# CERTAIN ASPECTS OF SPECTRA OF UNICYCLIC GRAPHS

*Milan Nath*

Department of Mathematics

**INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI**

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*Milan Nath*
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# Certificate

It is certified that the work contained in this thesis entitled **“Certain Aspects of Spectra of Unicyclic Graphs”** by **Milan Nath,** a student of Department of Mathematics, Indian Institute of Technology Guwahati, for the award of the degree of Doctor of Philosophy has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

28 December, 2006

**Dr. Bhaba Kumar Sarma**
Associate Professor
Department of Mathematics
Indian Institute of Technology Guwahati
Guwahati 781039, India

*Dedicated*

*To my wife Preeti*

*and*

*Childhood of our four year son Ayan (popi babu)*

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# ABSTRACT

**Keywords.** Unicyclic graph; Bipartite graph; Adjacency matrix; Spectrum of a graph; Spectral radius of a graph; Singular graph; Matching; Energy of a graph; Corona of graphs.

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This thesis aims at filling some conspicuous gaps in the study of spectra of unicyclic graphs, and answering some recent questions on relations between the structure of a unicyclic graph and the spectrum of its adjacency matrix.

A necessary condition for a graph to be singular in terms of its graph properties is derived. A sufficient condition for a graph to be singular is also obtained. Moreover, it is shown that the necessary condition is also sufficient for acyclic and unicyclic graphs. This characterization is shown to be useful for constructing bases for the null-spaces of trees and unicyclic graphs. All unicyclic graphs which are *minimal configurations* (a very special type of singular graphs of nullity one, defined by Sciriha and Gutman recently) are characterized.

A nonsingular graph is said to have property (SR) if the reciprocal of each of its eigenvalues is also an eigenvalue with same multiplicity. In this thesis, the structure of a unicyclic graph having property (SR) is discussed. It has been shown that such a graph is bipartite; and is a *corona graph* unless it has girth four. In the case it is not a corona, it is shown that the graph can have one of the three specified structures. Families of unicyclic graphs with property (SR) having each of these specific structures are provided.

The unicyclic graphs with maximal spectral radius are studied and four graphs in descending order occupying the highest positions in terms of their spectral radius in the class of all bipartite unicyclic graphs of order $n$ are obtained.

The unicyclic graphs with minimal energy are studied and two unique graphs in ascending order occupying the lowest positions in terms of their energy for each of the two classes, namely, the class of all unicyclic graphs of order $n$ and with a fixed girth $g$; and the class of all bipartite unicyclic graphs of order $n$.

# Contents

# Chapter 1

# Introduction

Combinatorial Matrix Theory, by and large, studies the interrelations between Linear Algebra and Graph Theory. Matrix completion problems, minimum rank problems and spectra of graphs are some of the main areas under this umbrella. 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 and their normalized forms.

The present thesis is the outcome of our study of the spectrum of the adjacency matrix of a unicyclic graph and its relation to the structure of the graph. We entered the scene of graph spectra as late as 2002. Though an extensive study has been made on spectra of graphs by many researchers, we noticed some conspicuous gaps between the known results on spectra of unicyclic graphs. For example, the complete classification of all singular unicyclic graphs was not known. This thesis is intended to fill up certain gaps with some concrete results on the spectra of unicyclic graphs. It also attempts to answer certain recent questions on spectral properties of unicyclic graphs.

## 1.1 Graph terminologies

All graphs we consider in this thesis are finite and simple: undirected and without loops and multiple edges. For a graph $G = (V, E)$ we write $V(G)$ and $E(G)$ for the vertex set $V$ and the edge set $E$ of $G$, respectively. By $|G|$ we mean the order of the graph $G$ and $d(v)$ denotes the degree of a vertex $v$ in $G$. For two vertices $u$ and $v$ in $G$, $d(u, v)$ denotes the distance between $u$ and $v$. We use the standard notations $C_n$, $K_n$, $P_n$ and $S_n$ for the cycle, the complete graph, the path and the star, respectively, on $n$ vertices. By an *empty* graph we mean the complement of $K_n$ for some $n$, that is, a graph having no edge.

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 $2k$ is the order of $G$, then a $k$-matching of $G$ is called a *perfect matching* of $G$.

A tree is a connected acyclic graph (i.e. one without a cycle), and a unicyclic graph is connected and has exactly one cycle. The cycle of the 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 $G$, by $G - S$ we mean the graph obtained by deleting all the elements of $S$ from $G$. 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 $K$ is *attached* at a vertex $v$ of $G$ to mean that a new graph is obtained by joining $v$ and a vertex of $K$ 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.

Let $G$ be a unicyclic graph. For a vertex $v \in V(G)$ we call a component of $G - v$ not containing any vertex of $C$ 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).

We denote the class of all unicyclic bipartite graphs on $n$ vertices by $\mathcal{U}_n^b$ and that of all unicyclic graphs on $n$ vertices with girth $g$ by $\mathcal{U}_{n,g}$.

## 1.2 The adjacency matrix of a graph

Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$. 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.

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.

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

## 1.3 Singularity of a graph

The problem of characterizing a singular graph by its graph theoretic properties was first posed by Collatz and Sinogowitz [13] almost fifty years back. The search for such a characterization was relevant 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. Though several partial answers to this central question are known for long, a characterization of a general singular graph by its graph properties is still elusive.

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

**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 [51, 52, 23, 58, 59].

In Chapter 2, we derive a necessary condition for a graph to be singular in terms of its graph properties. We also give a sufficient condition for a graph to be singular. Moreover, we show that our necessary condition is also sufficient for acyclic and unicyclic graphs. We show how this characterization can be used to construct bases for the null-spaces of trees and unicyclic graphs.

## 1.4 Minimal configuration graphs

Let $\mathbf{x}$ be a kernel eigenvector of the singular graph $G$. The subgraph $\chi = \chi_{\mathbf{x}}$ of $G$ induced by the vertices corresponding to the non-zero entries of $\mathbf{x}$ is called the *core* of $G$ with respect to $\mathbf{x}$ [52]. The set of vertices of $G$ which are not in the core $\chi_{\mathbf{x}}$ is called the periphery $\mathcal{P}$ of $G$ with respect to the core $\chi_{\mathbf{x}}$. If $\eta(G) = 1$, then $\mathbf{x}$ is uniquely determined (up to a multiplicative constant) and therefore $G$ has a unique core $\chi$ and a unique periphery $\mathcal{P}$. A particular class of singular graphs is the following: A graph $G$ with nullity one is called a *minimal configuration* if no two vertices in the periphery are adjacent and deletion of any vertex in the periphery increases the nullity.

A graph which is known to be a minimal configuration can be used to construct many singular graphs with the help of the following result.

**Theorem 1.4.1** [52] *Let $G$ be a singular graph with a core $\chi$ and periphery $\mathcal{P}$. Then the graph $G^N$ produced by joining one or more vertices in $\mathcal{P}$ to vertices of another graph $N$ is singular with $\chi$ as a core.*

Sciriha and Gutman [53] have recently characterized all trees which are minimal configurations.

**Theorem 1.4.2** [53] *A tree is a minimal configuration if and only if it is a subdivision of another tree.*

In Chapter 3, we characterize and single out all unicyclic graphs which are minimal configurations.

## 1.5 Reciprocal properties in the spectra of graphs

It is well known (see [19] Theorem 3.11 for example) that a graph $G$ is bipartite if and only if the negative of each eigenvalue of $G$ is also an eigenvalue of $G$. In contrast to the plus-minus pairs of eigenvalues of bipartite graphs, Barik, Pati and Sarma, [3], have introduced the notion of *graphs with property* (R). Such graphs $G$ have the property that $\frac{1}{\lambda}$ is an eigenvalue of $G$ whenever $\lambda$ is an eigenvalue of $G$. When each eigenvalue $\lambda$ of $G$ and its reciprocal have the same multiplicity, then $G$ is said to have *property* (SR). It has been proved in [3] that a graph $G$ obtained by attaching an additional pendant to each of the vertices of a bipartite graph $G_1$ has property (SR). Moreover, if $G$ is a tree, then $G$ has property (SR) if and only if $G$ is obtained this way from another tree $G_1$. Barik *et al.* [2] have recently shown that a nonsingular tree satisfies property (R) if and only if it satisfies (SR).

In Chapter 4, we study the structure of a unicyclic graph having property (SR). It has been shown that such a graph is bipartite; and is a corona (see Section 1.2 for definition) unless it has girth four. In the case it is not a corona, we show that the graph can have one of the three specified structures. We provide families of unicyclic graphs with property (SR) having each of these specific structures.

## 1.6 Spectral radius of a graph

The investigation of the spectral radius of graphs is an important topic in the theory of graph spectra. Many authors have studied the bounds for the spectral radius of graphs in terms of different parameters and for different subclasses of graphs. We give a brief review of the known results in this direction. Let $G$ be a graph with $n$ vertices and $m$ edges.

The earliest result was obtained in 1957 by Collatz and Sinogowitz [13]: If $G$ is a connected graph on $n$ vertices, then

$$2\cos(\pi(n+1)) = \lambda(P_n) \leq \lambda_1(G) \leq \lambda_1(K_n) = n-1.$$

Brualdi and Hoffman [6] showed in 1985 that if the number of edges in $G$ is $m = \begin{pmatrix} k \\ 2 \end{pmatrix}$ for some $k$, then $\lambda_1(G) \leq k-1$, and that the equality holds if and only if $G$ is a disjoint union of the complete graph $K_k$ and some isolated vertices. This upper bound was modified by Stanley [54] in 1987 as follows:

$$\lambda_1(G) \leq \frac{(-1+\sqrt{1+8m})}{2},$$

where equality occurs if and only if $m = \begin{pmatrix} k \\ 2 \end{pmatrix}$. Friedland [24] further modified this upper bound in 1988 as follows: Suppose that there is no complete graph with $m$ edges so that $m = \begin{pmatrix} k \\ 2 \end{pmatrix} + s,\ \ 0 < s < k$. Then

$$\lambda_1(G) \leq \frac{k-2+\sqrt{k^2+4s)}}{2}.$$

The equality holds if and only if $G$ is a complete graph with one edge removed.

Hong [37] independently showed in 1988 that for a connected graph $G$

$$\lambda_1(G) \leq \sqrt{2m-n+1},$$

and that the equality holds if and only if $G$ is either the star $K_{1,n-1}$ or the complete graph $K_n$.

Let $d_n$ be the minimum degree of the vertices of $G$. Hong *et al.* [39] have proved in 2001 that

$$\lambda_1(G) \leq \frac{d_n-1+\sqrt{(d_n+1)^2+4(2m-d_n n)}}{2},$$

and that the equality holds if and only if $G$ is either a regular graph or a graph (*bidegreed*) in which each vertex is of degree either $d_n$ or $n-1$.

Let $d_1 \geq d_2 \geq \cdots \geq d_n$ be the degree sequence in $G$ and $m_i$ denote the average of the degrees of the neighbours of the $i$-th vertex $v_i$. Favaron *et al.* [22] proved in 1993 that if $G$ does not have any isolated vertex, then

$$d_1 \leq \lambda_1(G) \leq max\{m_i d_i : v_i \in V\}.$$

In 2001 Berman and Zhang [4] found that if $G$ is connected and $d_i$ is the vertex degree of $v_i$, then

$$\lambda_1(G) \leq max\{\sqrt{d_i d_j} : 1 \leq i,j \leq n, v_i v_j \in E\},$$

and the equality holds if and only if $G$ is a regular or a bipartite semiregular graph. This result was further refined by Das and Kumar [21] in 2003 as follow: If $G$ is connected, then

$$\lambda_1(G) \leq max\{\sqrt{m_i m_j} : 1 \leq i,j \leq n, v_i v_j \in E\},$$

and the equality holds if and only if either all $m_i$ are equal or $G$ is a bipartite graph with vertices of same partitioned set have equal values of $m_i$. They also found the following upper bound for the spectral radius of $G$:

$$\lambda_1(G) \leq \sqrt{2m-(n-1)d_1+(d_1-1)d_n},$$

and the equality holds if and only if $G$ is a regular graph or a star graph; and for $d_n \neq 0$

$$\lambda_1(G) \geq \sqrt{\frac{(d_n+f_j-1)+\sqrt{(d_n+f_j-1)^2-4(d_n-1)(f_j-1)+4c_j^2+8c_j\sqrt{d_n}}}{2}},$$

where $f_j = max\{d_k : v_nv_k \in E\}$ and $c_j$ is the number of common neighbors between $v_n$ and $v_j$.

An upper bound for the spectral radius in terms of the girth of $G$ was obtained recently by Fang [56]: If $G$ has girth at least 5 and $d_n$ is the highest degree of $G$, then

$$\lambda_1(G) \leq \frac{-1+\sqrt{4n+4d_1-3}}{2},$$

and the equality holds if and only if $G = C_5$.

It is well-known that for any tree $T$ with $n$ vertices

$$\lambda_1(T) \leq \sqrt{n-1},$$

where the equality holds if and only if $T = S_n$, the star with $n$ vertices. Hofmeister [36] in 1997 has refined this result as follows: The spectral radii of the trees $S_n^k, n \geq 4$, in Figure 1.1 are given by

$$\begin{aligned}
\lambda_1(S_n^1) &= \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-6n+13})},\\
\lambda_1(S_n^2) &= \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-10n+33})},\\
\lambda_1(S_n^3) &= \sqrt{\frac{1}{2}(n-2+\sqrt{n^2-8n+24})},\\
\lambda_1(S_n^4) &= \sqrt{\frac{1}{2}(n-1+\sqrt{n^2-10n+29})},
\end{aligned}$$

and $\lambda_1(S_8^4) = \lambda_1(S_8^{4'})$. If $n \geq 6$ and $T \notin \{S_n, S_n^1, S_n^2, S_n^3, S_n^4, S_8^{4'}\}$, then

$$\lambda_1(T) \leq \lambda_1(S_n^4) \leq \lambda_1(S_n^3) \leq \lambda_1(S_n^2) \leq \lambda_1(S_n^1) \leq \lambda_1(S_n).$$

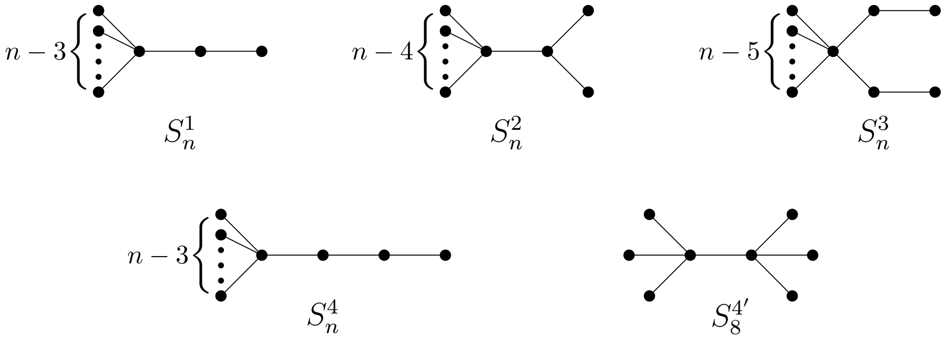


Figure 1.1: The trees $S_n^k$, $n \geq 4$

Moreover, if $n = 5$ and $T \notin \{S_5, S_5^1, S_5^2, S_5^3\}$, then

$$\lambda_1(T) \leq \lambda_1(S_5^3) \leq \lambda_1(S_5^2) \leq \lambda_1(S_5^1) \leq \lambda_1(S_5);$$

and, if $n = 4$ and $T \notin \{S_4, S_4^1, S_4^2, \}$, then

$$\lambda_1(T) \leq \lambda_1(S_4^2) \leq \lambda_1(S_4^1) \leq \lambda_1(S_4).$$

Some more results on the bounds of the spectral radius of a tree in terms of its largest vertex degree and the degree sequence can be seen in [55] and [48], respectively.

Xu *et al.* [62] have proved in 2001 that in the class of all $n$-vertex trees with a maximal matching of a fixed size $k$ the unique tree with largest spectral radius is the tree $K_{1,n-k}^{k-1}$ obtained from the star $K_{1,n-k}$ by attaching a pendent vertex to $k-1$ vertices of degree one in $K_{1,n-q}$.

Though there has been extensive studies on the spectral radius of a tree, the class of unicyclic graphs has not been explored much in this regard. Nevertheless, the following are some main results available in the literature.

Among all $n$-vertex unicyclic graphs, $U_n^3$ has the largest spectral radius, where $U_n^3$ is the graph obtained by joining two pendent vertices of the star $K_{1,n-1}$ by an edge. This is a long-known result obtained by Hong [38] in 1986.

Chang *et al.* [9] have proved in 2003 that the graphs having the largest and the second largest spectral radius in the class of all unicyclic graphs of order $n = 2k$ which have perfect matchings are $U_1$ and $U_2$ (not standard notations), respectively, where $U_1$ is the graph obtained from $C_3$ by attaching $k-2$ copies of $P_2$ together with a pendent vertex to one vertex of $C_3$; and $U_2$ is the graph on obtained from $C_3$ by attaching $k-3$ copies of $P_2$ together with a pendant to one of the three vertices and a pendant to each of the other two vertices of $C_3$. This result has been generalized in 2004 by Aimei *et al.* [66] to the class of all $n$-vertex unicyclic graphs each of which has a maximal matching of a fixed size $m \geq 4$. The graphs having the largest and the second largest spectral radius in this class are $U_1'$ and $U_2'$, respectively, where $U_1'$ is the graph obtained from $C_3$ by attaching $n-2m+1$ pendent vertices and $m-2$ copies of $P_2$ to one of three vertices of $C_3$; and $U_2'$ is the graph obtained from $C_3$ by attaching $m-3$ copies of $P_2$ together with $n-2m+1$ pendants to one of three vertices, and one pendant to each of the other two vertices of $C_3$.

However many other classes of graphs are yet to be studied in this line. Very little is known about the graphs with maximal spectral radius even in the class of bipartite graphs in general.

In Chapter 5, we have found four graphs in descending order occupying the highest positions in terms of their spectral radius in the class of all bipartite unicyclic graphs of order $n$ for $n \geq 10$, and the same four graphs in a different order for $n \leq 9$.

## 1.7 Energy of a graph

The study of 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 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. Triangles seldom appear in chemical graphs, but cycles of higher length can do. Regular graphs also appear very rarely.

In 1931, Hückel [44] 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 $\pi$-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 [19]. This prompted Gutman [30] in 1978 to define energy of a graph as follows: For an $n$-vertex graph $G$ with eigenvalues

$\lambda_i,\ i = 1, 2, \cdots, n$, the *energy* of $G$ is

$$E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1.7.1}$$

Since 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, 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:

$$E(G) \;=\; \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \frac{ix\phi'(G, ix)}{\phi(G, ix)}\right]dx \;=\; \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - x\frac{d}{dx}\ln\phi(G, ix)\right]dx. \tag{1.7.2}$$

The formula (1.7.2) is known as the *Coulson's formula for energy.* If $P(G; x) = \sum_{i=0}^{n} a_i x^{n-i}$, then (1.7.2) gives

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j+1}x^{2j+1}\right)^2\right]. \tag{1.7.3}$$

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

Various empirical and statistical studies (usually performed on graphs of chemical interest, which are connected and possess relatively few edges) in Quantum Chemistry had pointed towards a simple regularity: The energy of a graph increases with the increase of the number of vertices and edges. A famous approximation, quantifying the above regularity, is the McClelland formula [47]

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

which was found chemically quite satisfactory (see [32] for details). A naive extension of this rule to all graphs resulted in the conjecture Gutman [30] in 1978 that among $n$-vertex graphs, the complete graph $K_n$ has maximal energy. It was soon shown (first by Chris Godsil in the early 1980s) that there exist graphs whose energy exceeds $E(K_n)$. A graph $G$, such that $E(G) \geq E(K_n)$, is said to be *hyperenergetic.* There exist hyperenergetic graphs on $n$ vertices, for every $n \geq 9$. Walikar *et al.* [57] 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 [33] has shown in 2000 that

$$2\sqrt{m} \leq E(G) \leq 2m, \tag{1.7.4}$$

and, if $G$ has no isolated vertex, then

$$E(G) \leq 2\sqrt{n-1}. \tag{1.7.5}$$

Moreover, the bound (1.7.5) 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 [47] in 1971.

$$\sqrt{2m + n(n-1)|\det A(G)|^{\frac{2}{n}}} \leq E(G) \leq \sqrt{2mn}. \tag{1.7.6}$$

In 1978, Gutman [30] had shown that

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} = B_1. \tag{1.7.7}$$

For a $k$-regular graph $G$, $k = \frac{2m}{n}$, and we get, as an immediate consequence of (1.7.7),

$$E(G) \leq k + \sqrt{k(n-1)(n-k)} = B_2. \tag{1.7.8}$$

There are regular graphs (all complete graphs for example) for which the equality in (1.7.5) holds. In other words, the bounds $B_1$ and $B_2$ are both sharp. Recently, using (1.7.5) Balakrishnan [1] 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.* [45] has improved the upper bound (1.7.7) for bipartite graphs in 2003 and proved that for such graphs

$$E(G) \leq 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left[2m - 2\left(\frac{2m}{n}\right)^2\right]}. \tag{1.7.9}$$

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

$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{2} + \sqrt{n}), \tag{1.7.10}$$

and characterized the graphs for which (1.7.9) and (1.7.10) are sharp.

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

Graphs with extremal energy have been determined for $n$-vertex trees [29, 46, 69] and $n$-vertex trees with perfect matchings [68]. In [65], for a given positive integer $d$ the tree with the minimal energy having diameter at least $d$ is determined. In [42], 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. In [40] it is proved that for $n \geq 6$ the graph $S_n^3$ is the unique minimal energy graph among all unicyclic graphs of order $n$.

Caporossi *et al.* [8] 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 Hou *et al.* attempted in 2002 to solve the problem, but succeeded only partially.

In Chapter 6, we have found two unique graphs in ascending order occupying the lowest positions in terms of their energy for each of the two classes, namely, the class of all unicyclic graphs of order $n$ with a fixed girth $g$; and the class of all bipartite unicyclic graphs of order $n$.

# Chapter 2

# Singularity of Graphs and the Null Spaces of Trees and Unicyclic Graphs

## 2.1 Introduction

In Section 2 of this chapter, we derive a necessary condition for a graph to be singular in terms of its graph properties. We also give a sufficient condition for a graph to be singular. In Section 3, we show that our necessary condition is also sufficient for acyclic and unicyclic graphs. In Section 4, we show how this characterization can be used to construct bases for the null-spaces of trees and unicyclic graphs.

## 2.2 Singularity of a graph

Let $V(G)$ and $E(G)$ denote the vertex set $\{v_1, v_2, \ldots, v_n\}$ and the edge set of a graph $G$, respectively. The *neighborhood* of a vertex $v \in V$ in $G$ is defined to be $N(v) = \{u \in V(G) \mid \{u, v\} \in E(G)\}$.

**Theorem 2.2.1 (Zero-sum rule)** [16] *A nonzero vector* $(\alpha_1, \alpha_2, \ldots, \alpha_n)^t$ *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 $A(G) = [C_1, C_2, \ldots, C_n]$, 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 2.2.2** 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 2.2.3** *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).*

**Proof.** Let $G$ be singular and

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

be a kernel relation of $G$. 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

$$\sum_{v_j \in V_1} \alpha_j C_j + \sum_{v_j \in V_2} \alpha_j C_j = 0. \tag{2.2.1}$$

Let $X = \bigcup\{N(v) \mid v \in V_1\}$ and $Y = \bigcup\{N(v) \mid v \in V_2\}$. Let $v_k \in V_1$ and $v_i \in N(v_k)$. Then $a_{ik} = 1$. This implies that the $i$th entry of the vector $\sum_{v_j \in V_1} \alpha_j C_j$ is positive. Therefore, in view of (2.2.1), the $i$th entry of the vector $\sum_{v_j \in V_2} \alpha_j C_j$ must be negative. Consequently, $a_{il} = 1$, that is, $v_i \in N(v_l)$ for some $v_l \in V_2$. This shows that $X \subseteq Y$. Similarly, we have $Y \subseteq X$. $\square$

**Definition 2.2.4** 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 2.2.5** *Suppose that $V(G)$ has a pair of subsets $V_1$ and $V_2$ satisfying the property (S). Then $G$ is singular.*

**Proof.** Let $X = \bigcup\{N(v) \mid v \in V_1\} = \bigcup\{N(v) \mid v \in V_2\}$. For $v_i \in X$ we have a unique $v_j \in V_1$, such that $v_i \in N(v_j)$. Consequently, $a_{ij} = 1$ and $a_{it} = 0$ for all other $v_t \in V_1$. Similarly, there exists a unique $v_k \in V_2$ such that $a_{ik} = 1$. On the other hand, if $v_i \notin X$, then $a_{is} = 0$ for all $v_s \in V_1 \cup V_2$. Consequently,

$$\sum_{v_j \in V_1} C_j = \sum_{v_j \in V_2} C_j, \tag{2.2.2}$$

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

From the kernel relation (2.2.2) we have the following.

**Corollary 2.2.6** *Let $V_1, V_2$ be a pair in $V(G)$ satisfying the property (S). Let $\alpha_j$ be defined by*

$$\alpha_j = \begin{cases} 1 & \text{if } v_j \in V_1, \\ -1 & \text{if } v_j \in V_2, \\ 0 & \text{otherwise.} \end{cases} \tag{2.2.3}$$

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

Theorem 2.2.3 gives a necessary condition for $G$ to be singular. In general the condition is not sufficient. For example, consider the complete graph $K_4$ on the vertex set $\{1, 2, 3, 4\}$. Then $V_1 = \{1, 2\}$, $V_2 = \{3, 4\}$ is a minimal pair in $V(K_4)$ satisfying the property (N), though $K_4$ is nonsingular. However, in the next section we will show that for acyclic and unicyclic graphs the condition in Theorem 2.2.3 is also sufficient for the graph to be singular.

Theorem 2.2.5 gives a sufficient condition for $G$ to be singular. However, a singular graph may not satisfy the condition as can be seen from the following example.

**Example 2.2.7** The graph $G$ in Figure 2.1 is singular, $V_1 = \{2, 6\}$, $V_2 = \{4, 7\}$ is the only pair in $V(G)$ satisfying the property (N). However, $1 \in N(2) \cap N(6)$ and therefore $G$ does not satisfy the condition of Theorem 2.2.5.

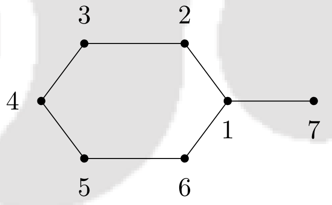


Figure 2.1: A singular graph

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

**Proposition 2.2.8** *Suppose $V_1, V_2$ be a minimal pair in $V(G)$ satisfying the property (N). Let $u$ and $v$ be distinct vertices in $V_1$ (or in $V_2$) and $x \in N(u) \cap N(v)$. Then $u, v$ and $x$ lie on a cycle in $G$.*

**Proof.** Let $u, v \in V_1$ and $x \in N(u) \cap N(v)$. Let $w \in V_2$ such that $x \in N(w)$. Clearly, $u$, $v$, $w$ and $x$ are all distinct. Suppose, if possible, $u, v$ and $x$ do not lie on any cycle in $G$. Then $u$ and $v$ are in different components of $G - x$. Without any loss of generality, we assume that $w$ is not a vertex of the component $G_1$ containing $u$. Let $U_1 = V_1 - V(G_1)$

and $U_2 = V_2 - V(G_1)$. Then $U_1$ and $U_2$ are disjoint and contain $v$ and $w$, respectively. We set $X = \bigcup\{N(z) \mid z \in U_1\}$ and $Y = \bigcup\{N(z) \mid z \in U_2\}$.

Let $u_1 \in U_1$ and $y \in N(u_1)$. If $y = x$, then $y \in N(w)$. Suppose that $y \neq x$. Since $u_1 \in V_1$, we have $u_2 \in V_2$ such that $y \in N(u_2)$. Since $G_1$ is a component of $G - x$, we must have $u_2 \in U_2$, otherwise both $u_1$ and $u_2$ would be vertices of $G_1$ contrary to our choice of $u_1$. Thus $X \subseteq Y$. Similarly, $Y \subseteq X$. This shows that $U_1, U_2$ satisfy the property (N), contradicting the minimality of the pair $V_1, V_2$. □

**Proposition 2.2.9** *Let $G$ be a unicyclic graph and $V_1, V_2$ be a minimal pair in $V(G)$ satisfying the property (N). Let $v$ be a vertex in $V_1 \cup V_2$ not on the cycle of $G$. Then $N(v)$ and $V_1 \cup V_2$ are disjoint.*

**Proof.** Let, if possible, $u_0 \in N(v) \cap (V_1 \cup V_2)$. Then $v \in N(u_0)$ and, therefore, there is $u_1 \in V_1 \cup V_2$ such that $u_0 \neq u_1$ and $v \in N(u_1)$. Since $v$ is not on the cycle of $G$, in view of Proposition 2.2.8, at least one of $u_0$ and $u_1$ (say $u_1$) is not on the cycle. Again, since $v \in N(u_1) \cap (V_1 \cup V_2)$, there is a vertex $u_2$ different from $v$ in $V_1 \cup V_2$ not on the cycle. By induction, for each $n \geq 1$ we get a path $vu_1 \cdots u_n$ with vertices in $V_1 \cup V_2$. However, this is not possible, $G$ being finite. Hence the result follows. □

## 2.3 Singularity of trees and unicyclic graphs

In this section, we show that the converse of Theorem 2.2.3 is true in case $G$ is acyclic or unicyclic. Thereby, we have a characterization of singular trees and singular unicyclic graphs.

By a *trivial tree* we mean a tree with a single vertex. Any other tree is *nontrivial.*

**Theorem 2.3.1** *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).*

**Proof.** (a) $\Rightarrow$ (b). Follows from Theorem 2.2.3.

(b) $\Rightarrow$ (c). Choose a minimal pair $V_1, V_2$ of subsets of $V(T)$ satisfying the property (N). Since $T$ is acyclic, in view of Proposition 2.2.8, $V_1$ and $V_2$ must satisfy the property (S).

(c) $\Rightarrow$ (a). Follows from Theorem 2.2.5. □

We need two lemmas before proving the result for unicyclic graphs.

**Lemma 2.3.2** *Let $G$ be a unicyclic graph. Let $V_1, V_2$ be a minimal pair in $V(G)$ satisfying the property (N). Then, for any distinct $u, v \in V_i$, ($i = 1$ or $2$), $|N(u) \cap N(v)| \leq 1$.*

**Proof.** If possible, let $|N(u) \cap N(v)| > 1$ for some distinct $u, v \in V_1$. Let $x, y \in N(u) \cap N(v)$, $x \neq y$. Then $u, v, x, y$ are all distinct and they form a four cycle in $G$. This must be the unique cycle $C$ of $G$. Let $T_1$ be the component (a tree) of $G - x - y$ containing $u$. Let $w_1, w_2$ be vertices in $V_2$ such that $x \in N(w_1)$ and $y \in N(w_2)$. Clearly, $w_i \notin V(C)$, otherwise $G$ will have another cycle (of length three). Since $x, u$ and $w_1$ do not lie on a cycle, $w_1 \notin V(T_1)$. Similarly, $w_2 \notin V(T_1)$. We put $U_1 = V_1 - V(T_1)$ and $U_2 = V_2 - V(T_1)$. Then $U_1$ and $U_2$ are disjoint. Moreover, $U_1$ contains $v$ and $U_2$ contains $w_1$ and $w_2$. Let $X = \bigcup\{N(w) \mid w \in U_1\}$ and $Y = \bigcup\{N(w) \mid w \in U_2\}$.

Let $z \in N(u_1)$ for some $u_1 \in U_1$. If $z$ is $x$ or $y$, then $z$ is in $N(w_1)$ or $N(w_2)$. Suppose that $z$ is neither of $x$ and $y$. Since $u_1 \in V_1$, we have $u_2 \in V_2$ such that $z \in N(u_2)$. Since $T_1$ is a component of $G - x - y$, we must have $u_2 \in U_2$, otherwise both $u_1$ and $u_2$ would be vertices of $T_1$ contrary to our choice of $u_1$. Thus $X \subseteq Y$. Similarly, $Y \subseteq X$. This shows that $U_1, U_2$ satisfy the property (N), contradicting the minimality of the pair $V_1, V_2$. $\square$

**Lemma 2.3.3** *Let $G$ be a unicyclic graph and $V_1, V_2$ be a minimal pair in $V(G)$ satisfying the property (N). Let $u, v$ be a pair of vertices in $V_1$ such that $N(u) \cap N(v) \neq \emptyset$. Then $N(u')$ and $N(v')$ are disjoint for all pairs $u', v' \in V_2$. Moreover, if $u', v'$ is a pair in $V_1$ different from $u, v$, then $N(u)$ and $N(v)$ are disjoint.*

**Proof.** In view of Lemma 2.3.2, $N(u) \cap N(v) = \{x\}$ for some $x \in V(G)$. Suppose, if possible, there is another pair $u', v'$ in either $V_1$ or $V_2$ such that $N(u') \cap N(v') = \{x'\}$, $x' \in V(G)$. In case $u', v'$ are in $V_1$, we assume that $u, v, u'$ are distinct. Now, in view of Proposition 2.2.8, the vertices $u, v, u', x, x'$ lie on the cycle $C$ of $G$. Since the vertices $u, v, u'$ are all distinct, $x \neq x'$. Moreover, $x'$ must be distinct from at least one of $u$ and $v$; so let $x' \neq u$. Let $T$ be the component (a tree) of $G - x - x'$ containing $u$. Consider the sets $U_1 = V_1 - V(T)$ and $U_2 = V_2 - V(T)$. It can be seen that $U_1$ and $U_2$ satisfy the property (N), contradicting the minimality of $V_1, V_2$. $\square$

**Theorem 2.3.4** *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).*

**Proof.** It is enough to show that the condition is sufficient. We choose a minimal pair $V_1, V_2$ of subsets of $V(G)$ satisfying the property (N). If $V_1, V_2$ satisfy the property (S), then we are done. Otherwise, there is a pair $u, v$ of vertices in $V_1$ (say) such that

$N(u) \cap N(v) \neq \emptyset$. Then, by Lemma 2.3.2, $N(u) \cap N(v) = \{x\}$ for some $x \in V(G)$. In view of Proposition 2.2.8, $u, v$ and $x$ are vertices of the cycle $C$ of $G$. Moreover, in view of Lemma 2.3.3, $N(u') \cap N(v') = \emptyset$ for all other pairs $u', v'$ in $V_1$ and all pairs $u', v'$ in $V_2$. Let $x \in N(w)$, $w \in V_2$. Clearly, $w \notin V(C)$. Let $T$ be the component (a tree) of $G - x$ containing $w$.

Define a function $\alpha$ on $V(G) = \{v_1, v_2, \ldots, v_n\}$ as follows:

$$\alpha(v_i) = \begin{cases} 2, & \text{if } v_i \in V_1 \cap V(T), \\ -2, & \text{if } v_i \in V_2 \cap V(T), \\ 1, & \text{if } v_i \in V_1 - V(T), \\ -1, & \text{if } v_i \in V_2 - V(T), \\ 0, & \text{otherwise.} \end{cases} \tag{2.3.4}$$

We show that $(\alpha(v_1), \alpha(v_2), \ldots, \alpha(v_n))^t$ is a null-eigenvector for $G$, that is, for each $v_i \in V(G)$

$$\sum_{z \in N(v_i)} \alpha(z) = 0. \tag{2.3.5}$$

If $v_i = x$, then

$$\sum_{z \in N(v_i)} \alpha(z) = \alpha(u) + \alpha(v) + \alpha(w) = 0.$$

If $v_i = w$, then $v_i \notin V(C)$ and $N(v_i) \cap (V_1 \cup V_2) = \emptyset$, by Proposition 2.2.9, and therefore (2.3.5) is satisfied. Now, let $v_i$ be different from $x$ and $w$. If $v_i \notin X = \bigcup\{N(z) \mid z \in V_1\} = \bigcup\{N(z) \mid z \in V_2\}$ then $\alpha(z) = 0$ for all $z \in N(v_i)$ and therefore (2.3.5) is satisfied. On the other hand, if $v_i \in X$, then $v_i \in N(u_1)$, $v_i \in N(u_2)$ for unique vertices $u_1 \in V_1$, $u_2 \in V_2$. Clearly, either both of $u_1$ and $u_2$ are in $T$ or both are outside $T$, and therefore (2.3.5) is satisfied. This completes the proof. $\square$

## 2.4 The null-spaces of singular trees and unicyclic graphs

In this section, we show how a basis for the null-space of a graph $G$ can be obtained, when $G$ is either a tree or a unicyclic graph. We note that for each minimal pair $V_1, V_2$ of subsets of $V(G)$ satisfying the property (N) a null-eigenvector is obtained using Corollary 2.2.6, if the pair satisfies the property (S), and using (2.3.4) of Theorem 2.3.4, otherwise. Moreover, the null-eigenvector will have entries in $\{0, \pm 1\}$ and $\{0, \pm 1, \pm 2\}$, respectively, in the two cases.

**Definition 2.4.1** An *elementary unicyclic* graph is a graph $G$ which is either a cycle or is obtained by attaching some pendants to a cycle.

The following result follows from Theorem 1.3.1.

**Proposition 2.4.2** *Let $G$ be an elementary unicyclic graph on $n$ vertices having a pendant. Then $\eta(G) = n - 2q$, where $q$ is the the maximum number of mutually nonadjacent edges in $G$.*

**Corollary 2.4.3** *Let $G$ be an elementary unicyclic graph. Then $G$ is singular if and only if one of the following holds:*

(a) $G = C_n,\ n = 0\ (mod\ 4)$.

(b) *$G$ is of odd order with a single pendant.*

(c) *There are two pendants attached to a vertex of the cycle in $G$.*

(d) *There is a pair of vertices with pendants on the cycle which have an odd number of consecutive vertices between them, none of which has a pendant attached.*

**Proof.** Let $G$ be an elementary unicyclic graph on $n$ vertices. If $G$ has no pendant, then $G = C_n$. We have $\eta(C_n)$ is 2 if $n = 0$ (mod 4) and 0, otherwise (see [19] p.53). Next, suppose that $G$ has a single pendent vertex. In view of Proposition 2.4.2, $G$ is singular if and only if $G$ does not have a perfect matching. This is the case if and only if $C_g$ is an even cycle, that is, $n\,(= g + 1)$ is odd.

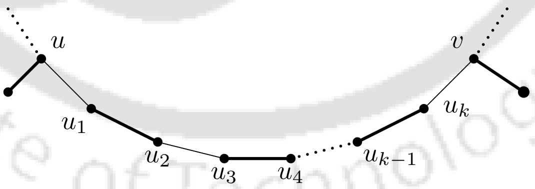


Figure 2.2: The $u$-$v$ path

Finally, let $G$ have more than one pendant. If there are two pendants attached to a vertex of $C_g$, then $G$ does not have a perfect matching, and therefore, $G$ is singular. Suppose that the pendants in $G$ are attached to the distinct vertices of $C_g$. Let $u, v$ be vertices on $C_g$ with pendants attached such that none of the vertices $u_i$ on the path $uu_1u_2 \cdots u_kv$ have pendants (Figure 2.2). If $G$ has a perfect matching $M$, then the edges $u_1u_2, u_3u_4, \ldots, u_{k-1}u_k$ must be in $M$, and therefore $k$ is even. Conversely, if there are even number (possibly zero) of vertices between each such pair of vertices, then $G$ has a perfect matching containing all pendent edges. In other words, if the pendent vertices are attached to distinct vertices of $C_g$, then $G$ is singular if and only if there is a pair of vertices with pendants on $C_g$ which have an odd number of consecutive vertices between them, none of which has a pendant attached. $\square$

**Definition 2.4.4** A matching $M_0$ in a unicyclic graph $G$ is an *outer matching* in $G$ if $G - V(M_0)$ is the disjoint union of an elementary unicyclic graph and a set of isolated vertices (possibly empty). (Note that $M_0 = \emptyset$, if $G$ is elementary.) A path $P$ in a graph $G$ is an *alternating path* relative to a matching $M$ in $G$, if alternate edges in $P$ are in $M$ (terminating edges may or may not be in $M$).

**Remark 2.4.5** (a) For a unicyclic graph $G$ which is not elementary, we construct an outer matching $M_0$ as follows. Let $u_1$ be a (pendent) vertex which is at a maximum distance from the cycle $C$ in $G$ and $v_1$ be the vertex adjacent to $u_1$. Then $v_1$ is not on $C$, since $G$ is not elementary. We choose $e_1 = \{u_1, v_1\}$ as an edge in $M_0$. Clearly, $G - u_1 - v_1$ is a disjoint union of a unicyclic graph $G_1$ and a set of isolated vertices (possibly empty). Suppose, the edges $e_i = \{u_i, v_i\}, 1 \leq i \leq k$, are already chosen for $M_0$ in this manner. Then $G - \{u_i, v_i : 1 \leq i \leq k\}$ is a disjoint union of a unicyclic graph $G_k$ and a set of isolated vertices (possibly empty). If $G_k$ is not elementary, we can choose another edge $e_{k+1} = \{u_{k+1}, v_{k+1}\}$ for $M_0$ by the same process. The process must terminate and an outer matching $M_0$ of $G$ is obtained.

(b) Let $T$ be a nontrivial tree. Using a similar recursive process for $T$, choosing the vertex $u_1$ to be at a maximum distance from the *center* of $T$ (see [35] for definition), we obtain a matching $M_0$ of $T$ such that $V(T) - V(M_0) = \Lambda_0$ is either empty or a set of vertices inducing an empty subgraph in $T$. In this case, we have $\eta(T) = |\Lambda_0|$ by Theorem 1.3.1 and therefore $M_0$ must be a maximal matching of $T$, in view of Theorem 1.3.3.

**Example 2.4.6** Consider the unicyclic graph $G$ in Figure 2.3. Here, the set $M_0$ of edges in bold face in the figure of $G$ is an outer matching of $G$. The corresponding elementary unicyclic graph is $G_0$ (depicted in the figure) and the set of isolated vertices of $G - V(M_0)$ is $\{7, 12, 19\}$.

For the rest of this section $G$ denotes either a tree or a unicyclic graph. We fix an outer matching (resp. a maximal matching) $M_0$ of $G$ constructed as in Remark 2.4.5, if

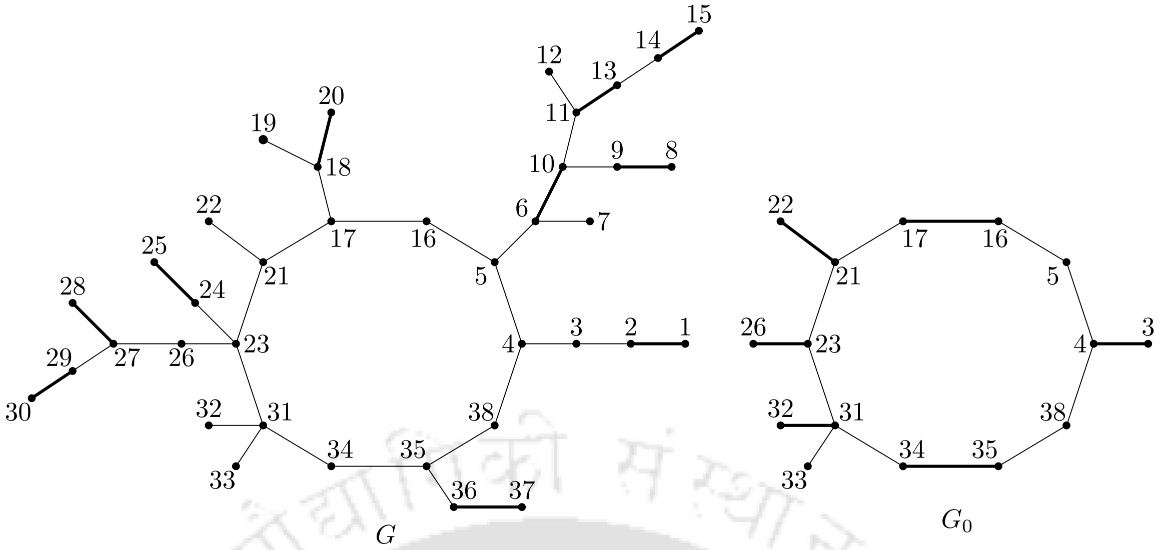


Figure 2.3: An outer matching and the resulting elementary component

$G$ is unicyclic (resp. acyclic). We denote the set of isolated vertices and the elementary unicyclic component (if $G$ is unicyclic) of $G - V(M_0)$ by $\Lambda_0$ and $G_0$, respectively.

**Theorem 2.4.7** *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 $\{u, v\}$ as the attaching edge such that none of $T_v$ and $T_v - v$ has a perfect matching.*

**Proof.** Suppose that $G$ is not elementary. We choose an outer matching $M_0$ of $G$. Let $G - V(M_0)$ be the disjoint union of the elementary unicyclic graph $G_0$ and a set $\Lambda$ of isolated vertices (possibly empty). We note that $G$ is obtained by attaching trees at the vertices of $G_0$. In view of Theorem 1.3.1, we have $\eta(G) = \eta(G_0) + |\Lambda|$. Therefore, $G$ is singular if and only if either $\Lambda \neq \emptyset$ or $G_0$ is singular. Suppose that $\Lambda = \emptyset$. Then $G - V(G_0)$ has a perfect matching, and therefore $G$ is singular if and only if (b) holds. Suppose that $\Lambda \neq \emptyset$ and $w \in \Lambda$. Let $T_v$ be a tree in $G$, attached at a vertex $u$ of the cycle with $\{u, v\}$ as the attaching edge, of which $w$ is a vertex. Since $w \in \Lambda$, $T_v$ 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, (c) holds. $\square$

**Lemma 2.4.8** *Let $x \in \Lambda_0$ and $T_{(x)}$ be the subgraph of $G$ induced by $x$ and the vertices $v$ in $G$ for which there are alternating $x$-$v$ paths. Then* *(a) The vertices in $T_{(x)}$ other than $x$ are in $V(M_0)$.*

*(b) $T_{(x)}$ is a tree.*

*(c) If $y$ in $T_{(x)}$ is at an even distance from $x$, then the degree of $y$ in $T_{(x)}$ is the same as the degree of $y$ in $G$.*

*(d) If $y$ in $T_{(x)}$ is at an odd distance from $x$, then the degree of $y$ in $T_{(x)}$ is two.*

**Proof.** (a) Let $y$ be any vertex on $T_{(x)}$, $y \neq x$. First, suppose that $y$ is adjacent to $x$. Then $y \notin \Lambda_0$, otherwise there would be an edge in the graph induced by $\Lambda_0$. Moreover, if $G$ is unicyclic, then $y \notin G_0$, since $x$ and $G_0$ are distinct components of $G - V(M_0)$. Therefore, $y \in V(M_0)$. Next, suppose that $y$ is not adjacent to $x$ and $[x, u_1, u_2, \ldots, u_r, y]$, $r \geq 1$, is an alternating $x$-$y$ path in $G$. If $r$ is odd, then $y \in V(M_0)$, since in that case the edges $\{u_1, u_2\}, \{u_3, u_4\}, \ldots, \{u_r, y\}$ are in $M_0$. Suppose that $r$ is even so that $\{u_1, u_2\}, \{u_3, u_4\}, \ldots, \{u_{r-1}, u_r\}$ are edges in $M_0$. It can be seen from our construction that if an edge is in $M_0$, then one of its terminating vertices must become pendent on deletion of a set of edges in $M_0$ from $G$. Therefore, since $x$ is not in $V(M_0)$, none of the above edges can be in $M_0$, unless $y \in V(M_0)$.

(b) If the path $P = [x, u_1, u_2, \ldots, u_r, y]$ is alternating, then so are $[x, u_1, u_2, \ldots, u_i]$, $1 \leq i \leq r$, and therefore the path $P$ is in $T_{(x)}$. Thus, $T_{(x)}$ is connected. Moreover, from (a) it follows that $T_{(x)}$ does not contain any vertex of $G_0$ in case $G$ is unicyclic.

(c) Let $y \in V(T_{(x)})$ be at an even distance from $x$. Let $z$ be a vertex in $G$ adjacent to $y$. If $y = x$, then $[x, z]$ is an alternating path and therefore $z \in V(T_{(x)})$. Suppose $y \neq x$ and $[x, u_1, u_2, \ldots, u_r, y]$ is an alternating $x$-$y$ path in $G$. Then $r$ is odd and $\{u_r, y\}$ is an edge in $M_0$. If $z = u_r$, then $z \in V(T_{(x)})$. Suppose $z \neq u_r$. Then $\{y, z\}$ is not an edge of $M_0$ and therefore $[x, u_1, u_2, \ldots, u_r, y, z]$ is an alternating path in $G$. Hence, $z \in V(T_{(x)})$.

(d) Let $y \in V(T_{(x)})$ be at an odd distance from $x$ and $[x, u_1, u_2, \ldots, u_r, y]$ be an alternating $x$-$y$ path in $G$. Then $r$ is even and $\{u_r, y\}$ is not an edge in $M_0$. Since $y \in V(M_0)$, there is a unique $z \in V(G)$ such that $\{y, z\}$ is an edge in $M_0$. Consequently, $[x, u_1, u_2, \ldots, u_r, y, z]$ is an alternating path in $G$. Moreover, since $T_{(x)}$ is a tree, the alternating $x$-$y$ path in $G$ is unique. Hence, $u_r$ and $z$ are the only vertices adjacent to $y$ in $T_{(x)}$. □

**Example 2.4.9** For the graph $G$ in Example 2.4.6 we have $\Lambda_0 = \{7, 12, 19\}$. It is easy to see that, $T_{19}$ is the path $[19, 18, 20]$, $T_{12}$ is the path $[12, 11, 13, 14, 15]$ and $T_7$ is the tree induced by the vertices $6, 7, 8, 9, 10, 11, 13, 14$ and $15$.

**Proposition 2.4.10** *Let $V_1, V_2$ be a minimal pair of subsets of $V(G_0)$ satisfying the property (N) in $G_0$. Let $W_1 = V_1 \cup U_1,\ W_2 = V_2 \cup U_2$, where $U_1$ and $U_2$ are subsets of $V(M_0)$ defined as follows: $y \in U_1$, if there is either an alternating path of length $0 \pmod 4$ from a vertex in $V_1$ or an alternating path of length $2 \pmod 4$ from a vertex in $V_2$ relative to $M_0$; $y \in U_2$, if there is either an alternating path of length $2 \pmod 4$ from a vertex in $V_1$ or an alternating path of length $0 \pmod 4$ from a vertex in $V_2$ relative to $M_0$. Then $W_1, W_2$ is a minimal pair of subsets of $V(G)$ satisfying the property (N) in $G$.*

**Proof.** For $y \in V(M_0)$ let $u$ be the vertex in $G_0$ nearest to $y$. Then $u$ is the unique vertex in $G_0$ such that the $u$-$y$ path is alternating relative to $M_0$. Therefore, $U_1$ and $U_2$ are disjoint. Since $V_1 \cup V_2$ and $V(M_0)$ are disjoint, we have $W_1 \cap W_2 = \emptyset$.

Let $X = \bigcup\{N(y) \mid y \in W_1\}$, $Y = \bigcup\{N(y) \mid y \in W_2\}$. First, let $y_1 \in V_1$ and $z \in N(y_1)$. If $z \in V(G_0)$, then $z \in N(y_2)$ for some $y_2 \in V_2$. If $z \notin V(G_0)$, then there is an alternating path $[y_1, z, y]$ in $G$. Consequently, $y \in U_2$ and $z \in N(y)$.

Next, let $y_1 \in U_1$ and $z \in N(y_1)$. Let $u$ be the vertex in $V_1 \cup V_2$ such that the $u$-$y_1$ path $[u, u_1, u_2, \ldots, u_r, y_1]$ is alternating in $G$ relative to $M_0$. Suppose $z = u_r$. If $r = 1$, then $u \in V_2$ and we put $y_2 = u$. If $r > 1$, then $u_{r-1} \in U_2$ and we put $y_2 = u_{r-1}$. Suppose that $z \neq u_r$. Then $[u, u_1, u_2, \ldots, u_r, y_1, z]$ is alternating and therefore $z \in V(M_0)$. Let $y_2$ be the vertex in $V(M_0)$ such that $\{z, y_2\} \in M_0$. Then the path $[u, u_1, u_2, \ldots, u_r, y_1, z, y_2]$ is alternating in $G$ and $y_2 \in U_2$. Thus, we have $y_2 \in W_2$ such that $z \in N(y_2)$. This shows that $X \subseteq Y$. The reverse inclusion is similar.

Suppose, if possible, there are subsets $W_1'$ and $W_2'$ of $W_1$ and $W_2$, respectively, such that $W_1', W_2'$ satisfy the property (N) in $G$ and at least one of the inclusions is proper. Since $N(y) \cap V(G_0) = \emptyset$ for $y \in U_1 \cup U_2$, the subsets $W_1' \cap V_1$ and $W_2' \cap V_2$ of $V(G_0)$ must satisfy the property (N) in $G_0$. Therefore, we must have $V_1 \subseteq W_1'$ and $V_2 \subseteq W_2'$. We choose a vertex $y \in (W_1 \cup W_2) - (W_1' \cup W_2')$ with minimum distance from $G_0$. Let $u$ be the vertex in $V_1 \cup V_2$ for which the $u$-$y$ path $[u = u_0, u_1, \ldots, u_r, y]$ is alternating. Since $y$ and $u_{r-1}$ are the only vertices in $W_1 \cup W_2$ adjacent to $u_r$, we must have $u_{r-1} \notin W_1' \cup W_2'$. This contradicts our choice of $y$ in case $r > 1$ and the fact that $V_i \subseteq W_i'$, $i = 1, 2$, in case $r = 1$. Hence $W_1, W_2$ form a minimal pair satisfying the property (N) in $G$. □

**Definition 2.4.11** The minimal pair $W_1, W_2$ (in Proposition 2.4.10) satisfying the property (N) in $G$ is said to be *generated by* the minimal pair $V_1, V_2$ in $G_0$.

**Example 2.4.12** Consider the unicyclic graph $G$ in Example 2.4.6. Note that $V_1 = \{3, 17\}$, $V_2 = \{5, 22\}$ is a minimal pair of subsets of $V(G_0)$ satisfying the property (N).

The minimal pair satisfying the property (N) generated by $V_1, V_2$ is

$$W_1 = \{3, 10, 15, 17\},\ W_2 = \{1, 5, 8, 13, 20, 22\}.$$

We now present a systematic approach for finding a basis for the null-space of $G$. The following result gives an overview of our approach.

**Proposition 2.4.13** *Let $\mathcal{V}$ be a collection of minimal pairs $V_1, V_2$ of subsets of $V(G)$ satisfying the property (N). Suppose $\mathcal{V}$ has the property that for each pair $V_1, V_2$ in $\mathcal{V}$ the set $V_1 \cup V_2$ contains a vertex which is not in $U_1 \cup U_2$ for any other pair $U_1, U_2$ in $\mathcal{V}$. Then, the null-eigenvectors obtained from the pairs in $\mathcal{V}$ by (2.2.3) and (2.3.4) are linearly independent.*

**Proof.** Let $V_1, V_2$ be a minimal pair of subsets of $V(G)$ satisfying the property (N). The coordinate corresponding to a vertex $v$ in the null-eigenvector obtained from $V_1, V_2$ by (2.2.3) or (2.3.4) is nonzero if and only if $v \in V_1 \cup V_2$. Therefore, with the given property of $\mathcal{V}$, the null-eigenvector obtained by any pair $V_1, V_2$ in $\mathcal{V}$, has a non-zero coordinate such that the corresponding coordinate in each of the null-eigenvectors obtained by the other pairs in $\mathcal{V}$ is zero. Hence, the result follows. $\square$

To obtain a basis for the null-space of a tree or a unicyclic graph $G$ it is enough to find a collection $\mathcal{V}$ of size $\eta(G)$ consisting of pairs of subsets of $V(G)$ as in Proposition 2.4.13. Then, the vectors obtained using (2.2.3) and (2.3.4) will form a basis for the null-space of $G$.

**Theorem 2.4.14** *Let $G$ be a singular elementary unicyclic graph.*

*(a) If $G$ has no pendant and $G = C_n = (v_1, v_2, \ldots, v_n = v_1)$, then $n = 0 \pmod 4$ and $\eta(G) = 2$. The two pairs $V_1, V_2$ and $V_1', V_2'$ given by*

$$V_1 = \{v_i \mid i = 2 \pmod 4\},\ V_2 = \{v_i \mid i = 0 \pmod 4\},$$

$$V_1' = \{v_i \mid i = 1 \pmod 4\},\ V_2' = \{v_i \mid i = 3 \pmod 4\},$$

*are minimal pairs satisfying the property (S).*

*(b) If $G$ has exactly one pendent vertex, then $n$ is odd and $\eta(G) = 1$. Moreover, if $w$ is the pendent vertex of $G$ attached to the vertex $v_1$ of the cycle $C_{n-1} = (v_1, v_2, \ldots, v_{n-1} = v_1)$, then $(V_1, V_2)$ as defined below is a minimal pair satisfying the property (N).*

*(i) In case* $n = 1 \pmod 4$,

$$V_1 = \{v_i \mid i = 2 \pmod 4\},\ V_2 = \{v_i \mid i = 0 \pmod 4\}.$$

*(The pair satisfies the property (S) in this case.)*

*(ii) In case* $n = 3 \pmod 4$,

$$V_1 = \{v_i \mid d(v_i, w) = 2 \pmod 4\},\ V_2 = \{v_i \mid d(v_i, w) = 0 \pmod 4\}.$$

*(The pair does not satisfy the property (S). The vertices* $v_2, v_{n-2}$ *are in* $V_1$ *and* $v_1 \in N(v_2) \cap N(v_{n-2})$*.)*

*(c) Suppose that* $G$ *has more than one pendent vertex and the pendants are attached at the vertices* $u_1, \ldots, u_k$ *of the cycle* $C$ *of* $G$*. Choose a pendent vertex* $w_i$ *attached at* $u_i$, $1 \leq i \leq k$*. Let* $M_1$ *be a maximal matching in* $G$ *containing the edges* $\{u_i, w_i\}$, $1 \leq i \leq k$*. Then* $\eta(G) = |\Lambda_1|$*, where* $\Lambda_1 = V(G) - V(M_1)$*. For each* $v \in \Lambda_1$, $(V_1, V_2)$ *as defined below is a minimal pair satisfying the property (N).*

*(i) In case* $v$ *is a pendant attached to* $u_i$, $V_1 = \{v\}, V_2 = \{w_i\}$*. (The pair satisfies the property (S).)*

*(ii) In case* $v$ *is on the cycle and* $k = 1$*, consider the subgraph induced by* $C$ *and* $w_1$*, and set* $V_1, V_2$ *as in (b).*

*(iii) In case* $v$ *is on the cycle and* $k \geq 2$*, choose* $w_i$ *and* $w_j$ *such that the* $w_i$*-*$w_j$ *path* $P$ *passing through* $v$ *is of minimum length. Then*

$$V_1 = \{u \in P \mid d(w_i, u) = 0 \pmod 4\},\ V_2 = \{u \in P \mid d(w_i, u) = 2 \pmod 4\}.$$

*(The pair satisfies the property (S).)*

*Moreover,* $V_1 \cup V_2$ *contains no vertex from* $\Lambda_0$ *other than* $v$*.*

**Proof.** The first assertion of (a) follows from the fact that the spectrum of $C_n$, the cycle of order $n$, is $\{2\cos\frac{2k\pi}{n} \mid 1 \leq k \leq n\}$ ([19], p53). Those in (b) and (c) follows from Propositions 2.4.2. Moreover, for the case (iii) of (c), the path $P$ has exactly one vertex from $\Lambda_0$, namely $v$, and therefore $V_1 \cup V_2$ contains no vertex from $\Lambda_0$ other than $v$. The rest of the assertions can be easily verified. □

We note that in each of the cases of Theorem 2.4.14, the collection $\mathcal{V}$ of minimal pairs $(V_1, V_2)$ satisfies the condition of Proposition 2.4.13 and therefore give rise to a basis for the null-space of the elementary unicyclic graph $G$. The final result of this chapter is the following which produces a basis for the null-space of an arbitrary acyclic or unicyclic graph.

**Theorem 2.4.15** *(a) If $G$ is a tree, then $\eta(G) = |\Lambda_0|$. If $G$ is unicyclic, then*

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

*(b) For each $x \in \Lambda_0$, consider the tree $T_{(x)}$ as defined in Lemma 2.4.8. Then*

$$V_1^{(x)} = \{v \in V(T_{(x)}) \mid d(v,x) = 0 \pmod 4\},$$

$$V_2^{(x)} = \{v \in V(T_{(x)}) \mid d(v,x) = 2 \pmod 4\}$$

*is a minimal pair of subsets of $V(G)$ satisfying the property (S). Moreover, $V_1^{(x)} \cup V_2^{(x)}$ contains no vertex from $\Lambda_0$ other than $x$. If $G$ is a tree, then the vectors obtained from these pairs using (2.2.3) form a basis for the null-space of $G$.*

*(c) Let $G$ be unicyclic and $\left\{\left(V_1^{(i)}, V_2^{(i)}\right) \mid 1 \le i \le \eta(G_0)\right\}$ be a collection of pairs of subsets of $V(G_0)$ satisfying the property (N) in $G_0$ giving rise to a basis for the null-space of $G_0$. If $\left(W_1^{(i)}, W_2^{(i)}\right)$ is the pair in $G$ generated by the pair $\left(V_1^{(i)}, V_2^{(i)}\right)$ as in Proposition 2.4.10, then the vectors obtained from the pairs in*

$$\mathcal{V} = \left\{\left(W_1^{(i)}, W_2^{(i)}\right) \mid 1 \le i \le \eta(G_0)\right\} \bigcup \left\{\left(V_1^{(x)}, V_2^{(x)}\right) \mid x \in \Lambda_0\right\}$$

*using (2.2.3) and (2.3.4) form a basis for the null-space of $G$.*

**Proof.** (a) Follows from the reduction formula of Theorem 1.3.1

(b) Since $G$ is connected, $x$ is not an isolated vertex in $G$. Therefore, $T_{(x)}$ is nontrivial and $V_i^{(x)}$ are nonempty. Clearly, the two sets are disjoint. Let $X = \bigcup\{N(z) \mid z \in V_1^{(x)}\}$, $Y = \bigcup\{N(z) \mid z \in V_2^{(x)}\}$. A vertex $z$ in $V_1^{(x)} \cup V_2^{(x)}$ is at even distance from $x$ and therefore have same degree in $T_{(x)}$ and $G$, by Lemma 2.4.8 (c). Consequently, $N(z)$ in $G$ is a subset of $V(T_{(x)})$ and therefore $X$ and $Y$ are subsets of $V(T_{(x)})$. Let $y$ be any vertex in $X$ (or in $Y$). Being adjacent to a vertex in the tree $T_{(x)}$ which is at an even distance from $x$, $y$ is at an odd distance from $x$. In view of Lemma 2.4.8 (d), there are exactly two vertices in $T_{(x)}$ adjacent to $y$. Clearly, one of them is in $V_1^{(x)}$ and the other is in $V_2^{(x)}$. This implies that $y \in X \cap Y$, that is, $X = Y$.

Suppose $U_1 \subseteq V_1^{(x)}$ and $U_2 \subseteq V_2^{(x)}$ is a pair satisfying the property (N). Let $y \in V_1^{(x)} \cup V_2^{(x)}$, $y \neq x$. Let $P = [x, u_1, \ldots, u_{2r} = y]$ be the alternating $x$-$y$ path in $G$. For odd $i$, $u_i$ are vertices of degree two in $T_{(x)}$. Therefore, if $y \notin U_1 \cup U_2$, then none of the vertices $u_{2r-2}, \ldots, u_2, x$ is in $U_1 \cup U_2$. Similarly, if $x \notin U_1$, then $y \notin U_1 \cup U_2$. Hence, we must have $U_1 = V_1^{(x)}$ and $U_2 = V_2^{(x)}$. This proves the first assertion.

The second assertion follows from Lemma 2.4.8(a). If $G$ is a tree, then the collection

$$\left\{\left(V_1^{(x)}, V_2^{(x)}\right) \mid x \in \Lambda_0\right\}$$

satisfies the condition of Proposition 2.4.13, and the third assertion follows.
(c) It is easy to see that $\mathcal{V}$ satisfies the condition of Proposition 2.4.13. $\square$

We illustrate some of the features presented in the last two theorems by two examples.

**Example 2.4.16** Each of the elementary unicyclic graphs in Figure 2.4 has a single pendant and is of odd order. By Theorem 2.4.14(b), each of them is of nullity one and we get a minimal pair of subsets for each of these graphs satisfying the property (N). For the first graph the pair $V_1 = \{2, 6\}$, $V_2 = \{4, 7\}$ satisfying the property (N) is obtained using (i) of Theorem 2.4.14(b). The pair does not satisfy the property (S) and the corresponding null-eigenvector is obtained by (2.3.4). For the second graph we use (ii) of Theorem 2.4.14(b) and obtain the pair $V_1 = \{2, 6\}$, $V_2 = \{4, 8\}$ satisfying the property (S). The corresponding null-eigenvector is obtained by (2.2.3). The two null-eigenvectors are depicted in the respective figure. The coordinate of a vertex in the null-eigenvector is shown as the suffix of the vertex.

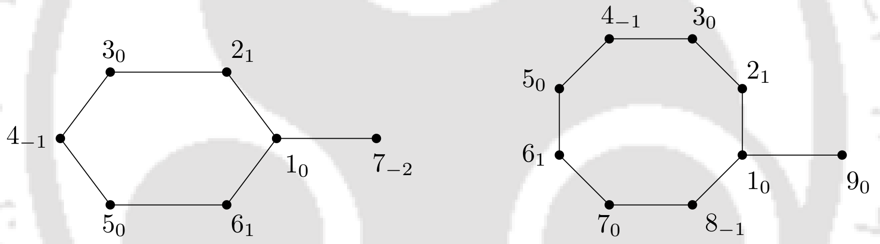


Figure 2.4: Null-eigenvector of elementary unicyclic graphs with a single pendant

**Example 2.4.17** Consider the graph $G$ in Example 2.4.6 (Figure 2.3). The three trees $T_{(19)}, T_{(12)}, T_{(7)}$ corresponding to the vertices in $\Lambda_0 = \{19, 12, 7\}$ give rise to minimal pairs

$$(\{19\}, \{20\}),\ (\{12, 15\}, \{13\}) \text{ and } (\{7, 8, 13\}, \{10, 15\})$$

in $G$, respectively.

Next, we fix a maximal matching $M_1$ of the elementary unicyclic component $G_0$ of $G - V(M_0)$ as one consisting of the edges in bold face in Figure 2.3. We have $\Lambda_1 = V(G_0) - V(M_1) = \{5, 33, 38\}$. Consequently, using Theorem 2.4.14(c), we get three minimal pairs

$$(\{3, 17\}, \{5, 22\}),\ (\{33\}, \{32\}) \text{ and } (\{3, 34\}, \{38, 32\})$$

in $G_0$. Using Proposition 2.4.10, we get minimal pairs

$$(\{3,10,15,17\},\{1,5,8,13,20,22\}),\ (\{33\},\{32\})\ \text{ and }\ (\{3,34\},\{1,32,38\})$$

of $G$ generated by the above minimal pairs in $G_0$.

Using the notation used in Example 2.4.16 and omitting the vertices with zero coordinates, we can now write down the basis for the null-space of $G$ with vectors given by these minimal pairs in $G$ as follows:

$$\begin{array}{l}
(19_1\,,\quad 20_{-1})\,;\\
(12_1\,,\quad 13_{-1},\quad 15_1)\,;\\
(7_1\,,\quad 8_1,\quad 10_{-1},\ 13_1,\ 15_{-1})\,;\\
(1_{-1}\,,\quad 3_1,\quad 5_{-1},\quad 8_{-1},\ 10_1,\quad 13_{-1},\ 15_1,\ 17_1,\ 20_{-1},\ 22_{-1})\,;\\
(32_{-1}\,,\ 33_1)\,;\\
(1_{-1}\,,\quad 3_1,\quad 32_{-1},\ 34_1,\ 38_{-1})\,.
\end{array}$$

# Chapter 3

# Minimal Configuration Unicyclic Graphs

## 3.1 Introduction

Let $\mathbf{x}$ be a null-eigenvector of the singular graph $G$. The subgraph $\chi = \chi_{\mathbf{x}}$ of $G$ induced by the vertices corresponding to the non-zero entries of $\mathbf{x}$ is called the *core* of $G$ with respect to $\mathbf{x}$ [52]. The set of vertices of $G$ which are not in the core $\chi_{\mathbf{x}}$ is called the periphery $\mathcal{P}$ of $G$ with respect to the core $\chi_{\mathbf{x}}$. If $\eta(G) = 1$, then $\mathbf{x}$ is uniquely determined (up to a multiplicative constant) and therefore $G$ has a unique core $\chi$ and a unique periphery $\mathcal{P}$. A particular class of singular graphs with nullity one is the following:

**Definition 3.1.1** [52] A singular graph $G$ of order $n \geq 3$, having a core $\chi$ and periphery $\mathcal{P} = V(G) - V(\chi)$, is a *minimal configuration*, if the following conditions are satisfied:

(i) $\eta(G) = 1$,

(ii) $\mathcal{P} = \emptyset$ or $\mathcal{P}$ induces a graph consisting of isolated vertices,

(iii) in the case when $\mathcal{P} \neq \emptyset$, the deletion of a vertex $v \in \mathcal{P}$ increases the nullity of $G$.

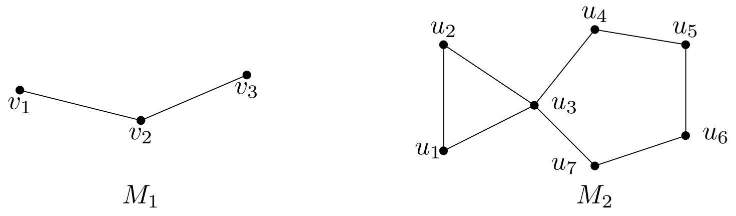


Figure 3.1: The graphs $M_1$ and $M_2$

**Example 3.1.2** *The graphs $M_1$ and $M_2$ in Figure 3.1 are of nullity one with $(1, 0, -1)$ and $(1, 1, -1, -1, 1, 1, -1)$ as a null-eigenvector respectively. Therefore the core of $M_1$ is the subgraph induced by $\{v_1, v_3\}$ and that of $M_2$ is $M_2$ itself. Peripheries of $M_1$ and $M_2$ are $P_1 = \{v_2\}$ and $P_2 = \emptyset$ respectively. Again deletion of $v_2$ in $M_1$ increases the nullity. Thus $M_1$ and $M_2$ are minimal configuration graphs.*

A graph which is known to be a minimal configuration can be used to construct many singular graphs with the help of the following result.

**Theorem 3.1.3** [52] *Let $G$ be a singular graph with a core $\chi$ and periphery $\mathcal{P}$. Then the graph $G^N$ produced by joining one or more vertices in $\mathcal{P}$ to vertices of another graph $N$ is singular with $\chi$ as a core.*

Sciriha and Gutman [53] have recently characterized all trees which are minimal configurations.

**Theorem 3.1.4** [53] *A tree is a minimal configuration if and only if it is a subdivision of another tree.*

In this chapter, we characterize all unicyclic graphs which are minimal configurations.

## 3.2 Minimal configuration unicyclic graphs

We call a tree which is the subdivision of another tree a *subdivision tree.* For $m \geq 1$, let $U_m$ denote the elementary unicyclic graph of order $4m + 3$ with a single pendent vertex $u_0$ (Fig. 3.2). A vertex in $U_m$ is said to be *even* (resp. *odd*) if it is at an even (resp. odd) distance from $u_0$. If $G$ is a graph obtained by attaching trees with perfect matchings at the even vertices of $U_m$, then the vertices in $G$ which are at even (resp. odd) distances from $u_0$ are also called the *even* (resp. *odd*) vertices of $G$.

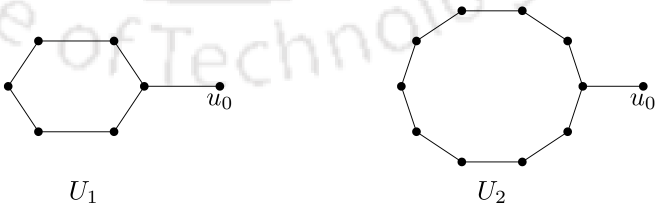


Figure 3.2: The graph $U_m$

We denote by $\mathcal{U}_m$ the class containing the graph $U_m$ and the unicyclic graphs obtained by identifying some pendent vertices of subdivision trees with even vertices of $U_m$. Figure 3.3 shows a graph in $\mathcal{M}_U^{(2)}$.

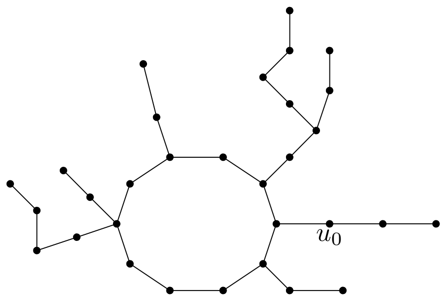


Figure 3.3: A graph in $\mathcal{M}_U^{(2)}$

It is easy to see that for a subdivision tree $T$, the tree $T - v$, where $v$ is pendent in $T$, has a unique perfect matching. Therefore, if $G \in \mathcal{U}_m$, then $G$ has a unique outer matching ( Definition 2.4.4 ) $M_0$ and $G - V(M_0) = U_m$.

The main result of this chapter is the following:

**Theorem 3.2.1** *A unicyclic graph $G$ is a minimal configuration if and only if $G \in \mathcal{U}_m$ for some $m \geq 1$.*

**Lemma 3.2.2** *Let $G$ be any graph in $\mathcal{U}_m$. Then $\eta(G) = 1$.*

**Proof.** It follows from Theorem 2.4.14(b) that $\eta(U_m) = 1$. Therefore by Theorem 1.3.1, we have $\eta(G) = \eta(G - V(M_0)) = \eta(U_m) = 1$. □

**Lemma 3.2.3** *Let $G$ be any graph in $\mathcal{U}_m$. Then the empty graph induced by the even vertices of $G$ is a core of $G$.*

**Proof.** Consider the subsets

$$V_1 = \{v \in V(U_m) \mid d(v, u_0) = 0 \ (\text{mod } 4)\},$$

$$V_2 = \{v \in V(U_m) \mid d(v, u_0) = 2 \ (\text{mod } 4)\}$$

of $V(U_m)$.

By Theorem 2.4.14(b)(ii), $(V_1, V_2)$ is a minimal pair in $U_m$ satisfying the property (N). The minimal pair $(W_1, W_2)$ in $G$ generated by $(V_1, V_2)$ (see Definition 2.4.11) is given by

$$W_1 = \{v \in V(G) \mid d(v, u_0) = 0 \ (\text{mod } 4)\},$$

$$W_2 = \{v \in V(G) \mid d(v, u_0) = 2 \ (\text{mod } 4)\}$$

Clearly $(W_1, W_2)$ is the set of all even vertices in $G$ and no two them are adjacent. □

**Lemma 3.2.4** *Let $G \in \mathcal{U}_m$ and $v$ be an odd vertex in $G$. Then $\eta(G - v) = 2$.*

**Proof.** First, we consider the case when $v$ is on the cycle of $G$. By Theorem 1.3.2, we have $\eta(G-v)=\eta(U_m-v)$. Now, if $v$ is adjacent to $u_0$, then $U_m-v$ is the disjoint union of a path of length $4m+1$ and an isolated vertex and, therefore, $\eta(G-v)=2$. If $v$ is not adjacent to $u_0$, then by repeated application of Theorem 1.3.1, we get $\eta(G-v)=\eta(U_m-v)=\eta(S_4)=2$, where $S_4$ is the star formed by $u_0$, the vertex $u_1$ on $C_g$ adjacent to $u_0$ and the two vertices on $C_g$ adjacent to $u_1$.

Next, consider the case when $v$ is not a vertex on the cycle of $G$. Since all pendent vertices of $G$ are at even distances from $u_0$, $v$ is not pendent in $G$. In fact, $G-v$ has exactly two components. The component of $G-v$ containing the cycle is in $\mathcal{U}_m$ and therefore has nullity one. The other component of $G-v$ is either an isolated vertex or a subdivision tree, and therefore has nullity one. Hence, the result follows. $\square$

***Proof of the sufficient part of Theorem 3.2.1.*** Since no two odd vertices in $G$ are adjacent, the periphery of $G$ consists of isolated vertices. The result follows now from the previous three lemmas. $\square$

**Lemma 3.2.5** *Let $G$ be unicyclic graph obtained by attaching trees with perfect matchings at some vertices of a singular elementary unicyclic graph $G_0$. Given a core $\chi_0$ of $G_0$, there is a core $\chi$ of $G$ such that $V(\chi_0)=V(\chi)\cap V(G_0)$.*

**Proof.** Let $\alpha_0$ be a kernel eigenvector of $G_0$ corresponding to the core $\chi_0$. Let $T_i, 1\leq i\leq r$, be the trees with perfect matchings attached to the vertices $w_i, 1\leq i\leq r$, (not necessarily distinct) of $G_0$. Since each $T_i$ has a perfect matching, $T_i+w_i$ is of odd order, and therefore is singular. For each $i$ let $\alpha_i$ be a kernel eigenvector corresponding to a core $\chi_i$ of $T_i+w_i$. Since $T_i$ is nonsingular, $w_i$ is a vertex of $\chi_i$, that is, $\alpha_i(w_i)\neq 0$. Moreover, $w_i$ being pendent in $T_i+w_i$, by the zero-sum rule, we must have $\alpha_i(w_i')=0$, where $w_i'$ is the vertex in $T_i+w_i$ adjacent to $w_i$. Now, consider the function $\alpha$ on $V(G)$ defined by

$$\alpha(v)=\begin{cases}\alpha_0(v), & \text{if } v\in V(G_0),\\ \alpha_0(w_i)\alpha_i(v)/\alpha_i(w_i), & \text{if } v\in V(T_i), 1\leq i\leq r.\end{cases}$$

It is easy to check that the sum of the values of $\alpha$ over the neighbors of any vertex $v$ in $G$ is zero. Therefore, by the zero-sum rule, $\alpha$ is a kernel eigenvector of $G$. Clearly, for the core corresponding to this eigenvector of $G$ the result holds. $\square$

**Lemma 3.2.6** *Let $G$ be a unicyclic graph and $T_v$ be a tree in $G$ attached at the vertex $u$ of the cycle with $\{u,v\}$ as the attaching edge. If both $T_v$ and $T_v-v$ are singular, then $G$ is not a minimal configuration.*

**Proof.** By Theorem 2.4.7, $G$ is singular. Suppose that $\eta(G) = 1$. We show that the core of $G$ is a subgraph of $T_v$ and therefore the vertices on the cycle of $G$ are in the periphery of $G$. In other words, the periphery is not consisting of isolated vertices, and the result will follow.

We first show by induction on the order $k$ of $T_v$ that $T_v$ has a core not containing $v$ as a vertex. We note that $k \geq 3$. If $k = 3$, then the only candidate for $T_v$ is the path $P_3$ with $v$ as the middle vertex. The empty subgraph of $T_v$ formed by its pendent vertices is the core of $T_v$ not containing $v$. Now, suppose that the result is true for all such $T_v$ with order less than $k > 3$.

Suppose that $T_v - v$ has two singular components (trees) $T_1$ and $T_2$. Let $\chi_1$ and $\chi_2$ be cores of $T_1$ and $T_2$, respectively. If $v$ is not adjacent to any vertex of one of $\chi_i$ $(i = 1, 2)$, then $\chi = \chi_i$ is a core of $T_v$ not containing $v$ as a vertex. Otherwise, the disjoint union $\chi$ of $\chi_1$ and $\chi_2$ is a core of $T_v$ not containing $v$ as a vertex.

Next, let $T_1$ be the only singular component of $T_v - v$, with $w$ as the vertex in $T_1$ adjacent to $v$ in $T_v$. Then, $T_1$ is nontrivial; otherwise $T_v$ will have a perfect matching, contradicting the fact that $T_v$ is singular. Moreover, if $T_1 - w$ has a perfect matching, then so does $T_v$, which is not true. Hence, both of $T_1$ and $T_1 - u$ are singular. Since $T_1$ has order less than $k$, by induction hypothesis, $T_1$ has a core $\chi$ not containing $w$.

Now, $w$ being in the periphery of $T_1$ with respect to $\chi$, in view of Theorem 1.4.1, $\chi$ is a core of $T_v$ not containing $v$.

Finally, the result follows by noting that a core of $T_v$ not containing $v$ as a vertex is a core of $G$, by Theorem 1.4.1. □

**Lemma 3.2.7** *Let $G$ be an elementary unicyclic graph. If $G$ is a minimal configuration, then $G = U_m$ for some $m \geq 1$.*

**Proof.** Suppose $G$ is a minimal configuration. Since $G$ is singular, $G$ satisfies one of the conditions stated in Corollary 2.4.3. Since $\eta(C_n) = 0$ or 2, $G$ is not a cycle. If there are two pendants attached at a vertex of the cycle of $G$, then these pendent vertices will form the unique core of $G$. However, this is not true since the periphery of $G$ induces a subgraph with isolated vertices. Hence, the pendants in $G$ are attached to distinct vertices of its cycle.

Suppose, if possible, $G$ has more than one pendant. Since $G$ is singular, by Corollary 2.4.3, we have a pair $u, u'$ of vertices on the cycle with pendants $v, v'$, respectively, such that there are odd number of vertices between them on the cycle none of which has a pendant attached. Now, let $P$ be the $v$-$v'$ path through these vertices. Then the vertices on $P$ which are at even distances from $v$ will induce the unique core of $G$. Consequently, $u$ and $u'$ are in the periphery of $G$. However, this implies that the vertices of the other $u$-$u'$ path on the cycle are in the periphery of $G$, contradicting the fact that the periphery of $G$ induces a subgraph with isolated vertices. Hence, $G$ contains exactly one pendant. Moreover, in view of Corollary 2.4.3(b), this implies that $G$ has order $2k+1$ for some integer $k$.

Let $u_0$ be the pendent vertex in $G$ and $v$ the vertex adjacent to $u_0$. If $k$ is even, then the subgraph of $G$ induced by the vertices on the cycle which are at even distances from $u_0$ form the core of $G$. Consequently, the periphery of $G$ does not induce a subgraph with isolated vertices, since both $u_0$ and $v$ are in the periphery. Hence, $k = 2m+1$ for some $m$ and $G = U_m$. □

**Corollary 3.2.8** *Let $G$ be a unicyclic graph obtained from an elementary unicyclic graph $G_0$ by attaching trees such that $G - V(G_0)$ has a perfect matching. If $G$ is a minimal configuration, then $G_0 = U_m$ for some $m \geq 1$.*

**Proof.** By the reduction formula of Theorem 1.3.1, we have $\eta(G_0) = \eta(G) = 1$. Let $\chi$ and $\chi_0$ be the unique cores of $G$ and $G_0$, respectively. Then by Lemma 3.2.5, $V(\chi_0) = V(\chi) \cap V(G_0)$. In particular, the periphery of $G_0$ is either empty or induces an empty subgraph of $G_0$. Now, let $v$ be any vertex in the periphery of $G_0$. Using Theorem 1.3.1, we have $\eta(G_0 - v) = \eta(G - v) \geq 2$. Thus, $G_0$ is a minimal configuration elementary unicyclic graph. The result is now follows from the previous lemma. □

**Lemma 3.2.9** *Let $G$ be a minimal configuration obtained by attaching trees with perfect matchings at some vertices of $U_m$. Let $v$ be a pendent vertex of $G$ which is at a maximum distance from $U_m$ and $u$ the vertex adjacent to $v$. Then $G-u-v$ is a minimal configuration unicyclic graph.*

**Proof.** Let $T$ be the tree attached to $U_m$ which contains the pendent vertex $v$. Since $T$ has a perfect matching and $v$ is at a maximum distance from $U_m$, $u$ must have degree 2. Therefore, $G - u - v$ is connected. Now, using Theorem 1.3.1, $\eta(G - u - v) = \eta(G) = 1$. Let $\alpha$ be a kernel eigenvector and $\chi$ the unique core of $G$. Using the zero-sum rule on $\alpha$ at $v$, we see that $\alpha(u) = 0$, that is, $u$ is in the periphery of $G$. This in turn implies that $v$ is in the core of $G$, since the periphery induces a null subgraph. Using the zero-sum rule, it can be easily checked that the restriction of $\alpha$ on $V(G - u - v)$ is a kernel eigenvector of $G - u - v$. In particular, the periphery of $G - u - v$ is contained in the periphery of $G$, and therefore is either empty or induces a null subgraph of $G - u - v$. Finally, for any $z$ in the periphery of $G-u-v$, we have $\eta(G-u-v-z)=\eta(G-z)\geq 2$, using Theorem 1.3.1. Hence, $G-u-v$ is a minimal configuration. $\square$

***Proof of the necessary part of Theorem 3.2.1.*** If $G$ is elementary, then by Lemma 3.2.7, we have $G=U_m$ for some $m\geq 1$. Therefore, suppose that $G$ is not elementary. Then, in view of Theorem 2.4.7, Lemma 3.2.6 and Corollary 3.2.8, $G$ is obtained from some $U_m$ by attaching trees $T_i$, $1\leq i\leq r$, with perfect matchings at vertices $w_i$, $1\leq i\leq r$, (not necessarily distinct) of $U_m$.

Suppose, if possible, $w_i$ is an odd vertex of $U_m$ for some $i$. Since the core of $U_m$ is induced by its even vertices, $w_i$ is in the periphery of $U_m$. Therefore, in view of Theorem 1.4.1, the nontrivial tree $T_i+w_i$ is in the periphery $\mathcal{P}$ of $G$, contradicting the fact that $\mathcal{P}$ induces a subgraph with isolated vertices. Hence, each $w_i$ is an even vertex of $U_m$.

The proof will be complete if we show that each of the trees $T_i+w_i$ is a subdivision tree. We show this by induction on the size $k$ of $V(G)-V(U_m)\geq 2$. If $k=2$, then there is a single tree $T_1=P_2$ attached to $w_1$. Then, $T_1+w_1=P_3$, which is a subdivision tree. Suppose that the result is true for $2\leq k\leq k_0$, and let the size of $V(G)-V(U_m)$ be $k_0$. Consider a pendent vertex $v$ of $G$ which is at a maximum distance from $U_m$ and let $u$ be the vertex adjacent to $v$. Without any loss of generality, let $v$ be on $T_1$. In view of Lemma 3.2.9, $G-u-v$ is a minimal configuration, and therefore, by induction hypothesis each of the trees $T_i+w_i, 2\leq i\leq r$, and $T_1+w_1-u-v$ are subdivision trees. It is easy to see that $T_1+w_1$ is also a subdivision tree. By induction, the result follows. $\square$

# Chapter 4

# A Strong Reciprocal Property of Unicyclic Graphs

## 4.1 Introduction

If a graph $G$ has property(SR), then the characteristic polynomial of $G$ has a palindrome-like behaviour with respect to the magnitudes of its co-efficients (see Lemma 4.2.1). We use heavily this property of $G$, to study the unicyclic graph which have property(SR). Moreover, we use the standard technique for computing the co-efficients of the characteristic polynomial of a graph. A *linear subgraph* $L$ of $G$ is a disjoint union of some paths of length one and some cycles in $G$. Let

$$P(G;x) = a_0x^n + a_1x^{n-1} + \cdots + a_n, \tag{4.1.1}$$

be the characteristic polynomial of $A(G)$. Then $a_0(G) = 1,\ a_1(G) = 0$ and $-a_2(G)$ is the number of edges in $G$. In general, we have (see [19] Theorem 1.3)

$$a_i = \sum_{L\in \mathcal{L}_i} (-1)^{c_1(L)}(-2)^{c_2(L)},\ i = 1, 2, \dots, n, \tag{4.1.2}$$

where $\mathcal{L}_i$ is the set of all linear subgraphs $L$ of $G$ of size $i$ and $c_1(L)$ denotes the number of components of size 2 in $L$ and $c_2(L)$ denotes the number of cycles in $L$. We note that if $G$ has two pendant vertices with a common neighbor, then $G$ is singular, because in that case $G$ cannot have a linear subgraph of size $n$. If $G$ is bipartite, then one gets $a_i = 0$, whenever $i$ is odd, and

$$P(G;x) = \sum_{i=0}^{[n/2]} (-1)^i\, b_{2i}\, x^{n-2i}, \tag{4.1.3}$$

where $b_{2i}$ are nonnegative. The following results are often used to calculate the characteristic polynomials of graphs.

**Lemma 4.1.1** [19] *Let $e = \{u, v\}$ be an edge of $G$, and $\mathcal{C}(e)$ be the set of all cycles containing $e$. Then*

$$P(G;x) = P(G-e;x) - P(G-u-v;x) - 2\sum_{Z\in\mathcal{C}(e)} P(G-Z;x).$$

**Lemma 4.1.2** [19] *Let $v$ be a vertex in the graph $G$ and $\mathcal{C}(v)$ be the set of all cycles containing $v$. Then*

$$P(G;x) = xP(G-v;x) - \sum_{u} P(G-u-v;x) - 2\sum_{Z\in\mathcal{C}(v)} P(G-Z;x),$$

*where the first summation extends over all $u$ adjacent to $v$.*

**Lemma 4.1.3** [19] *Let $v$ be a vertex of degree 1 in the graph $G$ and $u$ be the vertex adjacent to $v$. Then*

$$P(G;x) = xP(G-v;x) - P(G-u-v;x).$$

**Definition 4.1.4** [35] Let $G_1$ and $G_2$ be two graphs on disjoint sets of n and m vertices, respectively. The *corona* $G_1 \circ G_2$ of $G_1$ and $G_2$ is defined as the graph obtained by taking one copy of $G_1$ and $n$ copies of $G_2$, and then joining the $i$-th vertex of $G_1$ to every vertex in the $i$-th copy of $G_2$.

Note that the corona $G_1 \circ G_2$ has $n(m+1)$ vertices and $|E(G_1)| + n(|E(G_2)| + m)$ edges. Let us denote the cycle on $n$ vertices by $C_n$ and the complete graph on $n$ vertices by $K_n$. The coronas $C_3 \circ K_2$ and $K_2 \circ C_3$ are shown in Figure 4.1.

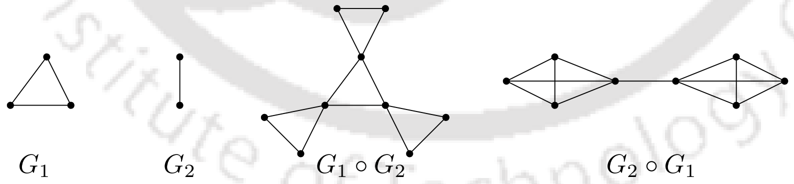


Figure 4.1: Corona of two graphs.

The following result gives a class of graphs with property (SR).

**Theorem 4.1.5** [3] *Let $G = G_1 \circ K_1$, where $G_1$ is any graph. Then $\lambda$ is an eigenvalue of $G$ if and only if $-1/\lambda$ is an eigenvalue of $G$. Further, if $G_1$ is bipartite then $G$ has property (SR).*

Trees with property (SR) has been classified as follows.

**Theorem 4.1.6** [3] *Let $T$ be a tree on $n$ vertices. Then $T$ has property (SR) if and only if $T = T_1 \circ K_1$, for some tree $T_1$.*

Moreover, the following result has recently been proved.

**Theorem 4.1.7** [2] *A nonsingular tree $T$ satisfies property (R) if and only if it satisfies (SR).*

**Example 4.1.8** There are bipartite and non-bipartite graphs with property (SR) which are not corona graphs. For example, one can easily verify that the graphs in Figure 4.2 have property (SR). In fact, the eigenvalues of the graph $H_1$ and $H_2$ are

$$\pm\sqrt{\frac{4+\sqrt{3}+\sqrt{15+8\sqrt{3}}}{2}}, \pm\sqrt{\frac{4+\sqrt{3}-\sqrt{15+8\sqrt{3}}}{2}},$$

$$\pm\sqrt{\frac{4-\sqrt{3}+\sqrt{15-8\sqrt{3}}}{2}}, \pm\sqrt{\frac{4-\sqrt{3}-\sqrt{15-8\sqrt{3}}}{2}};$$

$$1, 1, \frac{-3\pm\sqrt{5}}{2}, \frac{1+\sqrt{33}+\sqrt{18+2\sqrt{33}}}{4}, \frac{1+\sqrt{33}-\sqrt{18+2\sqrt{33}}}{4},$$

$$\frac{1-\sqrt{33}+\sqrt{18-2\sqrt{33}}}{4}, \frac{1-\sqrt{33}-\sqrt{18-2\sqrt{33}}}{4}.$$

respectively. $H_2$ is not a corona has been argued in [3]. Note also that the graph $H_1$ is unicyclic and $H_2$ is not even bipartite. We can argue that $H_1$ is not the corona of two graphs. Suppose that $H_1 = G_1 \circ G_2$. Thus $8 = |H_1| = (|G_2|+1)|G_1|$, where $|G|$ means the number of vertices of $G$. Note that $|G_1|$ cannot be 1 or 2, because in that case $H_1$ would have a vertex of degree more than 3. On the other hand, $|G_1|$ is not 4, otherwise $H_1$ would have four pendent vertices.

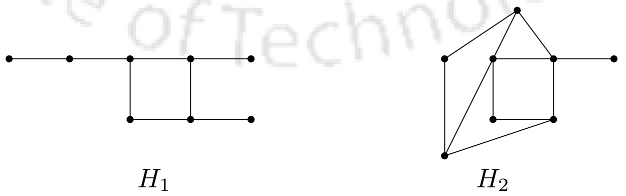


Figure 4.2: Graphs with property (SR) which are not coronas.

In view of the previous example it is clear that a unicyclic graph with property (SR) may not be a corona and this motivates us to study unicyclic graphs with property (SR).

## 4.2 Unicyclic graphs with property (SR)

In this section we study the structure of unicyclic graphs with girth $g$ and property (SR). We show that any such graph is bipartite. Further, if $g \neq 4$, then the graph is a corona graph.

**Lemma 4.2.1** *Let $G$ be a graph on $n$ vertices with property (SR) and $P(G;x)$ be as given in (4.1.1). Then $|a_i(G)| = |a_{n-i}(G)|$, for $i = 0, 1, \ldots, n$.*

**Proof.** Since $G$ has property (SR), $G$ is nonsingular. Moreover, $P(G;x)$ and $x^n P(G;\frac{1}{x})$ have the same roots. Since $P(G;x)$ is monic and the leading coefficient of $x^n P(G;\frac{1}{x})$ is $a_n = \pm 1$, it follows that $P(G;x) = \pm\, x^n P(G;\frac{1}{x})$ and the conclusion follows. □

**Lemma 4.2.2** *Let $G$ be a unicyclic graph of order $n$ with property (SR). Then $G$ has a unique perfect matching. In particular $n = 2m$, for some integer $m$ and there is an odd tree-branch of $G$ at a vertex of the cycle.*

**Proof.** A linear subgraphs of size $n$ in $G$ is either a perfect matching or the union of a perfect matching of $G - C$ and the cycle. Therefore, from (4.1.2), we have

$$a_n(G) = \pm\Big(m_0(G) \pm 2 \times m_0(G-C)\Big), \tag{4.2.4}$$

where $m_0(H)$ denotes the number of perfect matchings of a graph $H$. As $G$ has property (SR), it follows from Lemma 4.2.1 that $|a_0| = |a_n| = 1$.

Since $a_n$ is odd, it follows from (4.2.4) that $m_0(G) \neq 0$, that is, $G$ has a perfect matching. Consequently, $n$ is even. Let $n = 2m$.

Suppose, if possible, that $m_0(G - C) > 0$, i.e. $G - C$ has a perfect matching. Thus $C$ is an even cycle. As $m_0(C) = 2$, and since a matching of $G - C$ and a matching of $C$ give rise to a matching of $G$, we have

$$2m_0(G-C) = m_0(G-C)m_0(C) \leq m_0(G).$$

By (4.2.4) the above inequality is strict. Thus there is a perfect matching $M$ of $G$ which does not contain a perfect matching of $C$. That is, in $M$ a vertex $u$ of $C$ is matched to a vertex $v$ of $G - C$. So there is an odd tree-branch at $v$. But then $G - C$ cannot have a perfect matching. This is a contradiction.

Hence $m_0(G-C) = 0$ and so $m_0(G) = 1$. The final conclusion now follows easily. □

**Lemma 4.2.3** *Let $G$ be a unicyclic graph with property (SR). If $G = G_1 \circ G_2$ then $G_2 = K_1$.*

**Proof.** Let $G_1$ be of order $n_1$ and $G_1$ be of order $n_2$. Suppose that $G_2 \neq K_1$. Then $n_2 \geq 2$. Notice that if $G_2$ has more than one isolated vertex, then $G$ cannot have a perfect matching. Therefore, $G_2$ must have an edge. As $G$ is unicyclic, it follows that $n_1 = 1$ and $G_2 = K_2$ or $G_2 = K_2 + K_1$. In both the cases $G$ does not have the property (SR). $\square$

For the rest of this chapter, we write "$G$ is a corona" to mean that $G = G_1 \circ K_1$ for some graph $G_1$.

**Definition 4.2.4** Let $K$ be any graph with a perfect matching $M$. An alternating path $P$ (relative to $M$) (see Definition 2.4.4) in $K$ is said to be *strong*, if the terminating edges of $P$ are in $M$.

**Lemma 4.2.5** *Suppose $G$ is a unicyclic graph of order $n = 2m$ with a perfect matching. Then the number of $(m-1)$-matchings of $G$ is at least $n$.*

**Proof.** Let $M = \{e_1, e_2, \ldots, e_m\}$ be a perfect matching of $G$. Let $f_1, f_2, \ldots, f_m$ be the other $m$ edges of $G$, which are not in $M$. Now,

$$\{e_1, \ldots, e_m\} - \{e_1\}, \{e_1, \ldots, e_m\} - \{e_2\}, \ldots, \{e_1, \ldots, e_m\} - \{e_m\}$$

are $(m-1)$-matchings of $G$. Moreover, for each $f_j$ we have a unique alternate path $e_i f_j e_k$ of length three in $G$, and thereby an $(m-1)$-matching $(M - \{e_i, e_k\}) \cup \{f_j\}$ of $G$. $\square$

Let $\mathcal{L}_G$ denote the collection of linear subgraphs of the unicyclic graph $G$ of size $n-2$ with $C$ as a component. By $m_1$ we denote the number of $(m-1)$-matchings of $G$. We note that the linear subgraphs in $\mathcal{L}_G$ have the same number of components ($t$ say). Thus, from Equation (4.1.2), we have

$$a_{n-2}(G) = (-1)^{m-1} m_1 + (-1)^t 2|\mathcal{L}_G|. \tag{4.2.5}$$

**Lemma 4.2.6** *Let $G$ be a unicyclic graph of order $n$ with property (SR). Then the following are equivalent.*

*(i) $G$ is a corona,*

*(ii) there is no strong alternating path in $G$ of length 5,*

*(iii) $m_1 = n$,*

*(iv) $\mathcal{L}_G$ is empty.*

**Proof.** By Lemma 4.2.2, $n = 2m$, for some $m$.

(i)⇒(ii). If $G$ is a corona then $G$ has $m$ pendant vertices and has the unique perfect matching containing all the leaves. So there is no strong alternating path of length 5 in $G$.

(ii)⇒(iii). Since $G$ has a unique matching, arguing in the line of the previous lemma, we see that a $(m-1)$-matching is either a subset of the perfect matching or it corresponds to a strong alternating path. As there is no strong alternating path of length more than 3, it follows from the previous lemma that $m_1 = n$.

(iii)⇒(iv). Note that by Lemma 4.2.1 $|a_{n-2}| = |a_2| = n$, the number of edges in $G$. As $m_1 = n$, it follows now from (4.2.5) that $\mathcal{L}_G$ is empty.

(iv)⇒(i). If $\mathcal{L}_G$ is empty, using $|a_{n-2}| = |a_2| = n$, we get that $m_1 = n$ and hence by previous lemma there is no strong alternating path of length more than 3. If $G$ is not a corona, then there is an edge $(u, v) \in M$, the perfect matching such that $d(u), d(v) \geq 2$. Thus there is a path $[u_0, u, v, v_0]$ such that $(u_0, u), (v, v_0) \notin M$. Note that $u_0$ is matched to some vertex by $M$, and so is $v_0$. Then we get a strong alternating path of length 5, unless $(u_0, v_0) \in M$. But then $G$ has a cycle $C$ of girth 4 and $G$ has more than one perfect matchings. This is not possible, by Lemma 4.2.2. Thus $G$ is a corona. ☐

We know from Theorem 4.1.5 that if $G$ is a bipartite graph which is also a corona, then $G$ has property (SR). A unicyclic graph with property (SR) need not be a corona is evident from Example 4.1.8 ($H_1$ satisfies the property (SR) but is not a corona). However, the following lemma shows that such a graph is necessarily bipartite.

**Theorem 4.2.7** *Let $G$ be a unicyclic graph with property (SR). Then the girth $g$ of $G$ is even. Further, if $g \not\equiv 0 \pmod 4$ then $G$ is a corona.*

**Proof.** Suppose that $g$ is odd. Then $|\mathcal{L}_G| = 0$, and therefore by Lemma 4.2.6, $G$ is a corona. In view of Theorem 4.1.5, $\lambda, -\frac{1}{\lambda}$ have the same multiplicity in $\sigma(G)$. As $G$ has property (SR), $-\frac{1}{\lambda}, -\lambda$ have the same multiplicity in $\sigma(G)$. Thus $\lambda, -\lambda$ have the same multiplicity in $\sigma(G)$. Thus $G$ is bipartite, contradicting the fact that $G$ has an odd cycle. So $g$ is even.

Let $g = 2l$. Then by (4.2.5), we have

$$a_{n-2}(G) = (-1)^{m-1}m_1 + (-1)^{m-l}2|\mathcal{L}_G| = (-1)^{m-1}(m_1 + (-1)^{l-1}2|\mathcal{L}_G|). \qquad (4.2.6)$$

Since $l$ is odd in the present case, $n = |a_{n-2}(G)| = m_1 + 2|\mathcal{L}_G|$. As $m_1 \geq n$, by Lemma 4.2.5 we must have $|\mathcal{L}_G| = 0$, and the result follows from Lemma 4.2.6. ☐

**Lemma 4.2.8** *Let $G$ be a non-corona unicyclic graph with property (SR). Then $G$ has exactly two odd tree-branches at (say) $u, v \in C$. Every other vertex on $C$ is matched to a point on $C$ and the distance between $u$ and $v$ on $C$ is odd.*

**Proof.** From Theorem 4.2.7, $g \equiv 0 \pmod 4$. Moreover, by Lemma 4.2.6, we have $|\mathcal{L}_G| \neq 0$. By Lemma 4.2.2, there is at least one odd tree-branch at a vertex, say, $u \in C$. As the order of the graph and the cycle are both even, there must be another odd tree-branch, say, at $v \in C$.

Let $D$ be a linear subgraph of $G$ in $\mathcal{L}_G$. Clearly $D$ misses at least one vertex from each odd tree-branch at a vertex of $C$. Since $D$ covers $n-2$ vertices of $G$, it follows that the number of such odd tree-branches is at most 2. Thus $G$ has exactly two such odd tree-branches. Thus every other vertex on $C$ is matched to a point on $C$ and hence the distance between $u$ and $v$ on $C$ is odd. $\square$

**Lemma 4.2.9** *Let $G$ be a unicyclic graph with property (SR). Denote by $\mathcal{P}_G$ the set of all strong alternating paths of length more than 3. Then $|\mathcal{P}_G| = 2|\mathcal{L}_G|$.*

**Proof.** If $g \not\equiv 0 \pmod 4$ then $G$ is a corona, by Theorem 4.2.7. Hence $\mathcal{P}_G = \emptyset = \mathcal{L}_G$.

Suppose now that $g \equiv 0 \pmod 4$. It follows from (4.2.6) that

$$n = |a_{n-2}(G)| = m_1 - 2|\mathcal{L}_G|. \tag{4.2.7}$$

Let $M$ be the unique matching in $G$ and $m = |M|$. Note that any $(m-1)$-matching is either a subset of $M$ or is obtained uniquely by a strong alternating path. Following the argument in the proof of Lemma 4.2.5, we see that the number of $(m-1)$-matchings in $G$ (recall that it is $m_1$) is exactly $n + |\mathcal{P}_G|$. The result follows by using (4.2.7). $\square$

Suppose that $G$ is a non-corona unicyclic graph with property (SR). Then by Lemma 4.2.8, $G$ has exactly two odd tree-branches at vertices of $C$. For convenience, we shall always use that $T_1, T_2$ are the odd tree-branches of $G$ at the vertices $w_1, w_2 \in C$, respectively, and the edges $\{w_1, v_1\}, \{w_2, v_2\}$ are edges in the unique perfect matching, where $v_i \in T_i$, respectively. We call a vertex $u$ of $T_i$, $i = 1, 2$, a *distinguished vertex* if $T_i - u$ has a perfect matching. Let $r_i$ $(i = 1, 2)$ be the number of distinguished vertices in $T_i$. The following relation between $r_i$ and $\mathcal{L}_G$ is crucial for further developments.

**Lemma 4.2.10** *Let $G$ be a non-corona unicyclic graph with property (SR). Then $|\mathcal{L}_G| = r_1 r_2$.*

**Proof.** Let $D$ be any linear subgraph of $G$ of size $n-2$ containing $C$. Then $D$ will miss exactly one vertex from the trees $T_1$ and $T_2$. If these points are $u_1$ and $u_2$ respectively, then $D$ will induce a perfect matching of $T_i - u_i$, for $i = 1, 2$. Thus $u_i$ are distinguished points. Since the perfect matching of a forest (if it exists) is unique, each such pair $(u_1, u_2)$ will give rise to a unique linear subgraph of $G$ of size $n-2$ containing $C$. Hence the result follows. $\square$

The following lemma is crucial for further developments.

**Lemma 4.2.11** *Let $T$ be a tree such that $T - v$ has a perfect matching $M_v$ and $u$ be another vertex in $T$. Suppose that $[v = v_1, \cdots, v_r = u]$ is the unique path from $v$ to $u$ in $T$. Then $T - u$ has a perfect matching $M_u$ if and only if $r = 2k + 1$, for some $k$ and the edges $\{v_{2i}, v_{2i+1}\} \in M_v$.*

**Proof.** If $[v = v_1, \cdots, v_{2k+1} = u]$ be a path such that the edges $\{v_{2i}, v_{2i+1}\} \in M_v$, then clearly,

$$M_u = M_v \cup \Big\{\{v_{2i-1}, v_{2i}\} : i = 1, \cdots, k\Big\} \setminus \Big\{\{v_{2i}, v_{2i+1}\} : i = 1, \cdots, k\Big\}$$

is a perfect matching of $T - u$.

Conversely, take a $u$ such that $T-u$ has a perfect matching $M_u$. Let $[v = v_1, \cdots, v_r = u]$ is the unique path from $v$ to $u$ in $T$. Suppose if possible, that $\{v, x\} \in M_u, x \neq v_2$. In that case the component of $T - v$ which contains $x$ is odd. Thus $T - v$ could not be a perfect matching. Thus $\{v_1, v_2\} \in M_u$ and $\{v_2, v_3\} \notin M_u$. Thus $T - u - v_1 - v_2$ has no odd components.

Obviously $\{v_1, v_2\} \notin M_v$. If $\{v_2, y\} \in M_v, y \neq v_3$ then $T - v_1 - v_2$ has an odd component containing $y$. But then $T - u - v_1 - v_2$ has the same odd component, a contradiction. Thus $\{v_2, v_3\} \in M_v$. Hence $T - v_3$ has a perfect matching (apply the first paragraph). Hence as in the last paragraph, $\{v_3, v_4\} \in M_u$ and $\{v_3, v_4\} \notin M_v$.

Continuing this way, we see that $\{v_{2i}, v_{2i+1}\} \in M_v$ and $\{v_{2i-1}, v_{2i}\} \in M_u$. Since $\{v_{r-1}, v_r\} \notin M_u$, we see that $r$ is odd. $\square$

**Corollary 4.2.12** *Under the assumptions of Lemma 4.2.11, $T - u$ has a perfect matching if and only if $T - \{v = v_1, v_2, \cdots, v_r\}$ has each component of even order.*

**Proof.** To prove the 'if' part, note that $T - v$ has a perfect matching $M_v$. Let $S = \{v_i, i = 2, \cdots, 2k+1\}$. If any $v_i \in S$ is matched to a vertex $x \notin S$ in $M_v$, then $T - \{v = v_1, v_2, \cdots, v_{2k+1}\}$ should have an odd component. It follows that $v_2$ is matched to $v_3$ in $M_v$, $v_4$ is matched to $v_5$ in $M_v$ and so on. It now follows from Lemma 4.2.11 that $T - u$ has a perfect matching.

The 'only if' part is easier to see. ☐

**Theorem 4.2.13** *Let $G$ be a unicyclic graph with property (SR) and girth $g \neq 4$. Then $G$ is a corona.*

**Proof.** Suppose that $G$ is not a corona. Then by Theorem 4.2.7, $g = 4(k+1)$, for some positive integer $k$. Following Lemma 4.2.8, let $T_i, w_i, v_i$, $i = 1, 2$ be as discussed earlier. In view of Lemma 4.2.9 and Lemma 4.2.10 we have

$$|\mathcal{P}_G| = 2r_1r_2. \tag{4.2.8}$$

We prove that (4.2.8) cannot hold and the result will follow.

By Lemma 4.2.8, both the $v_1$-$v_2$ paths are strong alternating and their lengths are either $5, 7$ or $3, 9$. Let $x_1, x_2$ be the vertices on the longer paths, adjacent to $w_1, w_2$, respectively.

Note that from any distinguished vertex (other than $v_1$) $u_1$ of $T_1$ there are two strong alternating paths to each distinguished vertex of $T_2$ and these paths have lengths at least 5. Similarly, from any distinguished vertex (other than $v_2$) $u_2$ of $T_2$ there are two strong alternating paths to $v_1$ these paths have lengths at least 5. Thus

$$|\mathcal{P}_G| \geq 2(r_1 - 1)r_2 + 2(r_2 - 1) + 3 = 2r_1r_2 + 1,$$

where the term 3 counts the strong alternating path between $v_1, v_2$, the strong alternating path between $v_1, x_2$, and the strong alternating path between $v_2, x_1$. ☐

## 4.3 Non-corona unicyclic graphs with property (SR)

A necessary condition for a non-corona unicyclic graph to have property (SR) is that the girth is four. One can easily see that it is not sufficient. In this section, we study the structure of a non-corona unicyclic graph with property (SR) and show that it has one of three specific structures. We supply examples to show the existence of families of graphs with property (SR) in each of these cases.

**Lemma 4.3.1** *Let $G$ be a non-corona unicyclic graph with property (SR). Let $T_i$, $i = 1, 2$ be the two odd-tree branches of $G$ and $r_i$ be the number of distinguished vertices in $T_i$, $i = 1, 2$, respectively. Then $2 \leq r_1 + r_2 \leq 3$.*

**Proof.** It is obvious that $2 \leq r_1 + r_2$. Note that from any distinguished vertex (other than $v_1$) $u_1$ of $T_1$ there are two strong alternating paths to each distinguished vertex of

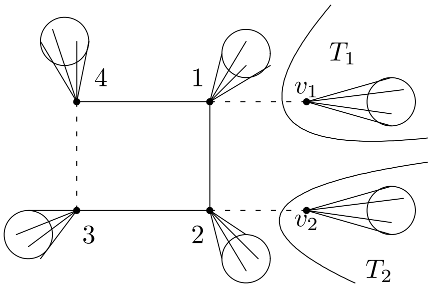


Figure 4.3: The graph $G$.

$T_2$, one strong alternating path to the vertex 3 and these paths have lengths at least 5. (See Figure 4.3).

From any distinguished vertex (other than $v_2$) $u_2$ of $T_2$ there are two strong alternating paths to $v_1$, one strong alternating path to the vertex 4 and these paths also have lengths at least 5.

There is one strong alternating path of length 5 from $v_1$ to $v_2$. Thus

$$|\mathcal{P}_G| \geq 2(r_1 - 1)r_2 + (r_1 - 1) + 2(r_2 - 1) + (r_2 - 1) + 1 = 2r_1r_2 + r_1 + r_2 - 3.$$

In view of Lemma 4.2.9 and Lemma 4.2.10, we have

$$|\mathcal{P}_G| = 2|\mathcal{L}_G| = 2r_1r_2.$$

So, $r_1 + r_2 \leq 3$. $\square$

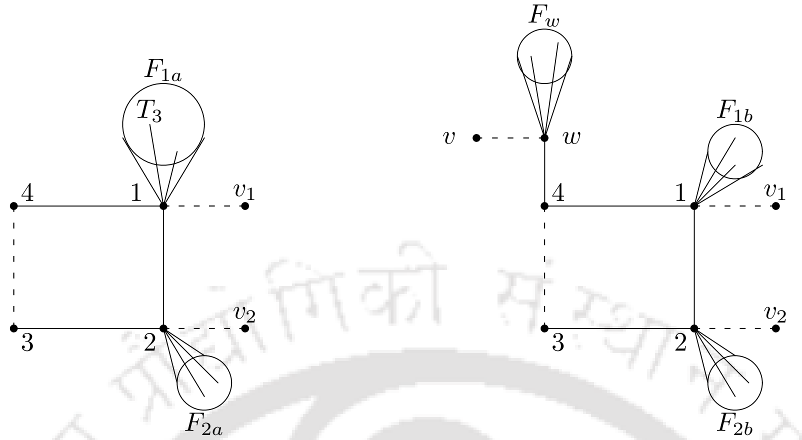
In view of the previous lemma, we have two cases: $r_1 = r_2 = 1$ or $r_1 = 1, r_2 = 2$. Accordingly, the necessary conditions on the structure of $G$ are described by the following results.

**Theorem 4.3.2** *Let $G$ be a non-corona unicyclic graph with property (SR) and $T_i, r_i$, $i = 1, 2$, be as discussed earlier. Suppose that $r_1 = r_2 = 1$. Then $G$ has one of the two structures as shown in Figure 4.4, where*

*(a) $F_{2a}, F_{2b}, F_{1b}, F_w$ are forests of corona trees; each of the trees in $F_{2a}$ and $F_{2b}$ is attached to the vertex 2, and each of the trees of $F_{1b}$ and $F_w$ is attached to 1 and $w$, respectively; the vertex adjacent to the attached vertex in each of these corona trees which have more than two vertices is non-pendent in the tree.*

*(b) $F_{1a}$ is a forest of trees attached to 1; all but one tree, say $T_3$, are coronas; and the vertex adjacent to 1 in each of these trees which have more than two vertices is non-pendent in the tree.*

*(c) The graph induced by $1, v_1$ and vertices of $T_3$ has exactly one strong alternating path of length 5 (thus it has no strong alternating paths of length more than 5).*



(A) (B)

Figure 4.4: Case of $r_1 = r_2 = 1$

**Proof.** As $r_1 = r_2 = 1$, the number of strong alternating paths of length more than 3 has to be exactly 2. The path $[v_1, 1, 4, 3, 2, v_2]$ is a strong alternating path of length 5. Therefore, there is exactly one more strong alternating path of length of length 5 in $G$.

We note that any even tree-branch at 3 or 4, will give us at least one more such path with starting from $v_1$ and $v_2$, respectively. Therefore, there is at most one (even) tree-branch at one of 3 and 4. Accordingly, we have two cases: (a) There is no tree-branch at 3 and 4. (b) There is an even tree-branch at 4 and no tree-branch at 3.

Consider the case (b) and suppose that $T$ is a tree-branch at 4. Let $w$ be the vertex adjacent to 4. Then $w$ is matched to a vertex $v$ outside the cycle, thus $v \in T$. So the path $[v_2, 2, 3, 4, w, v]$ is a strong alternating path of length 5. If $d(v) \geq 2$, then we will have a strong alternating path of length at least 7 and, therefore, more such paths of lengths at least 5 in $G$, which cannot be true. Therefore $d(v) = 1$. It follows that the other tree-branches at $w$ are even, have perfect matchings and does not have a strong alternating path of length at least 5. Thus they are corona trees. If $T'$ is such a tree-branch with more than two vertices, then $T'$ is attached to $w$ at a non-pendent vertex, otherwise there will be a strong alternating path of length 5 with $v$ as a terminating vertex. Further in this case, a similar argument shows that the forests $F_{1b}, F_{2b}$ consist of corona trees only, and for each tree $T'$ in these forests which have more than two vertices only a non-pendant vertex of $T'$ is adjacent to $1, 2$ respectively.

Now, in the case (a), there is exactly one tree-branch at one of the vertices 1 and 2 which give rise to a strong alternating path of length 5. Suppose that this tree-branch is at 1. By the argument as in the case (b), the rest of the assertions follows. □

**Theorem 4.3.3** *Let $G$ be a non-corona unicyclic graph with property (SR) and $T_i, r_i$, $i = 1, 2$, be as discussed earlier. Suppose that $r_1 = 1, r_2 = 2$. Then the structure of $G$ is as shown in Figure 4.5, where $F_1$ and $F_5$ are forests of corona trees; a non-pendant vertex of each tree having more than two vertices in $F_1$ (resp. $F_5$) is adjacent to the vertex 1 (resp. 5) in $G$.*

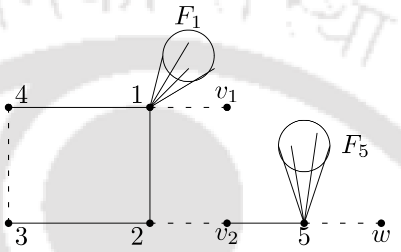


Figure 4.5: Case of $r_1 = 1, r_2 = 2$

**Proof.** The result follows with similar argument as in the previous theorem. □

We note that each of the graphs with structures described above can be obtained from certain corona graphs by deleting two specific pendent vertices with distance 3. The following two theorems give necessary and sufficient conditions for unicyclic graphs of structures as in Figure 4.4(B) and Figure 4.5 to have property (SR).

**Theorem 4.3.4** *Let $G$ be a unicyclic graph having structure as in Figure 4.4(B). Let $T$ and $T_4$ be the components of $G - 2 - 4$ containing the vertices 1 and $w$ respectively. Then $G$ has property (SR) if and only if*

$$P(T;x)P(T_4 - w - w';x) = P(T - 1 - v_1;x)P(T_4;x).$$

*In particular, if $T$ and $T_4$ in $G$ are isomorphic with 1 and $w$ as corresponding vertices, then $G$ has property (SR).*

**Proof.** Let $e$ be the edge with end vertices 2 and 3. Using Lemma 4.1.1 and Lemma 4.1.2, we get

$$
\begin{aligned}
P(G;x) &= P(G-e;x) - P(G-3-2;x) - 2P(G-C;x) \\
&= P(G-e;x) - \Big[xP(G-3-2-4;x) - P(G-3-2-4-w;x) \\
&\quad -P(G-3-2-4-1;x)\Big] - 2P(G-C;x) \\
&= P(G-e;x) - x^2P(G-3-2-4-v_2;x) + P(G-3-2-4-w;x) \\
&\quad -P(G-C;x) \\
&= P(G-e;x) - x^2P(G-3-2-4-v_2;x) \\
&\quad +x^2P(T;x)P(T_4-w-w';x)P(F_{2b};x) - x^2P(T-1-v_1;x)P(T_4;x) \\
&\quad \times P(F_{2b};x).
\end{aligned}
$$

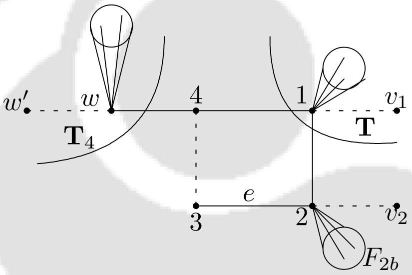


Figure 4.6: The trees $T$ and $T_4$ in $G$

The components of each of the graphs in the parentheses of the last expression are corona trees, and therefore have property (SR). Let $n = 2m$. Then for $P(G-e;x)$, the coefficient $a_n$ is $(-1)^m$, and we have

$$
P(G-e;x) = (-1)^m x^n \, P\left(G-e;\frac{1}{x}\right).
$$

Similarly, we have

$$
\begin{aligned}
P(G-3-2-4-v_2;x) &= (-1)^{m-2}x^{n-4}\, P\left(G-3-2-4-v_2;\frac{1}{x}\right), \\
P(T;x)P(T_4-w-w';x)P(F_{2b};x) &= (-1)^{m-3}x^{n-6}\, P\left(T;\frac{1}{x}\right) P\left(T_4-w-w';\frac{1}{x}\right) \\
&\quad \times P\left(F_{2b};\frac{1}{x}\right), \\
P(T-1-v_1;x)P(T_4;x)P(F_{2b};x) &= (-1)^{m-3}x^{n-6}\, P\left(T-1-v_1;\frac{1}{x}\right) P\left(T_4;\frac{1}{x}\right) \\
&\quad \times P\left(F_{2b};\frac{1}{x}\right).
\end{aligned}
$$

This gives

$$\begin{aligned}(-1)^m x^n\, P\left(G; \frac{1}{x}\right) &= P(G-e;x) - x^2 P(G-3-2-4-v_2;x) \\ &\quad -x^4 P(T;x)P(T_4-w-w';x)P(F_{2b};x) \\ &\quad +x^4 P(T-1-v_1;x)P(T_4;x)P(F_{2b};x).\end{aligned}$$

Thus $G$ has property (SR) if and only if

$$P(G;x) = (-1)^m x^n\, P\left(G; \frac{1}{x}\right),$$

which is the case if and only if

$$\begin{aligned} & x^2 P(T;x)P(T_4-w-w';x)P(F_{2b};x) - x^2 P(T-1-v_1;x)P(T_4;x)P(F_{2b};x) \\ = & -x^4 P(T;x)P(T_4-w-w';x)P(F_{2b};x) + x^4 P(T-1-v_1;x)P(T_4;x) \\ & \times P(F_{2b};x).\end{aligned}$$

That is $G$ has property (SR) if and only if

$$\begin{aligned}(x^4+x^2)P(T;x)P(T_4-w-w';x)P(F_{2b};x) &= (x^4+x^2)P(T-1-v_1;x) \\ &\quad \times P(T_4;x)P(F_{2b};x).\end{aligned}$$

This completes the proof of the first assertion. The second assertion now follows. □

**Theorem 4.3.5** *Let $G$ be a unicyclic graph having structure as in Figure 4.5. Let $T_1$ and $T_5$ be the components (trees) of the graph $G-2-4-v_2$ containing vertices 1 and 5 respectively. Then $G$ has property (SR) if and only if*

$$P(T_1;x)P(T_5-5-w;x) = P(T_1-1-v_1;x)P(T_5;x).$$

*In particular, if $T_1$ and $T_5$ in $G$ are isomorphic with 1 and 5 as corresponding vertices, then $G$ has property (SR).*

**Proof.** Using Lemma 4.1.2, we get

$$\begin{aligned}P(G;x) &= xP(G-2;x) - P(G-2-v_2;x) - P(G-2-1;x) - P(G-2-3;x) \\ &\quad -2P(G-2-1-4-3;x) \\ &= x^2 P(G-2-v_2;x) - xP(G-2-v_2-5;x) - P(G-2-v_2;x) \\ &\quad -xP(G-2-1-v_2;x) + P(G-2-1-v_2-5;x) - xP(G-2-3-4;x) \\ &\quad +P(G-C;x) - 2P(G-C;x)\end{aligned}$$

$$\begin{aligned}
&= x^2P(G-2-v_2;x) - xP(G-2-v_2-5;x) - P(G-2-v_2;x)\\
&\quad -xP(G-2-1-v_2;x) + (x^2-1)P(G-C-v_2-5;x)\\
&\quad -x^2P(G-2-3-4-v_2;x) - xP(G-2-3-4-v_2-5;x)\\
&\quad -xP(G-C-v_2;x) + P(G-C-v_2-5;x)\\
&= x^2P(G-2-v_2;x) - P(G-2-v_2;x) - x^2P(G-2-v_2-5-w;x)\\
&\quad -x^4P(F_1;x)P(T_5;x) + x^4P(F_1;x)P(F_5;x)\\
&\quad -x^2P(T_1;x)P(;x) + x^2P(T_1;x)P(F_5;x)
\end{aligned}$$

The components of each of the graphs in the parentheses of the last expression are corona trees, and therefore have property (SR). Let $n = 2m$. Then for $P(G-2-v_2;x)$, the coefficient $a_n$ is $(-1)^{m-1}$, and we have

$$P(G-2-v_2;x) = (-1)^{m-1}x^{n-2}\,P\left(G-2-v_2;\frac{1}{x}\right).$$

Similarly, we have

$$\begin{aligned}
P(G-2-v_2-5-w;x) &= (-1)^{m-2}x^{n-4}P\left(G-2-v_2-5-w;\frac{1}{x}\right),\\
P(F_1;x)P(T_5;x) &= (-1)^{m-3}x^{n-6}\,P(F_1;\frac{1}{x})P\left(T_5;\frac{1}{x}\right),\\
P(F_1;x)P(F_5;x) &= (-1)^{m-4}x^{n-8}\,P\left(F_1;\frac{1}{x}\right)P\left(F_5;\frac{1}{x}\right),\\
P(T_1;x)P(T_5;x) &= (-1)^{m-2}x^{n-4}\,P\left(T_1;\frac{1}{x}\right)P\left(T_5;\frac{1}{x}\right),\\
P(T_1;x)P(F_5;x) &= (-1)^{m-3}x^{n-6}\,P\left(T_1;\frac{1}{x}\right)P\left(F_5;\frac{1}{x}\right)
\end{aligned}$$

This gives

$$\begin{aligned}
(-1)^m x^n\,P\left(G;\frac{1}{x}\right) &= -P\left(G-2-v_2;x\right) + x^2P\left(G-2-v_2;x\right)\\
&\quad -x^2P\left(G-2-v_2-5-w;x\right) + x^4P\left(F_1;x\right)P\left(T_5;x\right)\\
&\quad +x^4P\left(F_1;x\right)P\left(F_5;x\right) - x^2P\left(T_1;x\right)P\left(T_5;x\right)\\
&\quad -x^4P\left(T_1;x\right)P\left(F_5;x\right)
\end{aligned}$$

Thus $G$ has property (SR) if and only if

$$P(G;x) = (-1)^m x^n\,P\left(G;\frac{1}{x}\right),$$

which is the case if and only if

$$\begin{aligned}
&-x^4P(T_1;x)P(F_5;x) + x^2P(F_1;x)P(T_5;x)\\
&= +x^2P\left(T_1;x\right)P\left(F_5;x\right) - x^4P\left(F_1;x\right)P\left(T_5;x\right)
\end{aligned}$$

That is $G$ has property (SR) if and only if

$$(x^4+x^2)P(T_1;x)P(T_5-5-w;x) \quad = \quad (x^4+x^2)P(T_5;x)P(T_1-1-v_1;x).$$

This completes the proof of the first assertion. The second assertion now follows. $\square$

Below we supply a class of non-corona unicyclic graphs with property (SR) which are in the form 4.4(A).

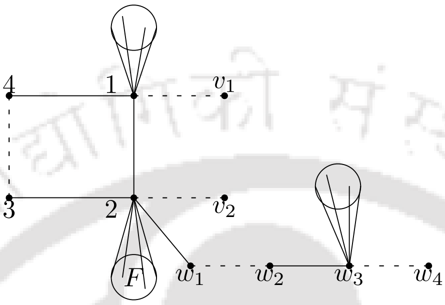


Figure 4.7: A subclass of graphs of Figure 4.4(A)

**Theorem 4.3.6** *Let $G$ be unicyclic graph of the form as shown in figure 4.7. Let $T_1$ and $T_2$ be the components of $G-2$ containing the vertices 1 and $w_1$ respectively. Then $G$ has property (SR) if and only if*

$$P(T_1;x)P(T_2-w_1-w_2-w_3-w_4;x) = P(T_1-3-4-1-v_1;x)P(T_2;x).$$

*In particular, if $T_1$ and $T_2$ are isomorphic with 1 and $w_3$ as corresponding vertices, then $G$ satisfies property SR.*

**Proof.** Using Lemma 4.1.2, we get

$$\begin{aligned}
P(G;x) &= xP(G-2;x)-P(G-2-v_2;x)-P(G-2-w_1;x)-P(G-2-3;x)\\
&\quad -P(G-2-1;x)-2P(G-2-3-v_2-4-1;x)\\
&= x^2P(G-2-v_2;x)-P(G-2-v_2;x)-x^2P(G-2-w_1-w_2-v_2;x)\\
&\quad +x^2P(G-2-w_1-w_2-w_3-w_4-v_2;x)-x^2P(G-2-3-v_2-4;x)\\
&\quad +x^2P(G-2-3-4-1-v_2-v_1;x)-2x^2P(G-2-v_2-3-4-1-v_1;x)\\
&= x^2P(G-2-v_2;x)-P(G-2-v_2;x)-x^2P(G-2-w_1-w_2-v_2;x)\\
&\quad +x^2P(G-2-w_1-w_2-w_3-w_4-v_2;x)-x^2P(G-2-3-v_2-4;x)\\
&\quad -x^2P(G-2-v_2-3-4-1-v_1;x)\\
&= (x^2-1)P(G-2-v_2;x)-x^2P(T_1;x)P(T_2-w_1-w_2;x)P(F;x)
\end{aligned}$$

$$
\begin{aligned}
&+x^2P(T_1;x)P(T_2-w_1-w_2-w_3-w_4;x)P(F;x)\\
&-x^2P(T_1-3-4;x)P(T_2;x)P(F;x)\\
&-x^2P(T_1-3-4-1-v_1;x)P(T_2;x)P(F;x).
\end{aligned}
$$

The components of each of the graphs in the parentheses of the last expression are corona trees, and therefore have property (SR). Let $n = 2m$. Then for $P(G-2-v_2;x)$, the coefficient $a_n$ is $(-1)^{m-1}$, and we have

$$P(G-2-v_2;x) \;=\; (-1)^{m-1}x^{n-2}\,P\left(G-2-v_2;\frac{1}{x}\right).$$

Similarly, we have

$$
\begin{aligned}
P(T_1;x)P(T_2-w_1-w_2;x)P(F;x) &= (-1)^{m-2}x^{n-4}P\left(T_1;\frac{1}{x}\right)P\left(T_2-w_1-w_2;\frac{1}{x}\right)\\
&\quad\times P\left(F;\frac{1}{x}\right)
\end{aligned}
$$

$$
\begin{aligned}
P(T_1;x)P(T_2-w_1-w_2-w_3-w_4;x)P(F;x) &= (-1)^{m-3}x^{n-6}P\left(T_1;\frac{1}{x}\right)\\
&\quad\times P\left(T_2-w_1-w_2-w_3-w_4;\frac{1}{x}\right)\\
&\quad\times P\left(F;\frac{1}{x}\right)
\end{aligned}
$$

$$
\begin{aligned}
P(T_1-3-4;x)P(T_2;x)P(F;x) &= (-1)^{m-2}x^{n-4}P\left(T_1-3-4;\frac{1}{x}\right)P\left(T_2;\frac{1}{x}\right)\\
&\quad\times P\left(F;\frac{1}{x}\right)\\
P(T_1-3-4-1-v_1;x)P(T_2;x)P(F;x) &= (-1)^{m-3}x^{n-6}P\left(T_1-3-4-1-v_1;\frac{1}{x}\right)\\
&\quad\times P\left(T_2;\frac{1}{x}\right)P\left(F;\frac{1}{x}\right)
\end{aligned}
$$

This gives

$$
\begin{aligned}
(-1)^m x^n\,P\left(G;\frac{1}{x}\right) &= (x^2-1)P(G-2-v_2;x)-x^2P(T_1;x)P(T_2-w_1-w_2;x)P(F;x)\\
&\quad -x^4P(T_1;x)P(T_2-w_1-w_2-w_3-w_4;x)P(F;x)\\
&\quad -x^2P(T_1-3-4;x)P(T_2;x)P(F;x)\\
&\quad +x^4P(T_1-3-4-1-v_1;x)P(T_2;x)P(F;x)
\end{aligned}
$$

Thus, $G$ has property (SR) if and only if

$$P(G;x) \quad = \quad (-1)^m x^n\, P\left(G;\frac{1}{x}\right),$$

which is the case if and only if

$$\begin{aligned} & -x^4P(T_1;x)P(T_2-w_1-w_2-w_3-w_4;x)P(F;x) \\ & +x^4P(T_1-3-4-1-v_1;x)P(T_2;x)P(F;x) \\ = \;& x^2P(T_1;x)P(T_2-w_1-w_2-w_3-w_4;x)P(F;x) \\ & -x^2P(T_1-3-4-1-v_1;x)P(T_2;x)P(F;x) \end{aligned}$$

That is $G$ has property (SR) if and only if

$$\begin{aligned} & (x^4+x^2)P(T_1-3-4-1-v_1;x)P(T_2;x)P(F;x) \\ = \;& (x^4+x^2)P(T_1;x) \\ & \times P(T_2-w_1-w_2-w_3-w_4;x)P(F;x). \end{aligned}$$

This completes the proof of the first assertion. The second assertion now follows. □

To sum up our discussion, we have seen that a unicyclic graph $G$ with girth $g \neq 4$ has property (SR) if and only if it is a corona. In case $g = 4$, $G$ has property (SR) if it is either a corona or has one of the forms as described in Figures 4.4(A), 4.4(B) and 4.5. Theorems 4.3.4, 4.3.5 and 4.3.6 supply classes of non-corona unicyclic graphs with property (SR) which are in the forms 4.4(B), 4.5 and 4.4(A), respectively.

# Chapter 5

# On Spectral Radius of Bipartite Unicyclic Graphs

## 5.1 Introduction

For $n \geq 4$, let $G_1(n)$ denote the graph in $\mathcal{U}_{n,4}$, the class of all unicyclic graph of girth four on $n$ vertices, having $n-4$ pendants attached at a vertex of $C$. Similarly, $G_2(n)$ $(n \geq 5)$ denotes the graph having $n-5$ pendants attached at a vertex $v$ on $C$ and another pendant attached at a vertex adjacent to $v$ on $C$; $G_3(n)$ $(n \geq 6)$ denotes the graph having $n-6$ pendants together with a copy of $P_2$ attached at a vertex of the cycle; $G_4(n)$ $(n \geq 6)$ denotes the graph having $n-5$ pendants attached at a vertex $v$ on $C$ and another pendant attached at a vertex at distance two from $v$ on $C$ (see Figure 5.1).

Since the girth of each of $G_i(n)$ is even, the graphs are bipartite. In this chapter, we show that these are the graphs in the class of $\mathcal{U}_n^b$, having the first four largest spectral radius. However we will see in the sequel that the ordering between these four graphs are not exactly the same for the two cases viz. $n \geq 10$ and $n < 10$.

In our pursuit, we will be extensively using two basic results. The first is known as *interlacing theorem* and the other is a proposition comparing the largest roots of two polynomials. The two results are as follows:

**Theorem 5.1.1** [19] **(Interlacing theorem)** *Let $S$ be a subset of $V(G)$ of size $k$. Then*

$$\lambda_{i+k}(G) \leq \lambda_i(G-S) \leq \lambda_i(G), \quad i = 1, 2, \ldots, n-k.$$

**Proposition 5.1.2** *Let $G$ and $H$ be the two graphs of order $n$.*

*(a) If $P(H;x) > P(G;x)$ for $x \geq \lambda_1(G)$, then $\lambda_1(H) < \lambda_1(G)$;*

*(b) If $P(H;\lambda_1(G)) < 0$ then $\lambda_1(H) > \lambda_1(G)$.*

**Proof.** The result can be seen easily, since $P(G;x)$ and $P(H;x)$ are monic polynomials of same degree with real roots. $\square$

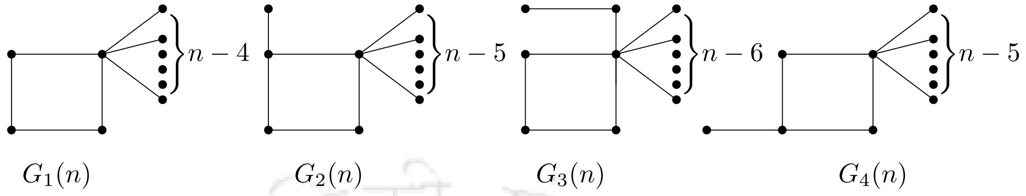


Figure 5.1: The graphs $G_i(n)$

## 5.2 The graph in $\mathcal{U}_n^b$ with maximal spectral radius

It is known that $(i,i)$-th entry of $A(G)^2$ is the degree of the $i$-th vertex in $G$ (see Corollary 13.1(a) of [35], for example). Therefore, for any graph $G$ with $m$ edges

$$2m = \sum_{v\in V(G)} d(v) = tr(A(G)^2) = \sum_{i=1}^{n} \lambda_i^2.$$

If $G$ is unicyclic, then $m = n$. Moreover for a bipartite graph $G$, $\lambda \in \sigma(G)$ if and only if $-\lambda \in \sigma(G)$ with equal multiplicity. Thus for a graph $G$ in $\mathcal{U}_n^b$

$$2n = tr(A(G)^2) = \sum_{i=1}^{n} \lambda_i^2 = 2\lambda_1^2 + 2\sum_{i=2}^{[\frac{n}{2}]} \lambda_i^2,$$

and therefore

$$n = \lambda_1^2 + \sum_{i=2}^{[\frac{n}{2}]} \lambda_i^2 \tag{5.2.1}$$

We define $S(G)$

$$S(G) = \sum_{i=2}^{[\frac{n}{2}]} \lambda_i^2 \tag{5.2.2}$$

**Lemma 5.2.1** *Let $G$ be a unicyclic bipartite graph with $n$ vertices and*

$$\lambda_1(G) \geq \sqrt{\frac{1}{2}\left(n + \sqrt{n^2 - 8n + 32}\right)}. \tag{5.2.3}$$

*Then* $S(G) < 2$.

**Proof.** From 5.2.2 we have

$$\begin{aligned} S(G) &= n-\lambda_1^2 \\ &\leq n-\frac{1}{2}(n+\sqrt{n^2-8n+32}) \\ &= \frac{1}{2}(n-\sqrt{n^2-8n+32}) \\ &< 2. \qquad \square \end{aligned}$$

**Lemma 5.2.2** *Let $G \in \mathcal{U}_{n,g}^b$ and $S(G) < 2$. Then $G$ has none of $P_7$ and $C_6$ as an induced subgraph.*

**Proof.** We have $\sigma(P_7) = \{\pm 1.848, \pm 1.4, \pm .765, 0\}$ ( Table 2 of Appendix in [19] ), and therefore $S(P_7) = 1.4^2 + .765^2 > 2$. Similarly, $S(C_6) = 2$. By interlacing, the result follows. $\square$

**Corollary 5.2.3** *Let $G \in \mathcal{U}_{n,g}^b$ and $S(G) < 2$. Then $g = 4$, that is, the cycle in $G$ is $C_4$.*

**Proof.** If $g \geq 6$, then $G$ has either $C_6$ or $P_7$ as an induced subgraph. $\square$

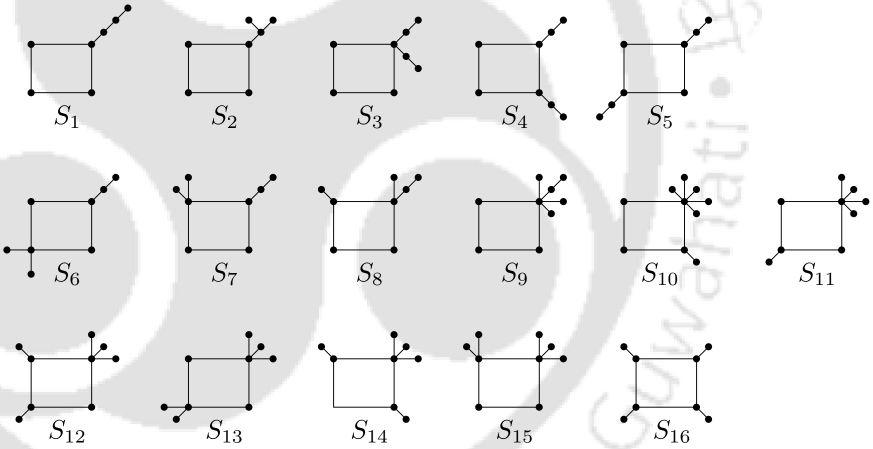


Figure 5.2: Forbidden subgraphs $S_i$

**Lemma 5.2.4** *Let $G \in \mathcal{U}_{n,4}$, $n \geq 10$ and $S(G) < 2$. Then none of the graphs $S_i$, $1 \leq i \leq 16$, (Figure 5.2) can be an induced subgraph of $G$.*

**Proof.** The result can be seen by showing that 2 is a lower bound for $S(S_i)$ looking at the characteristic polynomial of $S_i$. For example,

$$\begin{aligned} P(S_1;x) &= x(x^6-7x^4+11x^2-2) \\ &= x[x^4(x^2-5)-2x^2(x^2-5)+(x^2-5)+3] \\ &> 0 \end{aligned}$$

| $S_i$ | $\lambda_1(S_i)$ | $S(S_i)$ |
|---|---|---|
| $S_1$ | 2.1889 | 2.2087 |
| $S_2$ | 2.23607 | 2 |
| $S_3$ | 2.3799 | 2.3394 |
| $S_4$ | 2.30278 | 2.6972 |
| $S_5$ | 2.28825 | 2.7639 |
| $S_6$ | 2.37608 | 2.3542 |
| $S_7$ | 2.39684 | 2.2552 |
| $S_8$ | 2.40651 | 2.2087 |
| $S_9$ | 2.64044 | 2.0281 |
| $S_{10}$ | 2.81739 | 2.0623 |
| $S_{11}$ | 2.64375 | 2 |
| $S_{12}$ | 2.55761 | 2.4586 |
| $S_{13}$ | 2.56155 | 2.4385 |
| $S_{14}$ | 2.449 | 2.3542 |
| $S_{15}$ | 2.60123 | 2.2336 |
| $S_{16}$ | 2.414 | 2.1726 |

Table 5.1: Spectral radius and $S(G)$ for $S_i$

for all $x^2 \geq 5$. Therefore, $\lambda_1^2 < 5$. Since $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 7$, we have $S(S_1) > 2$. In fact, Table 5.1 shows the approximate values of $S(S_i)$ (computed with MATLAB). Therefore, by interlacing, if $G$ has some $S_i$ as an induced subgraph, then $S(G) \geq 2$ and the result follows. $\square$

**Lemma 5.2.5** *Let $G \in \mathcal{U}_{n,4}$, $n \geq 10$ and $S(G) < 2$. Then $G$ has no vertex at a distance two from the cycle.*

**Proof.** By Lemma 5.2.4, $G$ does not have any of $S_i$, $1 \leq i \leq 16$, as an induced subgraph. Since $G$ does not have $S_1$ as an induced subgraph, $G$ has no vertex at distance more than two from the cycle. Moreover, because none of $S_2, S_3, S_4, S_5$ is an induced subgraph of $G$, there can be at most one vertex at distance two from the cycle. Suppose that $P_2$ is a branch at the vertex 1 of the cycle $C = (1234)$ of $G$. The vertices neither on $C$ nor on the branch $P_2$ are all pendent at the cycle and they are $n-6$ in number. Since $n \geq 10$, $G$ has at least four such pendent vertices shared by the vertices of the cycle. Consider a subgraph $H$ of $G$ induced by the vertices of $C$, the branch $P_2$ and any four of the pendants to the

| $(x_1, x_2, x_3, x_4)$ | $S_i$ | $(x_1, x_2, x_3, x_4)$ | $S_i$ |
|---|---|---|---|
| $(4, 0, 0, 0)$ | $S_9$ | $(1, 1, 2, 0)$ | $S_6$ |
| $(3, 1, 0, 0)$ | $S_8$ | $(1, 1, 1, 1)$ | $S_8$ |
| $(3, 0, 1, 0)$ | $S_9$ | $(0, 4, 0, 0)$ | $S_7$ |
| $(2, 2, 0, 0)$ | $S_8$ | $(0, 0, 4, 0)$ | $S_6$ |
| $(2, 0, 2, 0)$ | $S_6$ | $(0, 3, 1, 0)$ | $S_7$ |
| $(2, 1, 1, 0)$ | $S_8$ | $(0, 3, 0, 0)$ | $S_7$ |
| $(2, 1, 0, 1)$ | $S_8$ | $(0, 1, 3, 0)$ | $S_6$ |
| $(1, 3, 0, 0)$ | $S_7$ | $(0, 2, 2, 0)$ | $S_6$ |
| $(1, 0, 3, 0)$ | $S_6$ | $(0, 2, 0, 2)$ | $S_7$ |
| $(1, 2, 1, 0)$ | $S_7$ | $(0, 2, 1, 1)$ | $S_7$ |
| $(1, 2, 0, 1)$ | $S_7$ | $(0, 1, 2, 1)$ | $S_6$ |

Table 5.2: Induced subgraph $S_i$ of $H$

cycle. Suppose out of the four pendent vertices, $x_1$, $x_2$, $x_3$ and $x_4$ numbers of pendants are allotted to the vertices $1, 2, 3$ and $4$ respectively in $H$. Then, there is an one-one correspondence between the possible 4-tuples $(x_1, x_2, x_3, x_4)$ and possible subgraphs $H$. However, Table 5.2 shows that in each of the cases $H$ has (not necessarily unique) some $S_i$ as an induced subgraph. Therefore, by Lemma 5.2.4, the result follows. □

**Lemma 5.2.6** *If $G \in \mathcal{U}_{n,4}$, $n \geq 10$ and $S(G) < 2$. Then $G = G_1(n)$.*

**Proof.** By Lemma 5.2.5, $G$ has no vertex at distance two from the cycle. The pendants in $G$, which are at least six in number, are distributed at the vertices $1, 2, 3$ and $4$ of the cycle. Let $G \neq G_1(n)$ and $K$ be an induced unicyclic subgraph of $G$ having six pendants with distribution $(y_1, y_2, y_3, y_4)$. Because $S_{16}$ is not an induced subgraph of $G$, at least one vertex on the cycle of $K$ has no pendant. Now, Table 5.3 shows that $K$ has one of the graphs $S_i$ as an induced subgraph. Therefore, by Lemma 5.2.4, the result follows. □

**Theorem 5.2.7** *Let $G \in \mathcal{U}_n^b$, $n \geq 10$. Then $\lambda_1(G) \leq \sqrt{\frac{1}{2}\left(n + \sqrt{n^2 - 8n + 32}\right)}$ and equality holds if and only if $G = G_1(n)$.*

**Proof.** Follows from above Lemma 5.2.1 and 5.2.6, and the fact that

$$\lambda_1(G_1(n)) = \sqrt{\frac{1}{2}\left(n + \sqrt{n^2 - 8n + 32}\right)}. \quad \square$$

| $(y_1, y_2, y_3, y_4)$ | $S_i$ | $(y_1, y_2, y_3, y_4)$ | $S_i$ |
|---|---|---|---|
| $(5,1,0,0)$ | $S_{10}$ | $(5,0,1,0)$ | $S_{11}$ |
| $(4,2,0,0)$ | $S_{15}$ | $(4,0,2,0)$ | $S_{13}$ |
| $(3,3,0,0)$ | $S_{15}$ | $(3,0,3,0)$ | $S_{13}$ |
| $(4,1,1,0)$ | $S_{12}$ | $(1,4,1,0)$ | $S_{14}$ |
| $(3,2,1,0)$ | $S_{12}$ | $(3,1,2,0)$ | $S_{12}$ |
| $(2,2,2,0)$ | $S_{15}$ | $(2,3,1,0)$ | $S_{14}$ |

Table 5.3: Induced subgraph $S_i$ of $K$

## 5.3 The graphs in $\mathcal{U}_n^b$ with the second, third and fourth largest spectral radius

**Lemma 5.3.1** *Let $G \in \mathcal{U}_n^b$ with $\lambda_1(G) \geq \lambda_1(G_4(n))$. Then $S(G) < 3$.*

**Proof.** We have

$$\begin{aligned} P(G_4(n); x) &= x^{n-4}(x^4 - nx^2 + 3n - 13) \\ \lambda_1(G_4(n)) &= \left[\frac{1}{2}\left(n + \sqrt{n^2 - 4(3n - 13)}\right)\right]^{\frac{1}{2}} \end{aligned}$$

Let $G \in \mathcal{U}_n^b$ and $\lambda_1(G) \geq \lambda_1(G_4(n))$, that is,

$$\lambda_1(G) \geq \left[\frac{1}{2}\left(n + \sqrt{n^2 - 4(3n - 13)}\right)\right]^{\frac{1}{2}}$$

Therefore, from 5.2.2, we have

$$\begin{aligned} S(G) &= n - \lambda_1^2 \\ &\leq n - \frac{1}{2}\left(n + \sqrt{n^2 - 4(3n - 13)}\right) \\ &< n - \frac{1}{2}(n + n - 6) \\ &= 3. \end{aligned}$$

□

**Lemma 5.3.2** *Let $G \in \mathcal{U}_{n,g}^b$, $n \geq 10$ and $S(G) < 3$. Then $G$ does not have $P_8$ or any of the graphs $X_i$, $1 \leq i \leq 5$ (Figure 5.3) as an induced subgraph.*

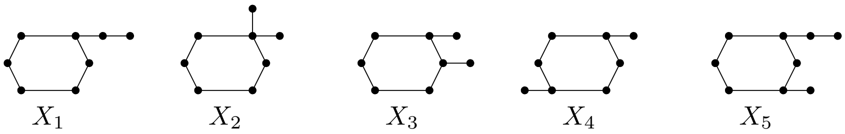


Figure 5.3: Forbidden subgraphs $X_i$

**Proof.** We have $\sigma(P_8) = \{\pm 1.879, \pm 1.932, \pm 1, \pm .347\}$. Therefore, $S(P_8) > 3$. This is also the case for $X_1$,$X_2$,$X_3$,$X_4$ and $X_5$. Thus by interlacing none of these can be an induced subgraph of $G$. $\square$

As an immediate consequence of the above lemma we have the following.

**Corollary 5.3.3** *Let $G \in \mathcal{U}^b_{n,g}$, $n \geq 10$ and $S(G) < 3$. Then $g = 4$.*

**Lemma 5.3.4** *Let $G \in \mathcal{U}_{n,4}$, $n \geq 10$ and satisfies $S(G) < 3$. Then $G$ does not have any of the graphs $Y_i, 1 \leq i \leq 56$, (Figure 5.4) as an induced subgraph.*

**Proof.** It can be seen that $S(Y_i) \geq 3$ for $1 \leq i \leq 56$. Indeed, we have

$$\begin{aligned} P(Y_1; x) &= x^3(x^8 - 11x^6 + 27x^4 - 23x^2 + 7) \\ &= x^3[x^6(x^2-8) - 3x^4(x^2-8) + 3x^2(x^2 - 8 + (x^2-7)) \\ &= x^3[x^4(x^2-8)(x^2-3) + 3x^2(x^2-8) + (x^2-7) \\ &> 0 \text{ for all } x^2 \geq 8, \end{aligned}$$

and therefore, $\lambda_1^2 \leq 8$. Since

$$\lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 11,$$

we have $S(Y_1) \geq 3$. The result can be verified similarly (or with computation) for other $Y_i$. By interlacing, the assertion of the lemma follows. $\square$

**Lemma 5.3.5** *Suppose that $G \in \mathcal{U}_{n,4}$, $G \neq G_1(n)$, does not have any of the graphs $Y_i$ (of Figure 5.4) as an induced subgraph. If $n > 12$ then $G$ is one of $G_i(n)$, $i = 2, 3, 4$. If $G \notin \{G_i(n) \mid 1 \leq i \leq 4\}$, then $G$ one of $H_i$, $1 \leq i \leq 16$, for $n = 10$; $H_{17}$, $H_{18}$ or $H_{19}$ for $n = 11$; and $H_{20}$ for $n = 12$.*

The graphs $H_i$ in Figure 5.6 have been obtained considering the restrictions given by the graphs $Y_i$ on the number and size of the branches in possible $H_i$. Though a table in the line of Table 5.1 and Table 5.2, we refrain from doing so, because it would be too space-consuming.

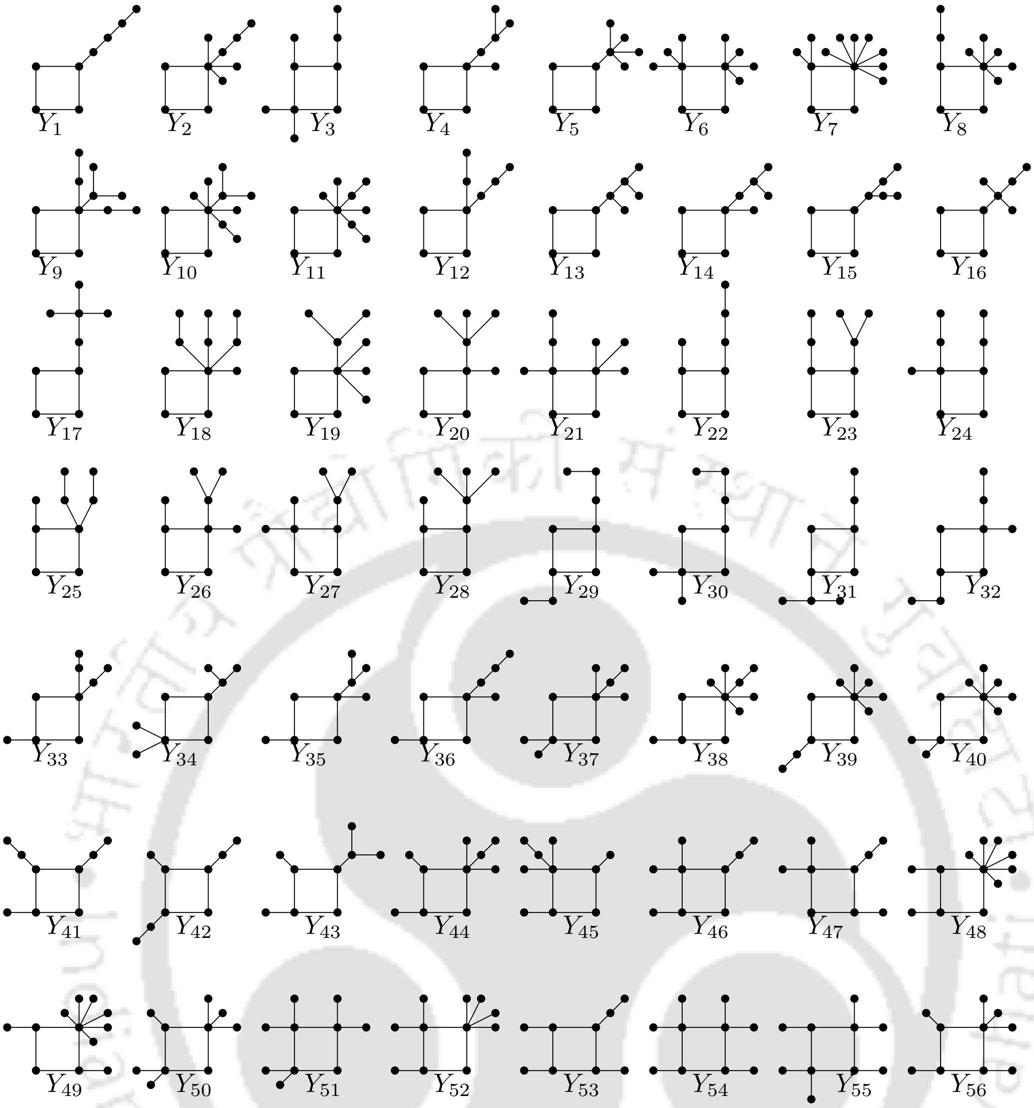


Figure 5.4: The forbidden subgraphs $Y_i$, $1 \leq i \leq 56$

**Lemma 5.3.6** *For* $1 \leq i \leq 20$, $\lambda_1(G_4(n)) > \lambda_1(H_i)$, *where* $H_i$ *is of order* $n$.

**Proof.** We have

$$\begin{aligned} P(H_1;x) &= x^2(x^8 - 10x^6 + 23x^4 - 18x^2 + 4) \\ P(G_4(10);x) &= x^6(x^4 - 10x^2 + 17) \end{aligned}$$

and, therefore,

$$\begin{aligned} P(G_4(10);x) - P(H_1;x) &= -6x^6 + 18x^4 - 4x^2 \\ &= -6x^2\left[\left(x^2 - \frac{3}{2}\right)^2 - \frac{19}{12}\right] \\ &< 0 \qquad \text{for all } \ x^2 > \sqrt{\tfrac{19}{12}} + \tfrac{3}{2} \end{aligned}$$

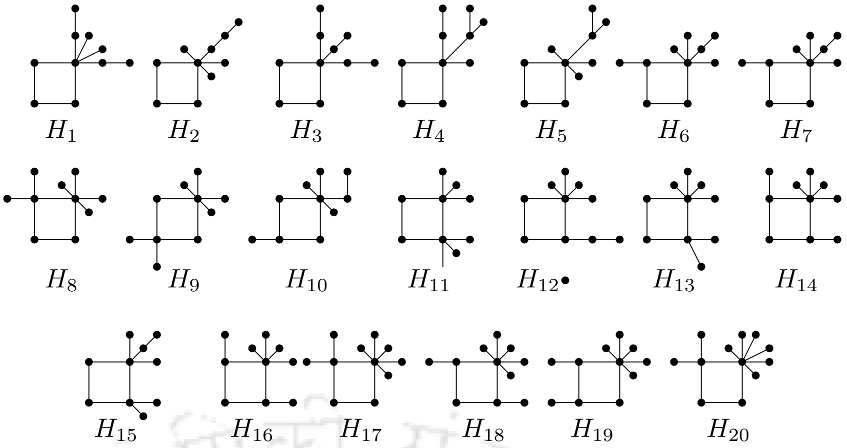


Figure 5.5: The graphs $H_i$, $1 \leq i \leq 20$.

Therefore, $P(H_1;x) > P(G_4(10);x)$ for all $x > \lambda_1(G_4(10))$ as $\lambda_1(G_4(10)) > \sqrt{7}$. By Proposition 5.1.2, we have

$$\lambda_1(H_1) \quad < \quad \lambda_1(G_4(10)).$$

The spectral radius of the other $H_i$ can be similarly compared with those of $G_4(n)$. (Alternately, they can be compared with numerical computations.) $\square$

**Lemma 5.3.7** *Let $n \geq 10$. Then*

$$\lambda_1(G_1(n)) > \lambda_1(G_2(n)) > \lambda_1(G_3(n)) > \lambda_1(G_4(n)).$$

**Proof.** We have

$$\begin{aligned} P(G_1(n);x) &= x^{n-4}(x^4 - nx^2 + 2n - 8) \\ P(G_2(n);x) &= x^{n-6}(x^6 - nx^4 + (3n-13)x^2 - (n-5)) \\ P(G_3(n);x) &= x^{n-6}(x^6 - nx^4 + (3n-12)x^2 - (2n-12)) \\ P(G_4(n);x) &= x^{n-4}(x^4 - nx^2 + 3n - 13) \end{aligned}$$

Therefore, we get

$$\begin{aligned} P(G_3(n),x) - P(G_2(n),x) &= x^{n-4} + (n-7)x^{n-6} \\ &= x^{n-6}\left[x^2 + (n-7)\right] \end{aligned}$$

If $f(x) = x^2 + (n-7)$ then $f'(x) = 2x > 0$ for $x > 0$, and therefore $f(x)$ is an increasing function. Moreover, $f(\sqrt{7}) = n$. For $n \geq 10$, $\lambda_1(G_2(n) > \sqrt{7}$ , and we have

$$P(G_3(n),x) > P(G_2(n),x)$$

whenever $x \geq \lambda_1(G_2(n))$. Therefore, by Proposition 5.1.2(a), we have $\lambda_1(G_2(n)) > \lambda_1(G_3(n))$ for $n \geq 10$. Similarly, for $n \geq 6$, we have

$$\begin{aligned} \lambda_1(G_1(n)) &> \lambda_1(G_2(n)), \\ \lambda_1(G_2(n)) &> \lambda_1(G_4(n)). \end{aligned}$$

Next,

$$P(G_3(n); x) = P(G_4(n); x) + x^{n-6}[x^2 - 2n + 12],$$

and, therefore,

$$P(G_3(n); \lambda_1(G_4(n))) = (\lambda_1(G_4(n)))^{n-6}\left[(\lambda_1(G_4(n)))^2 - 2n + 12\right]. \quad (5.3.4)$$

It is easy to see that the right side of (5.3.4) is negative, if $n \geq 10$, and therefore by Proposition 5.1.2(b), we get $\lambda_1(G_3(n)) > \lambda_1(G_4(n))$ for $n \geq 10$. □

**Lemma 5.3.8** *Let* $6 \leq n \leq 9$. *Then*

$$\lambda_1(G_1(n)) > \lambda_1(G_2(n)) > \lambda_1(G_4(n)) > \lambda_1(G_3(n)).$$

**Proof.** For $6 \leq n \leq 9$, in view of (5.3.4), we have $P(G_3(n); x) > 0$ for $x \geq \lambda_1(G_4(n))$. Therefore, we must have $\lambda_1(G_4(n)) > \lambda_1(G_3(n))$. The other inequalities follow from the proof of Lemma 5.3.8. □

In view of the previous lemmas, we are now in a position to present the main result of this section.

**Theorem 5.3.9** *For* $n \geq 10$, $G_2(n), G_3(n)$ *and* $G_4(n)$ *are the graphs with the second, the third and the fourth largest spectral radius, respectively, among all graphs in* $\mathcal{U}_n^b$.

Thus, we have found four unique graphs in descending order occupying the highest positions in terms of their spectral radius in the class of all bipartite unicyclic graphs of order $n$, $n \geq 10$.

We now consider the cases $4 \leq n \leq 9$.

**Case:** $n = 9$. We have,

$$P(G_3(9); x) = x^3(x^6 - 9x^4 + 15x^2 - 6),$$

and $S(G_3(9)) = 2.0283$. Thus, if $G \in \mathcal{U}_{9,4}$ and $\lambda_1(G) > \lambda_1(G_3(9))$, then $S(G) < 2.0283$. Therefore, none of $S_i, i \neq 2, 9, 11$ and $R_i, i \neq 8, 9$, is an induced subgraph of $G$. Moreover, if $S_2$ is an induced subgraph of $G$ then $G$ will have an induced subgraph $S_i, i =$

| $R_i$ | $\lambda_1$ | $S(R_i)$ |
|---|---|---|
| $R_1$ | 2.3563 | 2.4479 |
| $R_2$ | 2.3583 | 2.4384 |
| $R_3$ | 2.3268 | 2.5860 |
| $R_4$ | 2.3761 | 2.3541 |
| $R_5$ | 2.3073 | 2.6764 |
| $R6$ | 2.4412 | 2.0405 |
| $R_7$ | 2.3213 | 2.6116 |
| $R_8$ | 2.4812 | 1.8436 |
| $R_9$ | 2.4495 | 1.999 |
| $R_{10}$ | 2.2360 | 4.003 |
| $R_{11}$ | 2.4325 | 2.0829 |

Table 5.4: $S(R_i),\ 1 \leq i \leq 11$

$1, 3, 4, 5, 6, 7, 8$ or $R_i, i = 1, 2, 3, 4, 5, 6, 7$. Therefore $S_2$ is not an induced subgraph of $G$. In this way we can argue that none of $S_i$ and $R_i$ is an induced subgraph of $G$. Thus, $G$ is one of $G_i(9),\ i = 1, 2, 4$.

**Case:** $n = 8$. We have

$$P(G_3(8); x) \quad = \quad x^2(x^6 - 8x^4 + 12x^2 - 4),$$

and $S(G_3(8)) = 1.8436$. Thus, if $G \in \mathcal{U}_{8,4}$ and $\lambda_1(G) > \lambda_1(G_3(8))$, then $S(G) < 1.8436$. Therefore, none of $S_i, i \neq 9, 10, 11$, is an induced subgraph of $G$. Moreover, for $1 \leq i \leq 11, i \neq 8$, $S(R_i) \geq 1.9$ (see Table 5.4), and, therefore, none of the graphs $R_i$ except $R_8$ is an induced subgraph of $G$. This forces $G$ to be one of $G_i(8),\ i = 1, 2, 4$ or $R_8$ again we have $\lambda_1(G_3(8)) = \lambda_1(R_8)$.

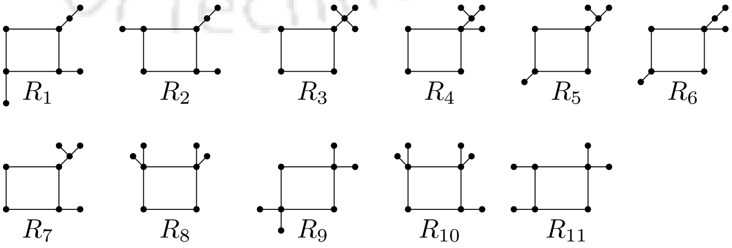


Figure 5.6: The graphs $R_i,\ 1 \leq i \leq 11$.

**Case:** $n = 7$. We have

$$P(G_3(7);x) = x(x^6 - 7x^4 + 9x^2 - 2),$$

and $S(G_3(7)) = 1.5973$. Thus, if $G \in \mathcal{U}_{7,4}$ and $\lambda_1(G) > \lambda_1(G_3(7))$, then $S(G) < 1.5973$. Since $S(P_6) = 1.753034$, $P_6$ can not be an induced subgraph of $G$, and $G$ is one of the graphs in Figure 5.7.

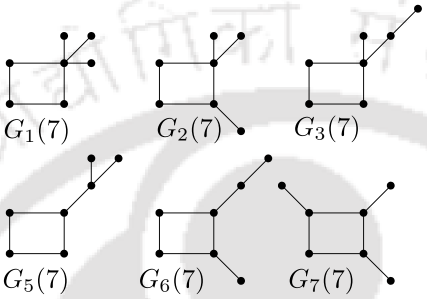


Figure 5.7:

Now,

$$\begin{aligned} P(G_5(7);x) &= x^3(x^4 - 7x^2 + 10) \\ P(G_6(7);x) &= x(x^6 - 7x^4 + 10x^2 - 3) \\ P(G_7(7);x) &= x(x^6 - 7x^4 + 10x^2 - 3) \end{aligned}$$

and using Proposition 5.1.2 we have $\lambda_1(G_3(7)) > \lambda_1(G_i)(7)$, for $i = 5, 6, 7$.

**Case:** $n = 6, 5, 4$. The possible graphs in $\mathcal{U}_{6,4}$ are $G_i(6)$, $1 \le i \le 4$; in $\mathcal{U}_{5,4}$ is $G_1(5)$; and $\mathcal{U}_{4,4}$ is $G_1(4) = C_4$.

We conclude the above discussion in the following theorem.

**Theorem 5.3.10** *Let* $6 \le n \le 9$. *Then*

$$\lambda_1(G_1(n)) > \lambda_1(G_2(n)) > \lambda_1(G_4(n)) > \lambda_1(G_3(n)).$$

*Moreover, if* $G \in \mathcal{U}_{n,g}$, $6 \le n \le 9$, *and* $G$ *is not one of* $G_i(n), 1 \le i \le 4$, *then* $\lambda_1(G) < \lambda_1(G_3(n))$ *for* $n \neq 8$, *and either* $G = R_8$ *or* $\lambda_1(G) < \lambda_1(G_3(n))$ *for* $n = 8$.

# Chapter 6

# Unicyclic graphs of minimal energy

## 6.1 Introduction

In this chapter, we devote ourselves in finding the graphs with minimal energy in the class of all unicyclic graphs with a fixed girth and that of all bipartite unicyclic graphs. Our main tool for this study will be the *Coulson's formula* (1.7.2) for energy of a graph. In particular, the formula (1.7.3) gives rise to a quasi-ordering (see Definition 6.1.2) in the class containing all trees and unicyclic graphs with a fixed girth of a given order. We explore this quasi-ordering in our effort and find two graphs each in $\mathcal{U}_{n,g}$ and $\mathcal{U}_n^b$ having the least energies.

For $3 \leq g \leq n$, let $S_n^g$ denote the graph in $\mathcal{U}_{n,g}$ obtained by attaching $n-g$ pendants to a vertex $u_0$ of the cycle $C_g$. Note that $S_n^n = C_n$ and $S_n^4 = G_1(n)$ (see Section 5.1). Moreover, for $n \geq 4$ let $T_n^g$ denote the graph obtained from $S_n^g$ by shifting one of its pendent edges from $u_0$ to another vertex on $C_g$ which is at a distance 2 from $u_0$, if $n-g > 1$, and $S_n^g$, if $n-g = 0$ or 1. Note that $T_n^4 = G_4(n)$ (see Section 5.1). We will see in the sequel that $S_n^g$ and $T_n^g$ are the unique graphs with minimum and second minimum energies among all graphs in $\mathcal{U}_{n,g}$ for given $n$ and $g \leq n$; and that $S_n^4$ and $T_n^4$ are the

$S_n^4 = G_1(n)$ $T_n^4 = G_4(n)$

Figure 6.1: The graphs $S_n^g$ and $T_n^g$

unique graphs with minimum and second minimum energies among all graphs in $\mathcal{U}_n^b$ for $n \geq 6$.

Let

$$P(G;x) = a_0(G)x^n + a_1(G)x^{n-1} + \cdots + a_n(G)$$

be the characteristic polynomial of $G$ and

$$b_i(G) = \mid a_i(G) \mid, \; i = 0, 1, \ldots, n.$$

If there is no confusion, then we write $b_i$ for $b_i(G)$. 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 6.1.1** [41] *If $G$ is a unicyclic graph with a cycle of size $g$, then for all $k \geq 0$, $(-1)^k a_{2k} \geq 0$. Further, $(-1)^k a_{2k+1} \geq$ (resp. $\leq$) $0$ if $g = 2r+1$ and $r$ is odd (resp. even).*

**Definition 6.1.2** [41] Let $\mathcal{T}_n$ denote the class of all trees of order $n$. The *quasi-ordering* $\succeq$ in the class $\mathcal{T}_n \cup \mathcal{U}_{n,g}$ is defined as follows: For graphs $G$ and $H$

$$G \succeq H \;\text{ if }\; b_i(G) \geq b_i(H), \; i = 1, 2, \ldots, n.$$

If $G \succeq H$, then we sometimes write $H \preceq G$. Moreover, if $G \succeq H$ holds but $H \succeq G$ does not, then we write $G \succ H$.

**Theorem 6.1.3** [41] *Let $G$ and $H$ be graphs in $\mathcal{T}_n \cup \mathcal{U}_{n,g}$. Then $G \succeq H$ implies $E(G) \geq E(H)$, and $G \succ H$ implies $E(G) > E(H)$.*

**Proof.** If $G$ is a unicyclic graph, in view of Lemma 6.1.1, the formula (1.7.3) reduces to

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil} b_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil} b_{2j+1}x^{2j+1}\right)^2\right]. \tag{6.1.1}$$

We note that (6.1.1) is also valid if $G$ is a tree, because then $b_{2j+1} = 0$ for all $j$. Thus, if $G$ is a tree or a unicyclic graph $E(G)$ is a monotonically increasing function of $b_i(G)$, $i = 1, 2, \ldots, n$. Hence, the result follows. □

The following lemma can be easily verified using Lemma 4.1.3.

**Lemma 6.1.4** [41] *Let $G$ be a tree or a unicyclic graphs and $\{u,v\}$ be a pendent edge of $G$ with the pendent vertex $v$. Then, for all $i$*

$$b_i(G) = b_i(G-v) + b_{i-2}(G-u-v). \tag{6.1.2}$$

## 6.2 Graphs in $\mathcal{U}_{n,g}$ with minimal energy

**Lemma 6.2.1** *Let* $G \in \mathcal{U}_{n,g}$ *then* $G \succeq S_n^g$*. Equality holds if and only if* $G = S_n^g$*.*

**Proof.** We prove the lemma by induction on $p = n - g$. In a trivial manner the result holds for $p = 0$ and 1, because then $\mathcal{U}_{n,g}$ consists of a single graph $S_n^g$. Suppose that $p \geq 2$ and that the result hold for all graphs for which $n - g = k < p$. Now, let $p = n - g$ for $G$. Since $G$ is unicyclic and not a cycle, $G$ must have a pendent edge $\{u, v\}$ with pendent vertex $v$. Therefore, by lemma 6.1.4, we have

$$\begin{aligned} b_i(G) &= b_i(G - v) + b_{i-2}(G - u - v), && (6.2.3) \\ b_i(S_n^g) &= b_i(S_{n-1}^g) + b_{i-2}(S_{n-1}^g - u_0). && (6.2.4) \end{aligned}$$

By the induction assumption, $G - v \succeq S_{n-1}^g$. If $G - u - v$ is connected and contains the cycle, then by induction assumption, $G - u - v \succeq S_{n-2}^g$. Now, for $2k \neq g$, we have

$$\begin{aligned} b_{2k-2}(S_{n-2}^g) &= m(S_{n-2}^g, k-1) \\ &\geq m(S_{n-1}^g - u_0, k-1) \\ &= b_{2k-2}(S_{n-1}^g - u_0). \end{aligned}$$

Since all other $b_i$ for $S_{n-1}^g - u_0$ are zero, we get $S_{n-2}^g \succeq S_{n-1}^g - u_0$ and, therefore,

$$G - u - v \succeq S_{n-1}^g - u_0.$$

If $G - u - v$ is acyclic (not necessarily connected), then we have

$$\begin{aligned} b_{2k-2}(G - u - v) &= m(G - u - v, k-1) \\ &\geq m(P_{g-1}, k-1) \\ &= m(S_{n-1}^g - u_0, k-1) \\ &= b_{2k-2}(S_{n-1}^g - u_0), \end{aligned}$$

yielding $G - u - v \succeq S_{n-1}^g - u_0$. If $G - u - v$ is not connected and contains the cycle, then again

$$\begin{aligned} b_{2k-2}(G - u - v) &= m(G - u - v, k-1) \\ &\geq m(P_{g-1}, k-1) \\ &= b_{2k-2}(S_{n-1}^g - u_0), \end{aligned}$$

for $2k-2 < g$. Since all other $b_i$ for $S^g_{n-1}-u_0$ are zero, we get $G-u-v \succeq S^g_{n-1}-u_0$. Hence from (6.2.3) and (6.2.4) we get $G \succeq S^g_n$. Moreover, if $G \neq S^g_n$, then we have $n > g \geq 3$ and

$$\begin{aligned} b_4(G) &= b_4(G-u) + b_2(G-u-v) \\ &\geq b_4(S^g_{n-1}) + m(G-u-v,1) \\ &> b_4(S^g_{n-1}) + m(P_{g-1},1) \\ &= b_4(S^g_{n-1}) + b_2(S^g_{n-1}-u_0) \\ &= b_4(S^g_n), \end{aligned}$$

yielding $G \succ S^g_n$. □

**Lemma 6.2.2** *Let $\mathcal{P}_{g-1}$ be the set of all graphs obtained from $P_{g-1}$ by attaching a pendant with any vertex of $P_{g-1}$. Let $P^1_{g-1}$ denote the tree obtained from $P_{g-1}$ by attaching a pendant at the vertex which is at a distance one from one end. If $Q \in \mathcal{P}_{g-1}$ then*

$$Q \succeq P^1_{g-1}.$$

**Proof.** If $Q = P_g$, then there is nothing to prove. Clearly the result is true for $g = 4$. Let $uv$ be a pendent edge with $v$ as pendant and degree of $u$ is two, by Lemma 6.1.4,

$$b_{2i}(Q) = b_{2i}(Q-v) + b_{2i-2}(Q-u-v), \tag{6.2.5}$$

$$b_{2i}(P^1_{g-1}) = b_{2i}(P^1_{g-1}-v) + b_{2i-2}(P^1_{g-1}-u-v). \tag{6.2.6}$$

By induction, we have

$$\begin{aligned} b_{2i}(Q-v) &\geq b_{2i}(P^1_{g-1}-v), \\ b_{2i-2}(Q-u-v) &\geq b_{2i-2}(P^1_{g-1}-u-v). \end{aligned}$$

Hence from (6.2.5) and (6.2.6) we get $b_{2i}(Q) \geq b_{2i}(P^1_{g-1})$ and therefore $Q \succeq P^1_{g-1}$. □

**Lemma 6.2.3** *Let $G \in \mathcal{U}_{n,g}$, $G \neq S^g_n, T^g_n$. Then $G \succ T^g_n$.*

**Proof.** We prove the lemma by induction on $p = n-g$. It is vacuously true for $p = 0$ and 1, because then $\mathcal{U}_{n,g}$ consists of a single graph $S^g_n$. Suppose that $p \geq 2$ and that the result hold for all graphs for which $n-g = k < p$. Now, let $p = n-g$ for $G$. Since $G$ is unicyclic and not a cycle, $G$ must have a pendent vertex. Let $v$ be a pendent vertex in $G$

which is at a maximum distance from the cycle and $u$ the vertex adjacent to $v$. Then by lemma 6.1.4, we have

$$\begin{aligned} b_i(G) &= b_i(G-v) + b_{i-2}(G-u-v), && (6.2.7) \\ b_i(T_n^g) &= b_i(T_{n-1}^g) + b_{i-2}(P_{g-1}^{(1)} \cup H). && (6.2.8) \end{aligned}$$

for all $i$, where $H$ is the empty graph on $n-g-2$ vertices. By the induction assumption, $G - v \succeq T_{n-1}^g$. Moreover, $G-u-v$ has an induced subgraph $K$, where $K$ is either $C_g$ or a tree in $\mathcal{P}_{g-1}$ $\left(\neq P_{g-1}^{(1)}\right)$. For $2k-2 < g$, we clearly have

$$m(P_{g-1}^{(1)}, k-1) \leq m(K, k-1),$$

with strict inequality for at least one $k$. Since

$$\begin{aligned} b_{2k-2}(P_{g-1}^{(1)} \cup H) &= m(P_{g-1}^{(1)}, k-1) \\ &\leq m(K, k-1) \\ &\leq b_{2k-2}(G-u-v), \end{aligned}$$

for $2k-2 < g$, and because all other $b_i$ for $P_{g-1}^{(1)} \cup H$ are zero, we get

$$b_{i-2}(P_{g-1}^{(1)} \cup H) \leq b_{i-2}(G-u-v)$$

for all $i$, with strict inequality for at least one $i$. Hence, by (6.2.7) and (6.2.8) we get $G \succ T_n^g$. □

**Theorem 6.2.4** *If $G \in \mathcal{U}(n,g)$ then $E(G) \geq E(S_n^g)$. Equality holds if and only if $G = S_n^g$.*

**Proof.** The theorem follows from Lemma 6.1.3 and Lemma 6.2.1. □

**Theorem 6.2.5** *Let $G \in \mathcal{U}(n,g), G \neq S_n^g, T_n^g$. Then $E(G) > E(T_n^g)$.*

**Proof.** The theorem follows from Lemma 6.1.3 and Lemma 6.2.3. □

The above two theorems show that among all unicyclic graphs on $n$ vertices and having girth $g$, the two graphs $S_n^g$ and $T_n^g$ have the minimum and the next minimum energies, respectively.

## 6.3 Unicyclic bipartite graphs with minimal energy

**Theorem 6.3.1** *If $G$ is a connected unicyclic bipartite graph on $n$ vertices, then $E(G) \geq E(S_n^4)$. Equality holds if and only if $G = S_n^4$.*

**Proof.** Let $G$ be of girth $g$. If $g = 4$, then the result follows from Theorem 6.2.4. So, suppose that $g \geq 6$. Now, we have

$$\begin{aligned} b_0(S_n^g) &= b_0(S_n^4) = 1, \\ b_2(S_n^g) &= b_2(S_n^4) = n, \\ b_4(S_n^4) &= 2n - 8, \end{aligned}$$

and $b_i(S_n^4) = 0$ for $i \neq 0, 2, 4$. On the other hand, $b_4(S_n^g) = f(g)$, where

$$\begin{aligned} f(g) &= m(S_n^g, 2) \\ &= (g-2)(n-g) + m(C_g, 2) \\ &= (g-2)(n-g) + \frac{g(g-3)}{2}. \end{aligned}$$

Now, $f^{'}(g) = n - g + \frac{1}{2} > 0$, for $g \leq n$, and, therefore $f(g)$ is an increasing function of $g$. Therefore, we have

$$b_4(S_n^g) \geq b_4(S_n^6) = 4n - 15 > 2n - 8 = b_4(S_n^4),$$

yielding $S_n^g \succ S_n^4$. Hence, by Theorem 6.2.4, $G \succeq S_n^g \succ S_n^4$, and the result follows from Theorem 6.1.3. $\square$

**Theorem 6.3.2** *If $G$ is a unicyclic bipartite graph on $n$ vertices, $G \neq S_n^4, T_n^4$, then $E(G) \succ E(T_n^4)$.*

**Proof.** Let $G$ be of grith $g$. If $g = 4$, then the result follows from Theorem 6.2.5. Therefore, suppose that $g \geq 6$. Now, we have

$$\begin{aligned} b_0(G) &= b_0(T_n^4) = 1, \\ b_2(G) &= b_2(T_n^4) = n, \\ b_4(T_n^4) &= 3n - 13, \end{aligned}$$

and $b_i(T_n^4) = 0$ for $i \neq 0, 2, 4$. Since

$$b_4(S_n^6) = 4n - 15 > 3n - 13 = b_4(T_n^4),$$

we have $S_n^6 \succ T_n^4$. Thus, we have $G \succeq S_n^g \succeq S_n^6 \succ T_n^4$ and therefore $E(G) \succ E(T_n^4)$. □

Theorem 6.3.1 and Theorem 6.3.2 show, respectively, that among all bipartite unicyclic graphs on $n$ vertices, the two graphs $S_n^4$ and $T_n^4$ have the minimum and the next minimum energies, respectively.

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