1) \prec \ldots \prec G_4\left(l, l, \left[\frac{n-2}{3}\right]\right)$.

Theorem 5.3.10. *If $G_5(k, n-k-5)$ is a unicyclic graph as shown in Figure 5.2 then* $G_5(0,n-5) \prec G_5(1,n-6) \prec \ldots \prec G_5\left(\left[\frac{n-5}{2}\right], n-5-\left[\frac{n-5}{2}\right]\right)$.

Proof. We have

$$\begin{aligned}
b_2(G_5(k, n-k-5)) &= n, \\
b_4(G_5(k, n-k-5)) &= k(n-k-2) + 2 + (n-k-3) + (n-k-4) + \\
&\quad (n-k-5), \\
b_5(G_5(k, n-k-5)) &= 2, \\
b_6(G_5(k, n-k-5)) &= 2k(n-k-5) + (n-k-5).
\end{aligned}$$

Since $b_4(G_5(k, n-k-5))$, $b_6(G_5(k, n-k-5))$ are increasing function of k in $0 \leq k \leq [\frac{n-5}{2}]$. Hence the result follows. ■

Theorem 5.3.11. *If $G_6(k, n-k-6)$ is a unicyclic graph as shown in Figure 5.2 then $G_6(0, n-6) \prec G_6(1, n-7) \prec \ldots \prec G_6\left(\left[\frac{n-7}{2}\right], n-6-\left[\frac{n-7}{2}\right]\right)$.*

Proof. We have

$$\begin{aligned}
b_2(G_6(k, n-k-6)) &= n, \\
b_4(G_6(k, n-k-6)) &= k(n-k-2) + 2(n-k-3) + (n-k-4) + (n-k-5), \\
b_6(G_6(k, n-k-6)) &= 3k(n-k-6) + 3(n-k-6).
\end{aligned}$$

Since $b_4(G_6(k, n-k-6))$ and $b_6(G_6(k, n-k-6))$ are increasing function of k in $0 \leq k \leq [\frac{n-7}{2}]$. Hence the result follows. ■

Chapter 6

On the distance spectral radius of graphs

In this chapter we study the distance spectral radius of graphs. In section 2, of this chapter we give a special type of operation on a class of simple graphs in order to increase its distance spectral radius.

Trees are very common in the theory and applications of combinatorics. In section 3, we have determined the graphs with maximal and minimal distance spectral radius in the class of tree like graphs.

6.1 Introduction

The distance between two vertices $u, v \in V$ is denoted by d_{uv} and is defined as the length of a shortest path between u and v in G. The distance matrix of G is denoted by $D(G)$ and is defined by $D(G) = (d_{uv})_{u,v \in V}$. Since $D(G)$ is a real symmetric matrix, all its eigenvalues are real. The *distance spectral radius* $\rho(G)$ of G is the largest eigenvalue of its distance matrix $D(G)$. Since $D(G)$ is irreducible, by the Perron-Frobenius Theorem, the eigenvalue $\rho(G)$ is simple, and there exists a unique (up to multiples) positive eigenvector corresponding to $\rho(G)$. The unique normalized eigenvector corresponding to $\rho(G)$ is referred as the *Perron vector* of

$D(G)$.

Let G be a connected graph. Let $\deg(v)$ (or $\deg_G(v)$) denote the degree of the vertex v in G. A pendant path of G is a walk $v_0v_1\ldots v_s (s \geq 1)$ such that the vertices $v_0, v_1, \ldots, v_s$ are distinct, $\deg(v_0) > 2$, $\deg(v_s) = 1$, and $\deg(v_i) = 2$, whenever $0 < i < s$. And v_0, s are called the root and the length of the pendant path, respectively.

Let $x(G) = (x_1, x_2, \cdots, x_n)^t$ be an eigenvector of $D(G)$ corresponding to $\rho(G)$. Then

$$\rho(G)x_i = \sum_{v_j \in V(G)} d_{ij}x_j. \tag{6.1.1}$$

6.2 Operating a graph to increase the distance spectral radius

Here we give a graph transformation which will increase the distance spectral radius for a special class of simple graphs.

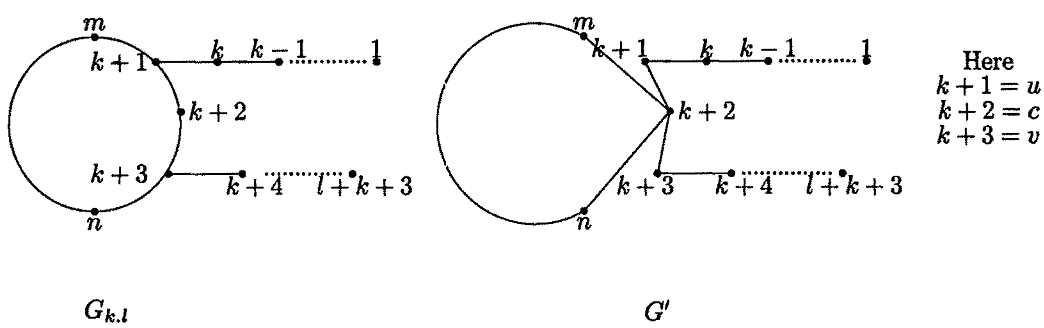


Figure 6.1: The graphs $G_{k,l}$ and G' in Lemma 6.2.1

Lemma 6.2.1. *Let u and v be two non adjacent vertices of a connected graph G such that $c \in N_G(u) \cap N_G(v)$ and all other vertices of G are equidistant from u and v. For positive integers k and l, let $G_{k,l}$ denote the graph obtained from G by adding paths of length k at u and length l at v. Let $m \in N_G(u)$ and $n \in N_G(v)$ and $G' = G_{k,l} - \{(u,m),(v,n)\} + \{(m,c),(n,c)\}$. Then $\rho_1(G') > \rho_1(G_{k,l})$.*

Proof. We label the vertices of $G_{k,l}, G'$ as in Figure 6.1. We partition $V(G_{k,l})$ into $A \cup \{k+2\} \cup \{k+3\} \cup B \cup C$, where $A = \{1, 2, \ldots, k+1\}$; $B = \{k+4, \ldots, l+k+3\}$; $C = \{j | dist(j, k+1) = dist(j, k+3)\}$.

When we pass from $G_{k,l}$ to G', the distances within $A \cup \{k+2\} \cup \{k+3\} \cup B$ and within C are unchanged; the distances between A and C, {k+3} and C are increased by 1; the distances between {k+2} and C is decreased by 1; the distances between B and C is increased by 1.

If the distance matrices are partitioned according to A, {k+2}, {k+3}, B and C, then their difference is

$$D(G') - D(G_{k,l}) = \begin{bmatrix} 0 & 0 & 0 & 0 & e_A(e_C)^t \\ 0 & 0 & 0 & 0 & -(e_C)^t \\ 0 & 0 & 0 & 0 & (e_C)^t \\ 0 & 0 & 0 & 0 & e_B(e_C)^t \\ e_C(e_A)^t & -e_C & e_C & e_C(e_B)^t & 0 \end{bmatrix}$$

where $e_i = \underbrace{(1, \ldots, 1)^t}_{|i|}$ and $i = A, B, C$.

Let $x = (x_1, \ldots, x_n)^t$ be a positive eigenvector corresponding to $\rho_1(G_{k,l})$. Then we have

$$\begin{aligned} \frac{1}{2}(\rho_1(G') - \rho_1(G_{k,l})) &\geq \frac{1}{2}x^t(D(G') - D(G_{k,l}))x \\ &= (\sum_{j\in A} x_j + \sum_{j\in B} x_j + x_{k+3} - x_{k+2}) \sum_{j\in C} x_j \qquad (6.2.1) \end{aligned}$$

By (6.1.1), we have

$$\begin{aligned}\rho_1(G_{k,l})x_{k+1} &= kx_1 + (k-1)x_2 + \ldots + x_k + x_{k+2} + 2x_{k+3} \\ &+ \ldots + (l+2)x_{l+k+3} + \sum_{j\in C} d(k+1,j)x_j \qquad \boxed{6.2.2}\end{aligned}$$

$$\begin{aligned}\rho_1(G_{k,l})x_{k+2} &= (k+1)x_1 + kx_2 + \ldots + 2x_k + x_{k+1} + x_{k+3} \\ &+2x_{k+4} + \ldots + (l+1)x_{l+k+3} + \sum_{j\in C} d(k+2,j)x_j \qquad \boxed{6.2.3}\end{aligned}$$

$$\begin{aligned}\rho_1(G_{k,l})x_{k+3} &= (k+2)x_1 + (k+1)x_2 + \ldots + 3x_k + 2x_{k+1} + x_{k+2} \\ &+x_{k+4} + \ldots + lx_{l+k+3} + \sum_{j\in C} d(k+3,j)x_j \qquad \boxed{6.2.4}\end{aligned}$$

Now (6.2.2)+(6.2.4)-(6.2.3) gives

$$\begin{aligned}\rho_1(G_{k,l})(x_{k+1} + x_{k+3} - x_{k+2}) &= (k+1)x_1 + kx_2 + \ldots + x_{k+1} + 2x_{k+2} + x_{k+3} \\ &+ \ldots + (l+1)x_{l+k+3} + \sum_{j\in C}(d(k+1,j) \\ &+d(k+3,j) - d(k+2,j))x_j > 0 \qquad \boxed{6.2.5}\end{aligned}$$

Since $\rho_1 > 0$, therefore by (6.2.5), we have

$$(x_{k+1} + x_{k+3} - x_{k+2}) > 0 \qquad \boxed{6.2.6}$$

Using (6.2.6) in (6.2.1) we get $\rho_1(G') > \rho_1(G_{k,l})$. ■

6.3 On the distance spectral radius of tree like graphs

Definition 6.3.1. *Let T be a tree on vertices $1, \ldots, n$ and G be any graph of order m. Then T^G is the graph obtained by taking n copies of G, and if $\{i, j\} \in E(T)$, then every vertex in the i^{th} copy of G is made adjacent to its corresponding vertex in the j^{th} copy of G.*

Observe that the order of T^G is nm, and when $G = K_1$, we have that $T^G = T$. We call the tree T the *parent* of T^G.

Example 6.3.2. *Here we consider $T = P_3$, the path on 3 vertices and $G = C_3$, the cycle on 3 vertices. The graph $P_3^{C_3}$ is shown in Figure 6.2.*

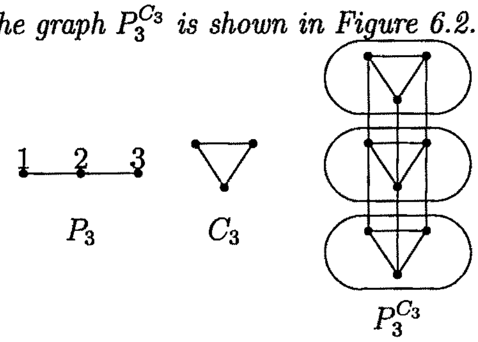


Figure 6.2: The graph $P_3^{C_3}$

Let $\mathcal{T}_G$ be the class containing all T^G, where T is a tree of order n and G is a graph The graphs $P_n^G, S_n^G \in \mathcal{T}_G$, are called a *G-comb* and a *G-bell*, respectively [see Figure 6.3]. By *length*, *centre* and *end vertex* of a G-comb we mean the length, centre and end vertex of its underlying parent path, respectively.

Definition 6.3.3. *A graph G is said to be obtained from a graph H by attaching a graph K to a vertex subset V_1 of $V(H)$, if $G - V_1$ has a component K.*

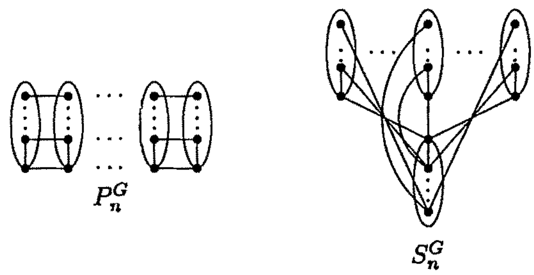


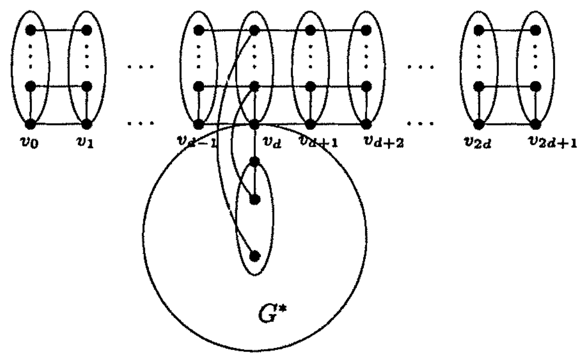
Figure 6.3: The graphs P_n^G and S_n^G

6.3.1 The transformation

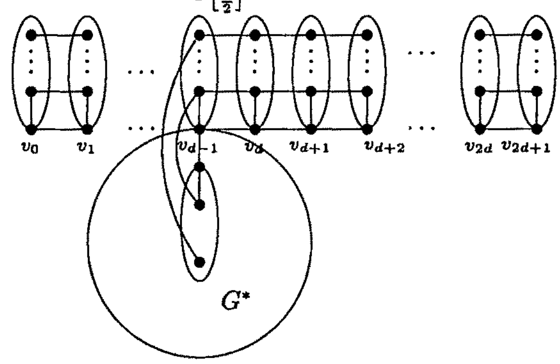
Here we give a graph transformation in the form of lemmas which will be useful to derive our main results.

Lemma 6.3.4. *If G_i is the graph obtained form $P_k^{G_0}$ by attaching a graph G^* to a subset of the vertex set of the i^{th} copy of G_0, in $P_k^{G_0}$, then $\rho(G_{i-1}) > \rho(G_i)$ for all $1 \le i \le \lfloor \frac{d}{2} \rfloor$.*

Proof. Let the vertices of $G_{\lfloor \frac{k}{2} \rfloor}$ be labeled as in Figure 6.4. Suppose k is even and $P_k = v_0 v_1 \dots v_{2d+1}$. Let $V_i = V(G^i) = \{w_i^1, w_i^2, \dots, w_i^m\}$ denote the vertex set corresponding to the i^{th} copy of G_0, where $w_i^1 = v_i$, for $0 \le i \le 2d+1$. Let $G_{\lfloor \frac{k}{2} \rfloor - 1} = G_{\lfloor \frac{k}{2} \rfloor} - \sum_{u \in V_d, v \in N_{G^*}(u)} uv + \sum_{u \in V_{d-1}, v \in N_{G^*}(u)} uv$, and X be the Perron vector of $D(G_{\lfloor \frac{k}{2} \rfloor})$. Suppose X_v denotes the component of X corresponding to



$G_{\lfloor \frac{k}{2} \rfloor}$



$G_{\lfloor \frac{k}{2} \rfloor - 1}$

Figure 6.4: The graphs $G_{\lfloor \frac{k}{2} \rfloor}$ and $G_{\lfloor \frac{k}{2} \rfloor - 1}$ in Lemma 6.3.4

the vertex $v \in G_{\lfloor \frac{k}{2} \rfloor}$. Let us denote $\rho(G_{\lfloor \frac{k}{2} \rfloor}) = \rho_1$ and $\rho(G_{\lfloor \frac{k}{2} \rfloor - 1}) = \rho_2$. Then from $G_{\lfloor \frac{k}{2} \rfloor}$ to $G_{\lfloor \frac{k}{2} \rfloor - 1}$, we have

$$\begin{aligned} \frac{1}{2}(\rho_2 - \rho_1) &\geq \frac{1}{2} X^t (D(G_{\lfloor \frac{k}{2} \rfloor - 1}) - D(G_{\lfloor \frac{k}{2} \rfloor}))X \\ &= \sum_{v \in G^*} X_v \left[\sum_{v \in \bigcup_{i=d}^{2d+1} V_i} X_v - \sum_{v \in \bigcup_{i=0}^{d-1} V_i} X_v \right] \end{aligned} \tag{6.3.1}$$

If $\sum_{v \in \bigcup_{i=d}^{2d+1} V_i} X_v > \sum_{v \in \bigcup_{i=0}^{d-1} V_i} X_v$, then by (6.3.1) we get,

$$\rho_2 > \rho_1. \tag{6.3.2}$$

Assume that $\sum_{v\in\bigcup_{i=d}^{2d+1}V_i} X_v \leq \sum_{v\in\bigcup_{i=0}^{d-1}V_i} X_v$. Then using (6.1.1) we get,

$$\begin{aligned}
&\rho_1(X_{v_d} - X_{v_{d+1}}) \\
&= \sum_{v\in\bigcup_{i=d+1}^{2d+1}V_i} X_v - \sum_{v\in\bigcup_{i=0}^{d-1}V_i} X_v - \sum_{v\in G^*} X_v \\
&\leq -\sum_{v\in V_d} X_v - \sum_{v\in G^*} X_v < 0 \\
\Rightarrow X_{v_d} &< X_{v_{d+1}}.
\end{aligned} \tag{6.3.3}$$

Similarly we get,

$$X_{w_i^j} < X_{w_{i+1}^j}, \tag{6.3.4}$$

where $d \leq i \leq 2d+1$, and $1 \leq j \leq m$.

Again by (6.1.1), when $2 \leq i \leq d$, we have

$$\begin{aligned}
&\rho_1(X_{v_{d-i}} - X_{v_{d+i+1}}) - \rho_1(X_{v_{d-i+1}} - X_{v_{d+i}}) \\
= \; & 2\left[\sum_{v\in\bigcup_{i=d}^{2d+1}V_i} X_v - \sum_{v\in\bigcup_{i=0}^{d}V_i} X_v\right. \\
&\left. -2\sum_{k=0}^{i-1}\left[\sum_{j=1}^{m}\left(X_{w_{d+k+1}^j} - X_{w_{d-k}^j}\right)\right]\right] X_v - \sum_{v\in V_d} X_v.
\end{aligned} \tag{6.3.5}$$

We now prove that $X_{w_{d-i}^j} < X_{w_{d+i+1}^j}$, for $1 \leq i \leq d$, and $1 \leq j \leq m$, by induction on i.

If $i = 1$, then

$$\begin{aligned}
\rho_1(X_{w_{d-1}^1} - X_{w_{d+2}^1}) - \rho_1(X_{w_d^1} - X_{v_{d+1}^1}) &= \rho_1(X_{v_{d-1}} - X_{v_{d+2}}) - \rho_1(X_{v_d} - X_{v_{d+1}}) \\
&= 2\left[\sum_{v\in\bigcup_{i=d+2}^{2d+1}V_i} X_v - \sum_{v\in\bigcup_{i=0}^{d-1}V_i} X_v\right] < 0.
\end{aligned}$$

Therefore, $X_{w^1_{d-1}} - X_{w^1_{d+2}}$ have the same sign as $X_{w^1_d} - X_{v^1_{d+1}}$. Hence by (6.3.4), $X_{w^1_{d-1}} < X_{w^1_{d+2}}$. Similarly we can prove $X_{w^j_{d-1}} < X_{w^j_{d+2}}$, where $2 \leq j \leq m$.

For $i \geq 2$, by induction hypothesis we have,

$$X_{w^j_{d-k}} < X_{w^j_{d+k+1}}, \quad \text{for } 0 \leq k \leq i-1, \quad \text{and } 1 \leq j \leq m.$$

Therefore,

$$-2\sum_{k=0}^{i-1}\left[\sum_{j=1}^{m}\left(X_{w^j_{d+k+1}} - X_{w^j_{d-k}}\right)\right] X_v < 0.$$

Thus by (6.3.5) and induction hypothesis, we have

$$\begin{aligned}
& \rho_1(X_{w^1_{d-i}} - X_{w^1_{d+i+1}}) - \rho_1(X_{w^1_{d-i+1}} - X_{w^1_{d+i}}) \\
= \;& \rho_1(X_{v_{d-i}} - X_{v_{d+i+1}}) - \rho_1(X_{v_{d-i+1}} - X_{v_{d+i}}) \\
< \;& 0 \\
\Rightarrow \rho_1(X_{w^1_{d-i}} - X_{w^1_{d+i+1}}) < \;& \rho_1(X_{w^1_{d-i+1}} - X_{w^1_{d+i}}) < 0, \\
\Rightarrow X_{w^1_{d-i}} - X_{w^1_{d+i+1}} < 0. &
\end{aligned} \tag{6.3.6}$$

Similarly we can prove that

$$X_{w^j_{d-i}} - X_{w^j_{d+i+1}} < 0,$$

for $1 \leq i \leq d$, and $2 \leq j \leq m$. Therefore we have,

$$\sum_{v \in \bigcup_{i=0}^{d-1} V_i} X_v < \sum_{v \in \bigcup_{i=d+2}^{2d+1} V_i} X_v < \sum_{v \in \bigcup_{i=d}^{2d+1} V_i} X_v,$$

a contradiction to our assumption $\sum_{v \in \bigcup_{i=d}^{2d+1} V_i} X_v \leq \sum_{v \in \bigcup_{i=0}^{d-1} V_i} X_v$. Hence

$$\sum_{v \in \bigcup_{i=d}^{2d+1} V_i} X_v > \sum_{v \in \bigcup_{i=0}^{d-1} V_i} X_v,$$

and (6.3.2) holds, i.e. $\rho_2 > \rho_1$.

Let Y be a Perron vector of $D(G_{\lfloor \frac{k}{2} \rfloor -1})$. Then we must have $\sum_{v\in \bigcup_{i=d}^{2d+1} V_i} Y_v > \sum_{v\in \bigcup_{i=0}^{d-1} V_i} Y_v$. Otherwise,

$$\begin{aligned} & \frac{1}{2}(\rho_1 - \rho_2) \\ \geq\ & \frac{1}{2}Y^t(D(G_{\lfloor \frac{k}{2} \rfloor}) - D(G_{\lfloor \frac{k}{2} \rfloor -1}))Y \\ =\ & \sum_{v\in G^*} Y_v \left[\sum_{v\in \bigcup_{i=0}^{d-1} V_i} Y_v - \sum_{v\in \bigcup_{i=d}^{2d+1} V_i} Y_v \right] \\ >\ & 0 \end{aligned}$$

$$\Rightarrow \rho_1 > \rho_2, \text{ a contradiction to (6.3.2).}$$

Let $G_{\lfloor \frac{k}{2} \rfloor -2} = G_{\lfloor \frac{k}{2} \rfloor -1} - \sum_{u\in V_{d-1}, v\in N_{G^*}(u)} uv + \sum_{u\in V_{d-2}, v\in N_{G^*}(u)} uv$. If ρ_3 denotes $\rho(G_{\lfloor \frac{k}{2} \rfloor -2})$, then

$$\begin{aligned} \frac{1}{2}(\rho_3 - \rho_2) &\geq \frac{1}{2}Y^t(D(G_{\lfloor \frac{k}{2} \rfloor -2}) - D(G_{\lfloor \frac{k}{2} \rfloor -1}))Y \\ &= \sum_{v\in G^*} Y_v \left[\sum_{v\in \bigcup_{i=d-1}^{2d+1} V_i} Y_v - \sum_{v\in \bigcup_{i=0}^{d-2} V_i} Y_v \right] > 0 \\ \Rightarrow \rho_3 &> \rho_2. \end{aligned}$$

Repeating the above procedure, we can get a sequence of graphs

$$G_{\lfloor \frac{k}{2} \rfloor}, G_{\lfloor \frac{k}{2} \rfloor -1}, G_{\lfloor \frac{k}{2} \rfloor -2}, \ldots, G_t, \quad \text{where } 2 \leq t \leq d+1,$$

such that

$$\rho(G_{\lfloor \frac{k}{2} \rfloor}) < \rho(G_{\lfloor \frac{k}{2} \rfloor -1}) < \ldots < \rho(G_t).$$

If we take $P = v_0 v_1 \ldots v_d$, then also proceeding as above we can get the same conclusion. ∎

6.3.2 Graphs with extremal distance spectral radius in $\mathcal{T}_G$

Theorem 6.3.5. *The G-bell S_n^G uniquely minimizes the distance spectral radius in $\mathcal{T}_G$.*

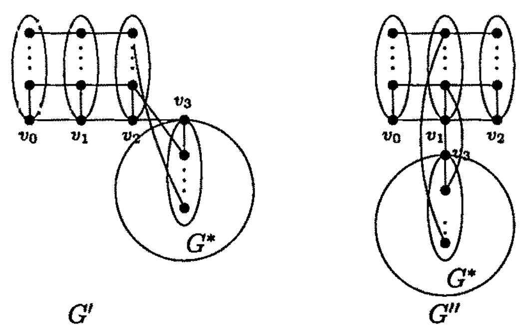


Figure 6.5: The graphs G' and G'' in Theorem 6.3.5

Proof. If the parent tree has order at most 3, then $\mathcal{T}_G = \{S_1^G\}$ or $\mathcal{T}_G = \{S_2^G\}$ or $\mathcal{T}_G = \{S_3^G\}$. So the discussion is trivial in this case. Assume that the parent tree has order at least 4. Let $G' \in \mathcal{T}_G$ be a graph with minimal distance spectral radius. We claim that G' is a G-bell. If not, then there exists one G-comb P_3^G of length 2 as an induced subgraph of G', such that G' is obtained by attaching a graph G^* at the vertex set of the first or the third copy of G in P_3^G [Figure 6.5]. If V_i is the vertex subset corresponding to the ith copy of the G-comb P_3^G, where $1 \leq i \leq 3$, and $G'' = G' - \sum_{u \in V_2, v \in N_{G^*}(u)} uv + \sum_{u \in V_1, v \in N_{G^*}(u)} uv$ is a graph in $\mathcal{T}_G$, then by Lemma 6.3.4, we get $\rho(G') < \rho(G'')$, a contradiction to the minimality of G'. ∎

Theorem 6.3.6. *The G-comb P_n^G uniquely maximizes the distance spectral radius* *in* $\mathcal{T}_G$.

Proof. Let G' be the graph in $\mathcal{T}_G$ with maximal distance spectral radius. If $G' \neq P_n^G$, then G' has an induced subgraph P_k^G for some k. Then by Lemma 6.3.4, we get another graph G'' in $\mathcal{T}_G$ with larger distance spectral radius, which is a contradiction. Therefore, $G' \cong P_n^G$. ■

Chapter 7

Open Problems for further research

From the literature it is apparent that although the spectral properties of graphs have been investigated quite extensively, only the surface of this subject has been scratched so far. Many interesting problems are still open and following are some of them.

7.1 Adjacency Spectrum

1. The characterization of singular graphs by their graph theoretic properties is not solved. Although the singular bipartite graphs have been studied to some extent, the singularity of non-bipartite graphs has not been studied that much.

2. The problem of determining the graphs with maximal adjacency spectral radius has received much attention and has been studied extensively. But the similar problem regarding the minimal adjacency spectral radius has not been investigated as much. For example, following are some open problems in this direction.

   (i) Determining the graphs with minimal adjacency spectral radius among all graphs with a given number of cut-vertices.

(ii) Determining the graphs with minimal adjacency spectral radius among all graphs with a given number of cut-edges.

(iii) Determining the graphs with minimal adjacency spectral radius among all graphs with a given vertex connectivity.

(iv) Determining the graphs with minimal adjacency spectral radius among all graphs with a given edge connectivity.

7.2 Distance Spectrum

The study of the spectral properties of the distance matrix of a graph is relatively new and is much more difficult than that of the adjacency matrix.

1. Some open extremal problems regarding the distance matrix are as follows.

   (i) Determining the graphs with maximal distance spectral radius among all graphs with a given number of cut-vertices.

   (ii) Determining the graphs with maximal distance spectral radius among all graphs with a given vertex connectivity.

   (ii) Determining the graphs with maximal distance spectral radius among all graphs with a given number of cut-vertices and given matching.

2. Even much less is known about the spectrum of the distance matrix of a graph as a whole. In other words, the characterization of graphs by their distance spectrum is an open problem, which is much more difficult than the corresponding problem regarding the adjacency matrix of a graph.

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