GRAPH INDICES AND GRAPH PRODUCTS

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GRAPH INDICES AND GRAPH PRODUCTS

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<u>DECLARATION</u>

I, Mr. **<u>Muhammad Kamran Jmail</u>** Registration No. **<u>63-GCU-PHD-SMS-13</u>** student at **Abdus Salam School of Mathematical Sciences GC University** in the subject of **Mathematics,** year of admission **2011**, hereby declare that the matter printed in thesis titled

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is my own work and that

(i) I am not registered for similar degree elsewhere contemporaneously.

(ii) No major work had already been done by me or anybody else on the topic; I worked on for the Ph.D degree.

(iii) The work I am submitting for the Ph.D degree has not already been submitted elsewhere and shall not in future be submitted by me for obtaining similar degree from any other institution.

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Date Signature of Student

RESEARCH COMPLETION CERTIFICATE

Certified that the research work contained in this thesis titled

“GRAPH INDICES AND GRAPH PRODUCTS”

has been carried out and completed by **Mr. Muhammad Kamran Jamil** Registration No. **63-GCU-PHD-SMS-11** under my supervision.

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Date	Prof. Dr. Ioan Tomescu Supervisor

Submitted Through

Prof. Dr. Shahid Saeed Siddiqui	--------------------------------
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Dedicated

To My Family

Table of Contents

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Abstract

Many chemical substances consists of molecules. One of the primary goals of chemistry is to build relations between the chemical and physical properties of substance and the structure of the corresponding molecules. Many results along these lines have been obtained. Majority of such chemical rules are qualitative in nature. For example, if a molecule have -COOH group then that molecule exhibits an acidic behavior.

A century-long tendency in chemistry is to go a step further and to find quantitative relations of same kind. But, molecular structure is a non-numerical notion. The measured physical and chemical properties of substances are quantities. So, to build a relation between molecular structure and any physico-chemical property, one must transform the information contained in the molecular structure into a number. A topological index is a quantity that is somehow calculated from the molecular graph and for which we believe that it reflects relevant structural features of the underlying molecule.

Chapter 1 of this dissertation deals with some basic definitions and notions from chemical graph theory.

In chapter 2, we discuss that the spur graph gives the maximum zeroth-order general Randić index for $\alpha > 1$ and general sum-connectivity index, $\alpha \geq 1$ for trees with given independence number.

We generalize the Du et. al. results for sum-connectivity index in chapter 3. We find the maximum value for the general sum-connectivity index of $n-$vertex trees and $n-$vertex unicyclic graphs and characterize the extremal graphs. We also discuss the $n-$vertex unicyclic graphs with second maximum general sum-connectivity index.

In chapter 4, we extend the Goubko's result for any connected graph with cyclomatic number and characterize the minimal first Zagreb index for graphs with fixed number of vertices, pendant vertices and cyclomatic number.

In chapter 5, we find some exact formulae for the first reformulated index of some graph operations i.e. cartesian product, composition, join, link of graphs etc. and

apply these results to graphs of general interest. In last chapter, we derive the exact formulas for distance based topological indices for double graphs and apply these results to special kinds of graphs.

Chapter 1

Basic Terminology and Graph Indices

1.1 Introduction

In this chapter, we recall some basic definitions, notations and results from graph theory which will be used throughout this dissertation. In this dissertation, we deal with simple, finite and connected graphs.

1.2 Preliminaries

A *graph* $G = (V(G), E(G), \sim)$ is a triple, where $V(G)$ and $E(G)$ is the set of vertices and the set of edges, respectively, and $\sim$ is the relation that associates each edge with two vertices. The number of elements in $V(G)$, $|V(G)|$, is called the *order* of G and the number of elements in $E(G)$, $|E(G)|$, is called the *size* of G. In this dissertation, we use m and n for the size and order, respectively. The order of a graph G is at least 1 and the graph G with order 1 is called a *trivial graph*. A graph with order 0 (and size 0) is called the *null graph*. A graph G is said to be finite if its order and size are

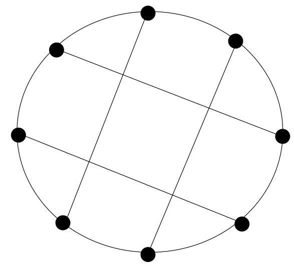

Figure 1.1: A 3-regular graph.

finite. In a graph G two vertices y and z are *adjacent* if $yz \in E(G)$, we also say y and z are *neighbors* of each other. An edge e is a *loop* if $e = zz$ and edges e_1, e_2 are *parallel* edges if $e_1 = e_2 = yz$. A graph G without loops and parallel edges is called a *simple graph*. The set $N(z)$ of the neighbors of vertex z, is called the *neighborhood* of z. In a graph G the number of vertices adjacent to a vertex z is called the *degree* of z in G, denoted as $d_G(z)$, also $d(z)$ when the graph G is obvious. Thus $d(z) = |N(z)|$ and $S_z = \sum_{y \in N(z)} d(y)$. A vertex z is said to be an *isolated* vertex if $d(z) = 0$ and *pendant* vertex if $d(z) = 1$. We denote the *maximum* and *minimum* degrees of a graph G by $\triangle(G)$ and $\delta(G)$, respectively. If for a graph G, $\delta(G) = \triangle(G) = t$, then G is called a *t-regular* graph. Figure 1.1 shows a 3-regular graph. For a graph G of order n and for any vertex z of G, the following inequalities hold:

$$0 \leq \delta(G) \leq d(z) \leq \triangle(G) \leq n - 1.$$

The following theorem relates the degrees of the vertices and the number of edges of a graph G.

Theorem 1.2.1. *[9] For any graph G*

$$\sum_{z \in V(G)} d(z) = 2m.$$

Corollary 1.2.2. *In any graph G, there is an even number of vertices of odd degree.*

For a graph G, a subset I of $V(G)$ is called an *independent set* of G if every two vertices of I are non-adjacent. The maximum number of vertices in I is called the *independence number* of G, denoted by $\alpha(G)$. In figure 1.2 white vertices form the independence set and these are maximum in numbers so $\alpha(G) = 4$. The maximum size of a set of pairwise adjacent vertices in a graph G is called the *clique number* of G, written as $\omega(G)$. In figure 1.3 the pairwise adjacent vertices are shown in white and these are maximum in numbers so $\omega(G) = 3$.

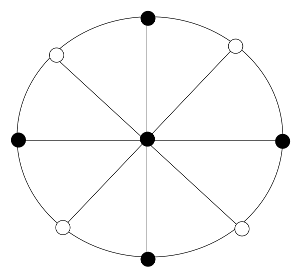

Figure 1.2: A graph with $\alpha = 4$.

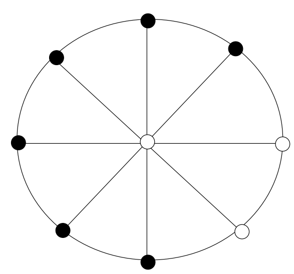

Figure 1.3: A graph with ω=3.

A graph K is called a *subgraph* of a graph G, denoted $K \subseteq G$, if $V(K) \subseteq V(G)$ and $E(K) \subseteq E(G)$. The subgraph K is said to be a *proper subgraph* of a graph G, if either $V(K)$ is a proper subset of $V(G)$ or $E(K)$ is a proper subset of $E(G)$ or both. If $V(K) = V(G)$ then the subgraph K is called *spanning subgraph* of the graph G. A subgraph K is said to be an *induced subgraph*, if whenever $y, z \in V(K)$ and $yz \in E(G)$, then $yz \in E(K)$ as well. Figure 1.4 shows a graph and its induced subgraph. Consider K be a nonempty set of vertices of a graph G, then the *subgraph of G induced* by K is the induced subgraph with vertex set K. This type of subgraph is denoted as $\langle K \rangle$. One can easily obtain a proper subgraph of a graph G by deleting some vertices and all edges incident to these vertices. The graphs $G-e$ and $G-v$ are the proper subgraphs of the graphs G, named as edge-deleted subgraph and vertex-deleted subgraph, respectively.

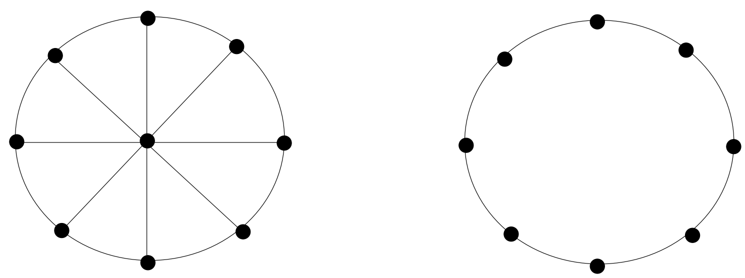

Figure 1.4: A graph and its induced subgraph.

1.3 Connectedness of Graphs

A *walk* (of length w) in a graph G is a sequence S with alternating terms of vertices and edges of G (not necessarily different), $S = z_0e_1z_1 \ldots z_{w-1}e_wz_w$, such that $e_i = z_{i-1}z_i, 1 \leq i \leq w$. If $z_0 = y$ and $z_w = z$, then this walk S connects y to z and refer to S as an $yz-$walk. A walk S is said to be closed walk if $z_0 = z_w$, i.e. its terminal vertices are identical. A walk is a *trail* if all its edge terms are different. If the vertices in a walk S are all different, then this walk is called a *path* in G. A *cycle* is a path with same initial and final vertex, i.e. $z_0 = z_w$. A path and a cycle of order n is denoted by P_n and C_n, respectively.

Theorem 1.3.1. *[10] If a graph G contains a yz-walk of length w, then G contains a yz-path of length at most w.*

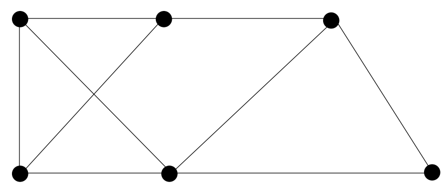

Figure 1.5: A connected graph.

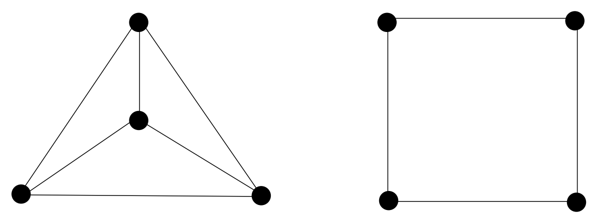

Figure 1.6: A disconnected graph with 2 components.

Theorem 1.3.2. *[9] Let G be a graph in which all vertices have degree at least two. Then G contains a cycle.*

A graph G is said to be *connected* if each pair of distinct vertices in G belongs to a path, otherwise graph G is disconnected. Let K be a connected subgraph of the graph G such that no other connected subgraph of the graph G properly contains K, then the subgraph K is called a *component* of the graph G. So, we can say that a graph G is connected if and only if it has exactly one component. Figures 1.5,1.6 shows a connected and a disconnected graph, respectively.

Proposition 1.3.3. *[66] Every graph with n vertices and m edges has at least $n - m$ components.*

Let G be a connected graph, the *distance* between two vertices y, z of G is the shortest length of any $y - z$ path in G and is denoted by $d_G(y, z)$ or simply $d(y, z)$, when the graph G is obvious. By definition, $d(x, x) = 0$. If there is no path containing y and z, i.e., if y and z lie in different components of G, in this case $d(y, z)$ is not

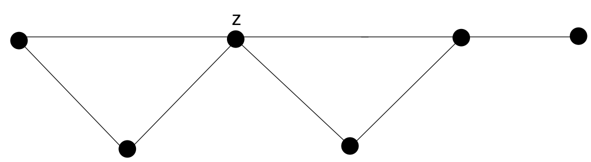

Figure 1.7: A graph with radius 2 and diameter 3.

defined. For every two vertices y and z of a connected graph G of order n

$$0 \leq d(y, z) \leq n - 1.$$

For a vertex z in a connected graph G, the *eccentricity* of z, $ecc(z)$, is the distance between z and a vertex farthest from z in G. The minimum and maximum eccentricities among the vertices of the graph G are called the *radius* and *diameter*, respectively, of the graph G. The graph in figure 1.7 has radius 2, diameter 3 and $ecc(z) = 2$.

A vertex z in a connected graph G is a *cut-vertex* of the graph G if $G - z$ is disconnected. If the graph G has more than one component, then the vertex z is a cut-vertex of G if z is a cut-vertex of a component of G. In figure 1.8 vertices a, b and c represent the cut vertices. A connected graph G without cut-vertices is called *nonseparable graph*. A maximal nonseparable subgraph of a graph G is called a *block*.

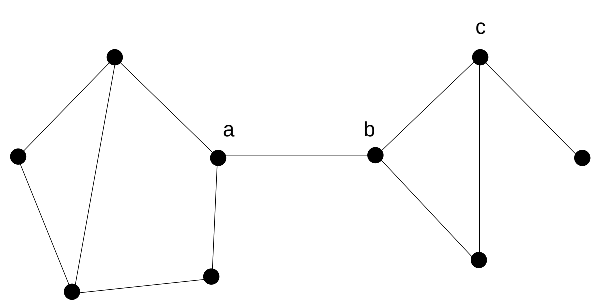

Figure 1.8: A graph with cut vertices.

1.4 Some Families of Graphs

A graph G is called a *complete* graph if any two vertices of G are adjacent, see figure 1.9. A complete graph of order n is denoted by K_n. It has maximum size, i.e., $\frac{n(n-1)}{2}$. A graph G is *bipartite* if its vertex set $V(G)$ can be partitioned into two subsets Y and Z such that every edge has one end in Y and one end in Z. If every vertex in Y is joined to every vertex in Z, then the graph G is called a *complete bipartite* graph. A complete bipartite graph with $|Y| = a$ and $|Z| = b$ is denoted by $K_{a,b}$. Figure 1.10 shows a complete bipartite graph.

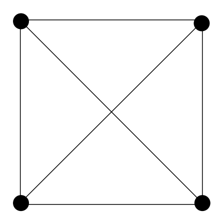

Figure 1.9: A complete graph with 4 vertices.

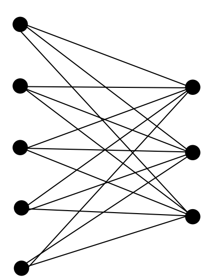

Figure 1.10: A complete bipartite graph.

Theorem 1.4.1. *[10] A graph G is bipartite if and only if there is no odd cycle in G.*

A graph G without cycles is an *acyclic* graph. A connected acyclic graph is known as a *tree*. We can say that each component of an acyclic graph is a tree. For this reason, acyclic graphs are called *forests*. A tree with n vertices is usually denoted as T_n.

Paths are trees. A tree is a path if and only if $\triangle(T) = 2$. A *star* graph is a tree consisting of one vertex adjacent to all other vertices. A star graph with order n is denoted by S_n and it has a vertex z such that $d(z) = n - 1$. Figure 1.11 shows a star graph. A star is a bipartite graph so it can also be represent as $K_{1,n-1}$. A *bistar* of order n, $BS(p, q)$, consists of two vertex disjoint stars, $K_{1,p}$ and $K_{1,q}$, where $p + q = n - 2$, and a new edge joining the centers of these stars, see figure 1.12. For every $n \geq 2$ and $n/2 \leq s \leq n - 1$, the *spur* [16] $S_{n,s}$ is a tree consisting of $2s - n + 1$ edges and $n - s - 1$ paths of length 2 having a common end vertex; in other words it is obtained from a star $K_{1,s}$ by attaching a pendant edge to $n - s - 1$ pendant vertices of $K_{1,s}$. Figure 1.13 illustrates the spur.

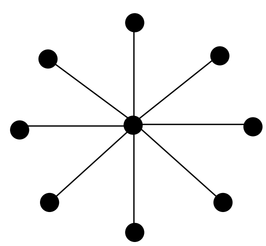

Figure 1.11: S_9

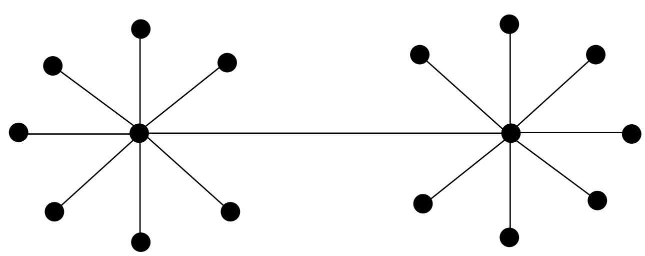

Figure 1.12: B(7,7)

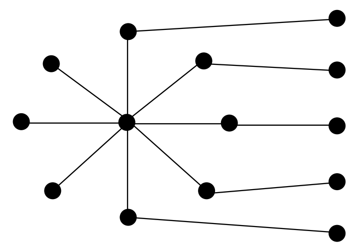

Figure 1.13: $S_{14,9}$

Theorem 1.4.2. *[10] A graph G is a tree if and only if every two distinct vertices of G are connected by a unique path.*

Theorem 1.4.3. *[5] The following statements are equivalent for a graph G:*

i. G is a tree.

ii. G is a minimal connected graph, that is G is connected and if $yz \in E(G)$ then $G - yz$ is disconnected.

iii. G is a maximal acyclic graph, that is G is acyclic and if x and y are non-adjacent vertices of G, then $G + xy$ contains a cycle.

Corollary 1.4.4. *[5] A tree of order at least 2 contains at least 2 pendant vertices.*

Theorem 1.4.5. *[9] Let G be a graph of order n and size m. If G satisfies any two of the properties:*

i. G is connected

ii. G is acyclic

iii. $m = n - 1$,

then G is a tree.

The *cyclomatic number* $\gamma(G)$ of a graph G is the number of independent cycles existing in G. For a connected graph G of order n and size m we have the relation $\gamma(G) = m - n + 1$. If G has p connected components, then $\gamma(G) = m - n + p$. A graph G with one cycle is called a *unicyclic* graph and a graph with two independent cycles called a *bicyclic* graph. Unicyclic and bicyclic graphs of order n has sizes n and $n+1$, respectively. If $\gamma = 0$, then G is a tree.

An *isomorphism* from a graph $G = (V(G), E(G))$ to a graph $K = (V(K), E(K))$ is a bijection $h : V(G) \to V(K)$ such that $yz \in E(G)$ if and only if $h(y)h(z) \in E(K)$. We write $G \cong K$ if there is an isomorphism from G to K and we say that G is *isomorphic* to K. Clearly, isomorphic graphs have same order and size. Figure 1.14 shows two isomorphic graphs.

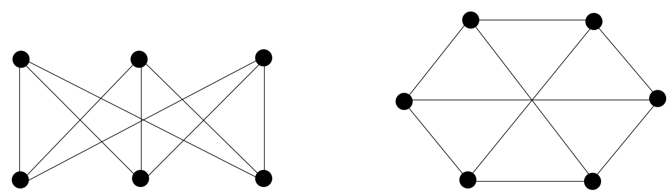

Figure 1.14: Two isomorphic graphs.

Theorem 1.4.6. *[66] The isomorphism relation is an equivalence relation on the set of graphs.*

1.5 Chemical Graph Theory

Graph theory applied in the study of molecular structure represents an interdisciplinary science, called chemical graph theory or molecular topology. By using tools taken from graph theory, set theory and statistics it attempt to identify structural features involved in structure-property activity relationship. The partitioning of a molecule and recombining its fragmental values by additive models is one of its main tasks. Topological characterization of chemical structures allows the classification of molecules and modeling unknown structures with desired properties.

A *chemical graph* is a model of a chemical system, used to characterize the interactions among its components: atoms, bonds, groups of atoms or molecules. Chemical graphs were first introduced in the latter half of the eighteenth century. Chemical graphs are now being used for many different purposes in all the major branches of chemistry. A structural formula of a chemical compound can be represented by a *molecular graph*, its vertices being atoms and edges corresponding to covalent bonds. Usually hydrogen atoms are not depicted in which case we speak of *hydrogen depleted molecular graphs.* The heavy atoms from carbon (i.e. heteroatoms) can be represented, as shown in figure 1.15. Similarly, a transform of a molecule (e.g. a chemical reaction) can be visualized by a *reaction graph*, whose vertices are chemical species and edges reaction pathways.

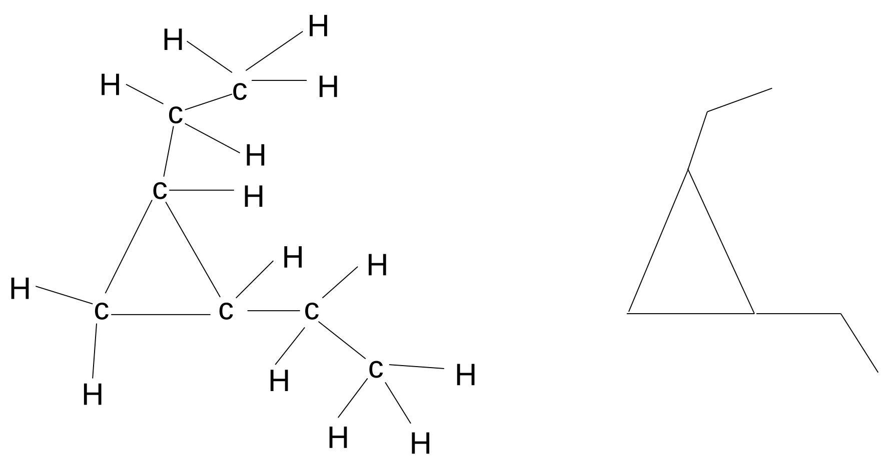

Figure 1.15: A molecular graph and its hydrogen depicted representation.

1.6 Topological Indices in Graph Theory

A *parameter* or an *invariant* of a graph G is a number associated with G which has the same value for any graph isomorphic to G [7]. These invariants may help us to distinguish non-isomorphic graphs. Some of very common graph invariants are the number of vertices, edges, components, radius, diameter, independence number, clique number, maximum or minimum degree etc.

A *topological index* is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. Many topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies [13, 15, 44, 63].

One of the oldest and widely used indices is the *Wiener index*, named after Harry Wiener, who introduced it in 1947 [33, 34]. It has been used to model various properties of chemical species [67]. The *Wiener index* of a graph G having $V(G) = \{z_1, z_2, \ldots, z_n\}$ is defined as the sum of distances between all unordered pairs of vertices of a graph G, i.e.,

$$W(G) = \sum_{1 \leq i < j \leq n} d_G(z_i, z_j).$$

Klein et. al. [46] introduced the *hyper-Wiener index* , as a generalization of the Wiener index. It is defined as

$$WW(G) = \frac{1}{2} W(G) + \frac{1}{2} \sum_{\{y,z\} \subseteq V(G)} d^2(y, z).$$

Many of mathematical properties of the hyper-Wiener index and its applications in chemistry are discussed in [27, 46, 49]. We introduce the *general hyper-Wiener* index [61], denoted by $WW_\alpha(G)$, for any real α by

$$WW_\alpha(G) = \frac{1}{2} \sum_{\{y,z\} \subseteq V(G)} (d(y, z)^\alpha + d(y, z)^{2\alpha}).$$

Sharma, Goswami and Madan [57] introduced an adjacency-cum-distance based topological index, called the *eccentric connectivity* index of the graph G, defined as

$$\zeta^c(G) = \sum_{z \in V(G)} d(z) ecc(z).$$

The *total eccentric connectivity* index is defined as

$$\zeta(G) = \sum_{z \in V(G)} ecc(z).$$

Another distance based topological index is the *Harary index*. The Harary index of a graph G, written as $H(G)$, is defined as follows [39, 54]:

$$H(G) = \sum_{1 \le i < j \le n} \frac{1}{d_G(z_i, z_j)}.$$

Mathematical properties and applications of this index can be seen in [14, 21].

Iranmmanesh et. al. [1] introduced a modification of the Harary index, called *additively Harary index*, defined by

$$H_A(G) = \sum_{1 \le i < j \le n} \frac{d(z_i) + d(z_j)}{d_G(z_i, z_j)}.$$

The *multiplicative Harary index* was introduced by Su et. al. [58], which can be seen as a product-degree-weight version of the Harary index:

$$H_M(G) = \sum_{1 \le i < j \le n} \frac{d(z_i)d(z_j)}{d_G(z_i, z_j)}.$$

A large number of topological indices have been derived depending on vertex degrees. We discussed some of them. *Randić* (product-connectivity) index was proposed by the chemist Milan Randić [55] in 1975. The Randić index $R(G)$ of a graph G is defined as

$$R(G) = \sum_{yz \in E(G)} \frac{1}{\sqrt{d(y)d(z)}}.$$

Erdős and Bollobás [23] proved that the star minimizes the Randić index for all graphs without isolated vertices and on a fixed number of vertices. Some properties of the Randić index concerning diameter, radius, chromatic number, average distance and eigenvalues of the adjacency matrix were discussed in [2, 3]. In 1998 Bollobás and Erdös [6] replaced $-\frac{1}{2}$ by any real number α to generalize this index, which is known as the general Randić index. Yuan, Li and Hu [70, 71] characterized the trees with extremal general Randić index. General Randić index is defined as:

$$R_\alpha(G) = \sum_{yz \in E(G)} (d(y)d(z))^\alpha.$$

The *zeroth-order general Randić index*, denoted by ${}^0R_\alpha(G)$ was defined in [37] and [45] as:

$${}^0R_\alpha(G) = \sum_{z\in V(G)} d(z)^\alpha.$$

For $\alpha = 2$ this index is also known as first Zagreb index and denoted by $M_1(G)$. The first and second *Zagreb indices* are among the oldest and most famous topological indices. These indices were introduced by Gutman and Trinajstić [36]. These are defined as follows:

$$M_1(G) = \sum_{z\in V(G)} d(z)^2,$$

$$M_2(G) = \sum_{yz\in E(G)} d(y)d(z).$$

The first Zagreb index can also be expressed as:

$$M_1(G) = \sum_{yz\in E(G)} (d(y) + d(z)).$$

For a historical background and properties of Zagreb indices see [8, 29, 53, 72, 73].

Recently, Todeschini et. al. [62, 64] proposed the *multiplicative* variants of ordinary Zagreb indices, defined as:

$$\prod\nolimits_1(G) = \prod_{z\in V(G)} d(z)^2,$$

$$\prod\nolimits_2(G) = \prod_{yz\in E(G)} d(y)d(z).$$

Various properties of multiplicative Zagreb indices were discussed in [24, 28, 43].

Narumi and Katayama [52] established an index by taking the product of degrees of all vertices of the graph G, which is known as *Narumi-Katayama index*, as follows:

$$NK(G) = \prod_{z\in V(G)} d(z).$$

Clearly, $\prod_1(G) = NK(G)^2$. So, the graphs for which NK assumes an extremal value, $\prod_1$ also assumes.

Miliçević et. al. [50] in 2004 *reformulated the Zagreb indices* by replacing vertex degrees by edge degrees as

$$EM_1(G) = \sum_{e\in E(G)} d(e)^2,$$

$$EM_2(G) = \sum_{e\sim f} d(e)d(f),$$

where $d(e)$ is the degree of the edge e in G, defined by $d(e) = d(y) + d(z) - 2$ with $e = yz$ and $e \sim f$ represents that the edges e and f are adjacent.

Zhou et. al. [75] proposed the *sum-connectivity index*. The sum-connectivity index is obtained from Randić index by replacing the term $d(y)d(z)$ by $d(y) + d(z)$.

$$\chi(G) = \sum_{yz\in E(G)} \frac{1}{\sqrt{d(y)+d(z)}}.$$

Du et. al. [21] found the minimum sum-connectivity indices of trees and unicyclic graphs. Some other properties can be seen in [69, 22]. The concept of sum-connectivity index was extend to the *general sum-connectivity index* in [76]:

$$\chi_\alpha(G) = \sum_{yz\in E(G)} (d(y) + d(z))^\alpha,$$

where $\alpha \in \mathbb{R}$. Several properties of the general sum-connectivity index were given in [18, 42, 60, 65].

Randić index has another variant, called *harmonic index* [25], defined as

$$H(G) = \sum_{yz\in E(G)} \frac{2}{d(y)+d(z)} = 2\chi_{-1}(G).$$

By the inequality between the arithmetic and geometric means we have inequality $H(G) \leq R(G)$ and equality holds if and only if the graph G is a regular graph.

1.7 Graph Operations

In this section, we discuss some graph operations. We can construct many interesting classes of graphs from simpler graphs by using graph operations also known as graph products [40].

The *cartesian product*, $G_1 \Box G_2$, of graphs G_1 and G_2 has the vertex set $V(G_1 \Box G_2) = V(G_1) \times V(G_2)$ and $(y_1, y_2)(z_1, z_2)$ is an edge of $G_1 \Box G_2$ if $y_1 = z_1$ and $y_2 z_2 \in E(G_2)$, or $y_1 z_1 \in E(G_1)$ and $y_2 = z_2$. If $G_1, G_2, \ldots, G_n$ are graphs, then we denote $G_1 \Box G_2 \Box \cdots \Box G_n$ by $\mathop{\Box}\limits_{1}^{n} G_i$. If $G_1 = G_2 = \cdots = G_n = G$, we denote $\mathop{\Box}\limits_{1}^{n} G_i$ by G^n.

The *composition* $G_1[G_2]$ (or lexicographic product) of graphs G_1 and G_2 with disjoint vertex sets and edge sets is again a graph on vertex set $V(G_1) \times V(G_2)$ in which (y_1, y_2) is adjacent with (z_1, z_2) whenever $y_1 z_1 \in E(G_1)$ or $y_1 = z_1$ and $y_2 z_2 \in E(G_2)$.

The *disjunction* $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and (y_1, z_1) is adjacent with (y_2, z_2) whenever $y_1 y_2 \in E(G_1)$ or $z_1 z_2 \in E(G_2)$.

The *symmetric difference* $G_1 \oplus G_2$ of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and $E(G_1 \oplus G_2) = \{(y_1, y_2)(z_1, z_2) | y_1 z_1 \in E(G_1) \textit{ or } y_2 z_2 \in E(G_2) \textit{ but not both}\}$.

The *direct product* of two graphs G_1 and G_2 is the graph $G_1 \times G_2$ with $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and the vertices (y_1, y_2) and (z_1, z_2) are adjacent if $y_1 z_1 \in E(G_1)$ and $y_2 z_2 \in E(G_2)$

Let G_1 and G_2 be two graphs on disjoint vertex sets. Their *sum* is the graph $G_1 + G_2$ on the vertex set $V(G_1) \cup V(G_2)$ and the edge set $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{yz : y \in V(G_1), z \in V(G_2)\}$. The sum of two graphs is also known as *join*.

For G_1 and G_2 we define their *corona product* $G_1 \circ G_2$ as the graph obtained by taking $|V(G_1)|$ copies of G_2 and joining each vertex of the i-th copy with vertex

$y_i \in V(G_1)$.

Suppose that G_1 and G_2 are graphs with disjoint vertex sets. For given vertices $y \in V(G_1)$ and $z \in V(G_2)$ a *splice* $(G_1.G_2; y, z)$ of G_1 and G_2 by vertices y and z is defined by identifying the vertices y and z in the union of G_1 and G_2 [11]. Similarly, a *link* $(G_1 \sim G_2; y, z)$ of G_1 and G_2 by vertices y and z is defined as the graph obtained by joining y and z by an edge in the union of these graphs.

Let $G_i, 1 \leq i \leq n$, be some graphs and $y_i \in V(G_i)$. A *chain* graph is obtained from the union of the graphs $G_i, i = 1, \ldots, n$, by adding the edges $y_i y_{i+1}$, where $y_i \in V(G_i)$ for $1 \leq i \leq n-1$, and denoted by $G = G(G_1, \ldots, G_n; y_1, \ldots, y_n)$. Note that $G(G_1, G_2; y_1, y_2) \cong (G_1 \sim G_2; y_1, y_2)$.

Sagan et. al. [59] computed some exact formulas for the Wiener polynomial of various graph operations. In [47, 48] Ashrafi et. al. computed index PI and Zagreb indices respectively, of some graph operations.

Munarini et. al. [51] defined the *double graph* of a simple graph denoted as $D[G]$. The double graph of a simple graph G can be build up by taking two distinct copies of the graph G and joining every vertex y in one copy to every vertex z' in the other copy corresponding to a vertex z adjacent to y in the first copy.

By adding a loop to every vertex of K_2 we obtained the graph K_2^s. The double graph of a simple graph G can be expressed as $D[G] = G \Box K_2^s$. Since the direct product of a simple graph with any graph is always a simple graph, it follows that the double of a simple graph is still a simple graph. Some of its elementary properties are discussed in [51]. If G has n vertices and m edges then $D[G]$ has $2n$ vertices and $4m$ edges. For an illustration see Fig 1.16.

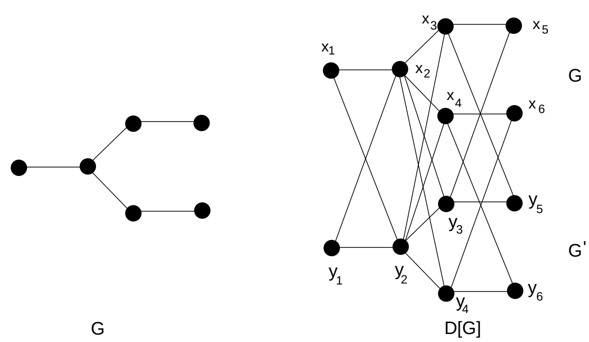

Figure 1.16: A graph G and its double graph $D[G]$.

Chapter 2

Maximum General Sum-Connectivity Index for Trees with Given Independence Number

Das, Xu and Gutman [16] proved that in the class of trees of order n and independence number s, the spur $S_{n,s}$ maximizes both first and second Zagreb indices and this graph is unique with these properties. In this chapter, we showed that in the same class of trees T, $S_{n,s}$ is the unique graph maximizing zeroth-order general Randić index ${}^0R_\alpha(T)$ for $\alpha > 1$ and general sum-connectivity index $\chi_\alpha(T)$ for $\alpha \geq 1$. This property does not hold for general Randić index $R_\alpha(T)$ if $\alpha \geq 2$.

2.1 Main Results

The zeroth-order general Randić index and general sum-connectivity index of $S_{n,s}$ are readily calculated:

$$ {}^0R_\alpha(S_{n,s}) = s^\alpha + s(1 - 2^\alpha) + 2^\alpha(n - 1); $$

$$ \chi_\alpha(S_{n,s}) = (2s - n + 1)(s + 1)^\alpha + (n - s - 1)((s + 2)^\alpha + 3^\alpha). $$

The path P_n has independence number equal to $\lceil n/2 \rceil$.

Lemma 2.1.1. *Let $n \geq 5$ and $\alpha > 1$. The following inequalities hold:*

$$^{0}R_{\alpha}(S_{n,\lceil n/2\rceil}) >^{0} R_{\alpha}(P_n) \tag{2.1.1}$$

$$\chi_{\alpha}(S_{n,\lceil n/2\rceil}) > \chi_{\alpha}(P_n). \tag{2.1.2}$$

Proof. We get $^{0}R_{\alpha}(P_n) = (n-2)2^{\alpha} + 2$ and $\chi_{\alpha}(P_n) = (n-3)4^{\alpha} + 2 \cdot 3^{\alpha}$. If n is even, $n = 2k$, (2.1.1) can be written as

$$k^{\alpha} - 2^{\alpha}k + k + 2^{\alpha} - 2 > 0, \tag{2.1.3}$$

where $k \geq 3$ and $\alpha > 1$. Consider the function $\varphi(x) = x^{\alpha} - 2^{\alpha}x + x$, where $x \geq 3$. We get $\varphi'(x) = \alpha x^{\alpha-1} - 2^{\alpha} + 1 \geq \alpha 3^{\alpha-1} - 2^{\alpha} + 1$. By letting $\psi(y) = y3^{y-1} - 2^{y} + 1$, where $y > 1$, we have $\psi'(y) = 3^{y-1}(1 + y\ln 3) - \ln 2 \cdot 2^{y}$. Since $(\frac{3}{2})^{y} > 1.5$ we deduce $\psi'(y) > 2^{y}(\frac{1+y\ln 3}{2} - \ln 2) > 2^{y}(\frac{1+\ln 3}{2} - \ln 2) = 2^{y-1}\ln\frac{3e}{4} > 0$.
Because $\psi(1) = 0$ we have $\psi(y) > 0$, thus $\varphi(x)$ is strictly increasing for $x \geq 3$ and $\alpha > 1$. It follows that it is sufficient to prove (2.1.3) for $k = 3$. For $k = 3$ (2.1.3) becomes

$$3^{\alpha} - 2 \cdot 2^{\alpha} + 1 > 0, \tag{2.1.4}$$

where $\alpha > 1$. (2.1.4) can be deduced by Jensen inequality written for the function x^{α}, which is strictly convex for $\alpha > 1$.

If $n = 2k+1$, where $k \geq 2$, we have $\alpha(P_{2k+1}) = k+1$ and (2.1.1) becomes (2.1.3) in which $k \geq 3$ has been replaced by $k+1 \geq 3$, which is true.

In order to prove (2.1.2) consider first the case n even, $n = 2k$. In this case (2.1.2) is

$$(k+1)^{\alpha} + (k-1)((k+2)^{\alpha} + 3^{\alpha}) - (2k-3)4^{\alpha} - 2 \cdot 3^{\alpha} > 0, \tag{2.1.5}$$

where $k \geq 3$ and $\alpha > 1$. For $k = 3$ (2.1.5) becomes $2 \cdot 5^{\alpha} - 2 \cdot 4^{\alpha} > 0$, which is true. Consider the function $\xi(x) = (x+1)^{\alpha} + (x-1)((x+2)^{\alpha} + 3^{\alpha}) - 2 \cdot 4^{\alpha}x$, where $x \geq 3$. We get $\xi'(x) = \alpha(x+1)^{\alpha-1} + (x+2)^{\alpha} + 3^{\alpha} + \alpha(x+2)^{\alpha-1}(x-1) - 2 \cdot 4^{\alpha}$. We have

$(x+2)^\alpha + 3^\alpha - 2\cdot 4^\alpha \geq 5^\alpha + 3^\alpha - 2\cdot 4^\alpha > 0$ by Jensen inequality. This implies that $\xi'(x) > 0$, hence $\xi(x)$ is strictly increasing. Thus (2.1.5) is valid since it holds for $k = 3$.

If $n = 2k+1$, where $k \geq 2$, the proof is similar, using in the same way Jensen inequality. □

The following observation will be useful.

Lemma 2.1.2. *Let T be a tree and $x \in V(T)$, which is adjacent to pendant vertices $v_1, \dots v_r$. If $r \geq 2$ then any maximum independent subset of $V(T)$ contains $v_1, \dots, v_r$.*

Theorem 2.1.1. *Let $n \geq 2$, $n/2 \leq s \leq n-1$ and T be a tree of order n with independence number s. Then for every $\alpha > 1$, ${}^0R_\alpha(T)$ is maximum if and only if $T = S_{n,s}$.*

Proof. The proof is by induction on n. For $n = 2$ we get $s = 1$ and $S_{2,1} = P_2$ and for $n = 3$ we deduce $s = 2$ and $S_{3,2} = P_3$. For $n = 4$ we have two possible values for s: $s = 2$, when $S_{4,2} = P_4$ and $s = 3$, when $S_{4,3} = K_{1,3}$. These trees are unique for respective values of parameters n and s, therefore they are extremal.

Let $n \geq 5$ and suppose that the property is true for all trees of order $n-1$. By Lemma 2.1.1 ${}^0R_\alpha(P_n)$ cannot be maximum. Since $n \geq 5$ we deduce $s \geq 3$. Suppose that $s = 3$. It follows that $n = 5$ or $n = 6$. For $n = 5$ we get only two trees of order 5 and independence number 3, namely P_5 and $S_{5,3}$ and for $n = 6$ we get P_6 and $S_{6,3}$. The theorem is verified in this case since P_5 and P_6 are not extremal. It follows that we can consider only the case when $\Delta(T) \geq 3$ and $s \geq 4$.

Let T be a tree of order $n \geq 5$ having $\Delta(T) \geq 3$ and independence number $s \geq 4$. As in [16] we shall consider a path $v_1, v_2, \dots, v_{d+1}$ of maximum length in T, where d is the diameter of T. We can suppose that $d \geq 3$ since otherwise $T = K_{1,n-1}$, $s = n-1$ and the theorem is verified. Both vertices v_1 and v_{d+1} are pendant. By letting $d(v_2) = d_2$, we obtain $s \geq \Delta(T) \geq d_2$.

First we consider the case when $\alpha(T-v_1)=\alpha(T)-1$. By the induction hypothesis we can write

$$\begin{aligned} {}^0R_\alpha(T) &= {}^0R_\alpha(T-v_1)+1+d_2^\alpha-(d_2-1)^\alpha \\ &\le {}^0R_\alpha(S_{n-1,s-1})+1+d_2^\alpha-(d_2-1)^\alpha \\ &= (s-1)^\alpha+(s-1)(1-2^\alpha)+2^\alpha(n-2)+1+d_2^\alpha-(d_2-1)^\alpha. \end{aligned}$$

Since the function $x^\alpha-(x-1)^\alpha$ is strictly increasing for $x\ge 1$ and $\alpha>1$, it follows that $d_2^\alpha-(d_2-1)^\alpha\le s^\alpha-(s-1)^\alpha$, equality holding if and only if $d_2=s$.

It follows that ${}^0R_\alpha(T)\le s^\alpha+s(1-2^\alpha)+2^\alpha(n-1)={}^0R_\alpha(S_{n,s})$ and equality holds if and only if $T-v_1=S_{n-1,s-1}$ and pendant vertex v_1 is adjacent to a vertex of degree $s-1$ in $S_{n-1,s-1}$. Since $s-1\ge 3$ it follows that for equality v_1 must be adjacent to the central vertex of the star $K_{1,s-1}$ of $S_{n-1,s-1}$. We deduce that $T=S_{n,s}$.

Next we assume that $\alpha(T-v_1)=\alpha(T)$. If v_2 would be adjacent to a vertex $w\ne v_1,v_3$, the degree of w cannot be greater than one, since in this case the path $v_1,\ldots,v_{d+1}$ has not maximum length in T. It follows that $d(w)=1$ and by Lemma 2.1.2 every maximum independent set of vertices of T include both v_1 and w. This implies $\alpha(T-v_1)=\alpha(T)-1$, which contradicts the hypothesis. It follows that $d_2=2$. We can write

$${}^0R_\alpha(T)={}^0R_\alpha(T-v_1)+2^\alpha\le {}^0R_\alpha(S_{n-1,s})+2^\alpha=s^\alpha+s(1-2^\alpha)+2^\alpha(n-1)={}^0R_\alpha(S_{n,s}).$$

The equality holds if and only if $T-v_1=S_{n-1,s}$ and pendant vertex v_1 is adjacent to a pendant vertex of $S_{n-1,s}$. Let x be the vertex of degree s of $S_{n-1,s}$. If v_1 is adjacent to a pendant vertex v_2 of $S_{n-1,s}$ such that $d(v_2,x)=2$, the resulting tree T has $\alpha(T)=s+1$,which contradicts the hypothesis. We deduce that v_1 is adjacent to a pendant vertex which is adjacent to x, which implies that $T=S_{n,s}$. □

A similar result holds for general sum-connectivity index.

Theorem 2.1.2. *Let $n \geq 2$, $n/2 \leq s \leq n-1$ and T be a tree of order n with independence number s. Then for every $\alpha \geq 1$, $\chi_\alpha(T)$ is maximum if and only if $T = S_{n,s}$.*

Proof. For $\alpha = 1$ we have $\chi_1(T) =^0 R_2(T)$ and by Theorem 2.3 the result holds true. Suppose that $\alpha > 1$. We shall use induction on n in the same way as in the proof of Theorem 2.3. By the same arguments and inequality (2) we can consider $n \geq 5$, $s \geq 4$, a tree T of order n and independence number s such that $\Delta(T) \geq 3$, and a path $v_1, v_2, \ldots, v_{d+1}$ of length d in T, where $d \geq 3$ is the diameter of T.
First we consider the case when $\alpha(T - v_1) = \alpha(T)$. As in the proof of Theorem 2.3 we deduce $d(v_2) = 2$ and $d(v_3) = d_3 \leq \Delta(T) \leq s$.
By the induction hypothesis we get

$$\chi_\alpha(T) = \chi_\alpha(T - v_1) + 3^\alpha + (d_3 + 2)^\alpha - (d_3 + 1)^\alpha$$

$$\leq (2s-n+2)(s+1)^\alpha + (n-s-2)(s+2)^\alpha + (n-s-2)3^\alpha + 3^\alpha + (d_3+2)^\alpha - (d_3+1)^\alpha.$$

Since $d_3 \leq s$ we have $(d_3 + 2)^\alpha - (d_3 + 1)^\alpha \leq (s + 2)^\alpha - (s + 1)^\alpha$ and equality holds if and only if $d_3 = s$.

It follows that $\chi_\alpha(T) \leq (2s-n+1)(s+1)^\alpha + (n-s-1)(s+2)^\alpha + (n-s-1)3^\alpha = \chi_\alpha(S_{n,s})$ and equality holds if and only if $T - v_1 = S_{n-1,s}, d(v_2) = 2$ and $d_3 = s$, which implies that $T = S_{n,s}$.

Next we assume that $\alpha(T - v_1) = \alpha(T) - 1$. Since $v_1, v_2, v_3, \ldots, v_{d+1}$ is a path of maximum length of T, v_3 is the only vertex in $N(v_2)$ having degree $d_3 \geq 2$. By letting $d(v_2) = d_2 \leq s$ we have

$$\chi_\alpha(T) = \chi_\alpha(T - v_1) + (d_2+1)^\alpha + (d_2-2)((d_2+1)^\alpha - d_2^\alpha) + (d_2+d_3)^\alpha - (d_2+d_3-1)^\alpha.$$

The function $(x-2)((x+1)^\alpha - x^\alpha)$ being strictly increasing in x for $x \geq 2$ and $\alpha \geq 1$, we have $(d_2-2)((d_2+1)^\alpha - d_2^\alpha) \leq (s-2)((s+1)^\alpha - s^\alpha)$; also $(d_2+1)^\alpha \leq (s+1)^\alpha$. v_2 is adjacent to $d_2 - 1$ pendant vertices and in the graph $T - v_2v_3$ the degree of v_3 is equal to $d_3 - 1$. It follows that $d_2 - 1 + d_3 - 1 \leq s$, or $d_2 + d_3 \leq s + 2$ since T has at least d_2+d_3-2 pendant vertices. This implies $(d_2+d_3)^\alpha-(d_2+d_3-1)^\alpha \leq (s+2)^\alpha-(s+1)^\alpha$ with equality if and only if $d_2 + d_3 = s + 2$. By the induction hypothesis we have $\chi_\alpha(T - v_1) \leq \chi_\alpha(S_{n-1,s-1})$. Thus we get $\chi_\alpha(T) \leq (2s - n)s^\alpha + (n - s - 1)(s + 1)^\alpha + (n - s - 1)3^\alpha + (s + 1)^\alpha + (s - 2)((s + 1)^\alpha - s^\alpha) + (s + 2)^\alpha - (s + 1)^\alpha = (s + 2)^\alpha + (n - 3)(s + 1)^\alpha + (s - n + 2)s^\alpha + (n - s - 1)3^\alpha$. By denoting the last expression by $E(n, s, \alpha)$, the inequality $E(n, s, \alpha) \leq \chi_\alpha(S_{n,s})$ is equivalent to

$$(n - s - 2)(s + 2)^\alpha + (n - s - 2)s^\alpha \geq 2(n - s - 2)(s + 1)^\alpha. \tag{2.1.6}$$

If $s = n - 1$ then $T = K_{1,n-1} = S_{n,n-1}$ and the theorem is true. If $s = n - 2$ then (2.1.6) becomes an equality. Otherwise $n - s - 2 \geq 1$ and (2.1.6) is equivalent to $(s + 2)^\alpha + s^\alpha \geq 2(s + 1)^\alpha$. By Jensen inequality this inequality is strict. It follows that if $\alpha(T - v_1) = \alpha(T) - 1$ we have $\chi_\alpha(T) \leq \chi_\alpha(S_{n,s})$ and the equality holds only if $s = n - 2, T - v_1 = S_{n-1,n-3}, d_2 = s$ and $d_2 + d_3 = s + 2$, i.e., $d_3 = 2$. It follows that the equality holds only if $T = S_{n,n-2}$ and the proof is complete.
Notice that only if $n - s - 1 \in \{0, 1\}$ a pendant vertex adjacent to the center of the star $K_{1,s}$ is the endvertex of a longest path in $S_{n,s}$, and this corresponds to the equality in (2.1.6). □

In the family of trees T of order n and independence number s the second Zagreb index $M_2(G) = R_1(T)$ is maximum if and only if $T = S_{n,s}$ [16]. But this property does not hold for $R_\alpha(T)$ if $\alpha \geq 2$, since in [38] it was shown that for $\alpha \geq 2$ and $n \geq 8$, only the balanced double star $S(p, q)$, where $p+q = n-2$ and $|p-q| \leq 1$ realizes the maximum value of $R_\alpha(T)$ in the set of trees of order n. The independence number of $S(p, q)$ is $n - 2$, but $S_{n,n-2}$ is not a balanced double star.

Chapter 3

General Sum-Connectivity Index of Trees and Unicyclic Graphs with Fixed Maximum Degree

In this chapter, we discussed the maximum value for the general sum-connectivity index of $n-$vertex trees for $-1.7036 \leq \alpha < 0$ and of $n-$vertex unicyclic graphs for $-1 \leq \alpha < 0$ respectively, with fixed maximum degree $\triangle$. We also characterized the corresponding extremal graphs, as well as the $n-$vertex unicyclic graphs with the second maximum general sum-connectivity index for $n \geq 4$. This extends the corresponding results by Du, $Zhou$ and $Trinajstić$ [19] about sum-connectivity index.

For $n \geq 3$, let $T(n, \triangle)$ be the set of trees with n vertices and maximum degree $\triangle$ and $U(n, \triangle)$ be the set of unicyclic graphs with n vertices and maximum degree $\triangle$ $(2 \leq \triangle \leq n-1)$. Let P_n and C_n be the path and the cycle, respectively, on $n \geq 3$ vertices. For $\triangle = 2$, $T(n, \triangle) = \{P_n\}$ and $U(n, \triangle) = \{C_n\}$. For $\frac{n}{2} \leq \triangle \leq n-1$, let $T_{n,\triangle}$ be the tree obtained by attaching $2\triangle + 1 - n$ pendant vertices and $n - \triangle - 1$ paths of length two to a vertex. For $\frac{n+2}{2} \leq \triangle \leq n-1$, let $U_{n,\triangle}$ be the unicyclic graph obtained by attaching $2\triangle - n - 1$ pendant vertices and $n - \triangle - 1$ paths of length two to the same vertex of a triangle.

3.1 General Sum Connectivity Index of n-vertex Trees

Lemma 3.1.1. *[18] Let Q be a connected graph with at least two vertices. For $a \geq b \geq 1$, let G_1 be the graph obtained from Q by attaching two paths P_a and P_b to $u \in V(Q)$ and G_2 the graph obtained from Q by attaching a path P_{a+b} to u. Then $\chi_\alpha(G_2) > \chi_\alpha(G_1)$, for $\alpha_1 \leq \alpha < 0$, where $\alpha_1 \approx -1.7036$ is the unique root of the equation $\frac{3^\alpha - 4^\alpha}{4^\alpha - 5^\alpha} = 2$.*

Theorem 3.1.1. *Let $G \in T(n, \triangle)$, where $2 \leq \triangle \leq n-1$ and $\alpha_1 \leq \alpha < 0$, where $\alpha_1 \approx -1.7036$ is the unique root of the equation $\frac{3^\alpha - 4^\alpha}{4^\alpha - 5^\alpha} = 2$. Then*

$$\chi_\alpha(G) \leq \begin{cases} ((\triangle+2)^\alpha - (\triangle+1)^\alpha + 3^\alpha)(n-\triangle-1) + \triangle(\triangle+1)^\alpha & if \ \dfrac{n}{2} \leq \triangle \leq n-1 \\ ((\triangle+2)^\alpha + 3^\alpha - 4^\alpha)\triangle + (n-\triangle-1)4^\alpha & if \ 2 \leq \triangle \leq \dfrac{n-1}{2} \end{cases}$$

and equality holds if and only if $G = T_{n,\triangle}$ for $\frac{n}{2} \leq \triangle \leq n-1$, and G is a tree obtained by attaching $\triangle$ paths of length at least two to a unique vertex for $2 \leq \triangle \leq \frac{n-1}{2}$.

Proof. The case $\triangle = 2$ is clear since in this case $G = P_n$. Suppose that $\triangle \geq 3$ and let G be a tree in $T(n, \triangle)$ having maximum general sum-connectivity index. Let v be a vertex of degree $\triangle$ in G. If there exists some vertex of degree greater than two in G different from v, then by Lemma 3.1.1, we may get a tree in $T(n, \triangle)$ with greater general sum-connectivity index, a contradiction. It follows that v is the unique vertex of degree greater than two in G. Let k be the number of neighbors of v with degree two. Since in $V(G) \backslash (\{v\} \cup N(v))$ there are $n - \triangle - 1$ vertices, it follows that $k \leq \min\{n - \triangle - 1, \triangle\}$. If $n - \triangle - 1 \geq \triangle$, i.e., $\triangle \leq \frac{n-1}{2}$, then $1 \leq k \leq \triangle$. If $n - \triangle - 1 < \triangle$, i.e., $\triangle \geq \frac{n}{2}$, then $0 \leq k \leq n - \triangle - 1$. We get

$$\begin{aligned} \chi_\alpha(G) &= (\triangle - k)(\triangle+1)^\alpha + k(\triangle+2)^\alpha + k \cdot 3^\alpha + (n - \triangle - k - 1)4^\alpha \\ &= k((\triangle+2)^\alpha - (\triangle+1)^\alpha + 3^\alpha - 4^\alpha) + \triangle(\triangle+1)^\alpha + (n-\triangle-1)4^\alpha. \end{aligned}$$

Since $(\triangle+2)^\alpha-(\triangle+1)^\alpha$ is increasing for $\triangle \geq 3$ we obtain $(\triangle+2)^\alpha-(\triangle+1)^\alpha+3^\alpha-4^\alpha \geq 5^\alpha+3^\alpha-2\cdot 4^\alpha > 0$, the last inequality holding by Jensen's inequality. Consequently,

$$\chi_\alpha(G) \leq \begin{cases} ((\triangle+2)^\alpha-(\triangle+1)^\alpha+3^\alpha)(n-\triangle-1)+\triangle(\triangle+1)^\alpha & if\ \dfrac{n}{2} \leq \triangle \leq n-1 \\ ((\triangle+2)^\alpha+3^\alpha-4^\alpha)\triangle+(n-\triangle-1)4^\alpha & if\ 2 \leq \triangle \leq \dfrac{n-1}{2}. \end{cases}$$

For $\frac{n}{2} \leq \triangle \leq n-1$, the equality holds if and only if $k=n-\triangle-1$, i.e., each of the $n-\triangle-1$ neighbors of degree two of the vertex v is adjacent to exactly a pendant vertex, i.e., $G=T_{n,\triangle}$. For $2 \leq \triangle \leq \frac{n-1}{2}$ the equality holds for $k=\triangle$, i.e., G is a tree obtained by attaching $\triangle$ paths of length at least two to a unique vertex. □

3.2 First and Second Maximum General Sum Connectivity index of n-vertex Unicyclic Graphs

Now we obtain the maximum general sum-connectivity index of graphs in $U(n,\triangle)$ and deduce the extremal graphs. As a consequence, we deduce the n-vertex unicyclic graphs with the first and second maximum general sum-connectivity indices for $n \geq 4$.

The following property is an extension of a transformation defined in [19].

Lemma 3.2.1. *[19] Let a connected graph M with $|V(M)| \geq 3$ and a vertex u of degree two of M. Let H be the graph obtained from M by attaching a path P_a to u. Denote by u_1 and u_2 the two neighbors of u in M, and by u' the pendant vertex of the path attached to u in H. If $d_H(u_2) \leq 3$, then for $H' = H-\{uu_2\}+\{u'u_2\}$ we have $\chi_\alpha(H') > \chi_\alpha(H)$, where $-1 \leq \alpha < 0$.*

Proof. If $d_H(u,u')=1$, then for $\alpha<0$ we have: $\chi_\alpha(H')-\chi_\alpha(H) = (d_H(u_1)+2)^\alpha + (d_H(u_2)+2)^\alpha - (d_H(u_1)+3)^\alpha - (d_H(u_2)+3)^\alpha > 0$.

If $d_H(u, u') \geq 2$, then

$$\begin{aligned}\chi_\alpha(H') - \chi_\alpha(H) =& (d_H(u_1)+2)^\alpha - (d_H(u_1)+3)^\alpha + (d_H(u_2)+2)^\alpha - (d_H(u_2)+3)^\alpha + \\ &+ 2\cdot 4^\alpha - 3^\alpha - 5^\alpha \\ &> (d_H(u_2)+2)^\alpha - (d_H(u_2)+3)^\alpha + 2\cdot 4^\alpha - 3^\alpha - 5^\alpha.\end{aligned}$$

Since $(x+2)^\alpha - (x+3)^\alpha$ is decreasing for $x \geq 0$, we have $(d_H(u_2)+2)^\alpha - (d_H(u_2)+3)^\alpha \geq 5^\alpha - 6^\alpha$. Therefore

$$\chi_\alpha(H') - \chi_\alpha(H) > 2\cdot 4^\alpha - 3^\alpha - 6^\alpha.$$

The function $\eta(x) = 2\cdot 4^x - 3^x - 6^x$ has roots $x_1 = -1$ and $x_2 = 0$ and $\eta(x) > 0$ for $x \in (-1, 0)$ [68]. It follows that $\chi_\alpha(H') > \chi_\alpha(H)$ for every $-1 \leq \alpha < 0$. □

Theorem 3.2.1. *Let $G \in U(n, \triangle)$, where $2 \leq \triangle \leq n-1$, and $-1 \leq \alpha < 0$. Then*

$$\chi_\alpha(G) \leq \begin{cases} (n-\triangle-1)3^\alpha + (n-\triangle+1)(\triangle+2)^\alpha + (2\triangle-n-1)(\triangle+1)^\alpha + 4^\alpha \\ \qquad\qquad ;if\ \dfrac{n+2}{2} \leq \triangle \leq n-1 \\ (\triangle-2)3^\alpha + \triangle(\triangle+2)^\alpha + (n-2\triangle+2)4^\alpha \qquad ;if\ 2 \leq \triangle \leq \dfrac{n+1}{2}. \end{cases}$$

For $\frac{n+2}{2} \leq \triangle \leq n-1$ the equality holds if and only if $G = U_{n,\triangle}$. If $2 \leq \triangle \leq \frac{n+1}{2}$ the equality holds if and only if G is a unicyclic graph obtained by attaching $\triangle - 2$ paths of length at least two to a fixed vertex of a cycle.

Proof. The case $\triangle = 2$ is trivial since in this case $G = C_n$. Suppose that $\triangle \geq 3$, G is a graph in $U(n, \triangle)$ with maximum general sum-connectivity index, and C is the unique cycle of G. Let v be a vertex of degree $\triangle$ in G. If $\triangle = 3$ and there exists some vertex outside C with degree three, then by Lemma 3.1.1, we may get a graph in $U(n, 3)$ with greater general sum-connectivity index, a contradiction. If there are at least two vertices on C with degree three, then by Lemma 3.2.1, we may deduce the same conclusion. Thus, $v \in V(C)$ and v is the unique vertex in G with degree three. Then either $\chi_\alpha(G) = (n-2)4^\alpha + 2 \cdot 5^\alpha$ when v is adjacent to a vertex of degree one and two vertices of degree two for $n \geq 4$, or $\chi_\alpha(G) = (n-4)4^\alpha + 3 \cdot 5^\alpha + 3^\alpha$ when v is adjacent to three vertices of degree two for $n \geq 5$. The difference of these two numbers equals $(n-2)4^\alpha + 2 \cdot 5^\alpha - (n-4)4^\alpha - 3 \cdot 5^\alpha - 3^\alpha = 2 \cdot 4^\alpha - 5^\alpha - 3^\alpha < 0$ by Jensen's inequality. Hence, G is the graph obtained by attaching a pendant vertex to a triangle for $n = 4$, i.e., $G = U_{4,3}$, and a graph obtained by attaching a path of length at least two to a cycle for $n \geq 5$.

Now suppose that $\triangle \geq 4$. As for the case $\triangle = 3$ we deduce that the vertex of maximum degree is unique, otherwise G has not a maximum general sum-connectivity index in $U(n, \triangle)$. We showed that the vertex of maximum degree v lies on C. Suppose that v is not on C. Let w be the vertex on C such that $d_G(v, w) = \min\{d_G(v, x) : x \in V(C)\}$. If there is some vertex outside C with degree greater than two different from v, or if there is some vertex on C with degree greater than two different from w, then by Lemmas 3.1.1 and 3.2.1, we may get a graph in $U(n, \triangle)$ with greater general sum-connectivity index, a contradiction. Thus, v and w are the only vertices of degree greater than two in G, and $d_G(v) = \triangle$ and $d_G(w) = 3$. Let Q be the path connecting v and w. Suppose that $v_1, v_2, \cdots, v_{\triangle-1}$ are the neighbors of v outside Q. Let $d_i = d_G(v_i)$ for $i = 1, \ldots, \triangle - 1$. Note that since G has maximum general sum-connectivity index, then $d_1, \ldots, d_{\triangle-1} \in \{1, 2\}$, since otherwise we can apply Lemma 3.1.1 and obtain a graph having a greater general sum-connectivity index. Consider $G_1 = G - \{vv_3, \cdots, vv_{\triangle-1}\} + \{wv_3, \cdots, wv_{\triangle-1}\} \in U(n, \triangle)$. Note that $d_{G_1}(w) = \triangle$ and $d_{G_1}(v) = 3$. Then

$$\begin{aligned}\chi_\alpha(G_1) - \chi_\alpha(G) =& (d_1+3)^\alpha - (d_1+\triangle)^\alpha + (d_2+3)^\alpha - (d_2+\triangle)^\alpha + 2(\triangle+2)^\alpha - \\ &- 2 \cdot 5^\alpha \\ &> 5^\alpha - (2+\triangle)^\alpha + 5^\alpha - (2+\triangle)^\alpha + 2(\triangle+2)^\alpha - 2 \cdot 5^\alpha = 0,\end{aligned}$$

since the function $(x+3)^\alpha - (x+\triangle)^\alpha$ is strictly decreasing in $x \geq 0$ for $\triangle \geq 4$.

Because $d_{G_1}(v) = 3$, then by Lemma 3.1.1, we may get a graph G' in $U(n, \triangle)$ such that $\chi_\alpha(G') > \chi_\alpha(G_1) \geq \chi_\alpha(G)$, a contradiction. Hence, we have shown that v lies on C.

If there is some vertex outside C with degree greater than two, then by Lemma 3.1.1 we may obtain a graph in $U(n, \triangle)$ with greater general sum-connectivity index, a contradiction. If there is some vertex on C with degree three, then by Lemma 3.2.1, we may get a graph in $U(n, \triangle)$ with greater general sum-connectivity index, a contradiction. Thus, G is a graph obtained from C by attaching $\triangle - 2$ paths to v. Let k be the number of neighbors of v with degree two outside C. Then as above we get $k \leq \min\{n - \triangle - 1, \triangle - 2\}$. If $n - \triangle - 1 \geq \triangle - 2$, i.e., $\triangle \leq \frac{n+1}{2}$, then $0 \leq k \leq \triangle - 2$. If $n - \triangle - 1 < \triangle - 2$, i.e., $\triangle \geq \frac{n+2}{2}$, then $0 \leq k \leq n - \triangle - 1$. We get

$$\begin{aligned}\chi_\alpha(G) =& k3^\alpha + (k+2)(\triangle + 2)^\alpha + (\triangle - k - 2)(\triangle + 1)^\alpha + (n - \triangle - k)4^\alpha \\ =& (3^\alpha + (\triangle + 2)^\alpha - (\triangle + 1)^\alpha - 4^\alpha)k + (\triangle - 2)(\triangle + 1)^\alpha + 2(\triangle + 2)^\alpha + \\ &+ 4^\alpha(n - \triangle).\end{aligned}$$

We have

$$3^\alpha - 4^\alpha + (\triangle + 2)^\alpha - (\triangle + 1)^\alpha \geq 3^\alpha - 4^\alpha + 6^\alpha - 5^\alpha > 0$$

since the function $f(x) = (x+2)^\alpha - (x+1)^\alpha$ is strictly increasing for $\alpha < 0$, hence $f(\triangle) \geq f(4)$ and $f(4) > f(2)$. It follows that $\chi_\alpha(G)$ is bounded above by

$$\begin{cases} (3^\alpha + (\triangle + 2)^\alpha - (\triangle + 1)^\alpha - 4^\alpha)(n - \triangle - 1) + (\triangle - 2)(\triangle + 1)^\alpha + 2(\triangle + 2)^\alpha + \\ 4^\alpha(n - \triangle) \qquad ; if \ \frac{n+2}{2} \leq \triangle \leq n - 1 \\ (3^\alpha + (\triangle + 2)^\alpha - (\triangle + 1)^\alpha - 4^\alpha)(\triangle - 2) + (\triangle - 2)(\triangle + 1)^\alpha + 2(\triangle + 2)^\alpha + 4^\alpha(n - \triangle) \\ \qquad ; if \ 2 \leq \triangle \leq \frac{n+1}{2} \end{cases}$$

$$= \begin{cases} (n-\triangle-1)3^\alpha+(n-\triangle+1)(\triangle+2)^\alpha+(2\triangle-n-1)(\triangle+1)^\alpha+4^\alpha \\ \qquad ;if\ \dfrac{n+2}{2}\le\triangle\le n-1 \\ (\triangle-2)3^\alpha+\triangle(\triangle+2)^\alpha+(n-2\triangle+2)4^\alpha \qquad ;if\ 2\le\triangle\le\dfrac{n+1}{2} \end{cases}$$

Equality holds for $\frac{n+2}{2}\le\triangle\le n-1$ if and only if $k=n-\triangle-1$, i.e., $G=U_{n,\triangle}$; if $2\le\triangle\le\frac{n+1}{2}$ then equality is reached if and only if $k=\triangle-2$, i.e., G is a unicyclic graph obtained by attaching $\triangle-2$ paths of length at least two to a unique vertex of a cycle. □

Theorem 3.2.2. *If $-1\le\alpha<0$, among the unicyclic graphs on $n\ge4$ vertices, C_n is the unique graph with maximum general sum-connectivity index, which is equal to $n4^\alpha$. For $n=4$, $U_{4,3}$ is the unique graph with the second maximum general sum-connectivity index, which is equal to $2\cdot4^\alpha+2\cdot5^\alpha$. For $n\ge5$, the graphs obtained by attaching a path of length at least two to a vertex of a cycle are the unique graphs with the second maximum general sum-connectivity index, which is equal to $(n-4)4^\alpha+3\cdot5^\alpha+3^\alpha$.*

Proof. For $n=4$ we get

$$\chi_\alpha(U_{4,3})-\chi_\alpha(C_4)=2\cdot5^\alpha-2\cdot4^\alpha<0.$$

Now, suppose that $n\ge5$ and G is a unicyclic graph on n vertices. Let $\triangle$ be the maximum degree of G, where $2\le\triangle\le n-1$. Let $f(x)=(x-2)3^\alpha+x(x+2)^\alpha+(n-2x+2)4^\alpha$ for $x\ge2$. If $\frac{n+2}{2}\le\triangle\le n-1$, then by Theorem 3.2.1,

$$\chi_\alpha(G)\le(n-\triangle-1)3^\alpha+(n-\triangle+1)(\triangle+2)^\alpha+(2\triangle-n-1)(\triangle+1)^\alpha+4^\alpha$$

$$=f(\triangle)+(n-2\triangle+1)(3^\alpha-4^\alpha+(\triangle+2)^\alpha-(\triangle+1)^\alpha)<f(\triangle)$$

since the function $x^\alpha-(x+1)^\alpha$ is strictly decreasing for $x\ge0$ and $\triangle\ge4$.
If $2\le\triangle\le\frac{n+1}{2}$, then by Theorem 3.2.1, $\chi_\alpha\le f(\triangle)$ and equality can be reached. We

shall prove that $f'(x) < 0$, which implies that $f(x)$ is strictly decreasing for $x \geq 2$. One deduces

$$f'(x) = 3^\alpha + (x+2)^\alpha + \alpha x(x+2)^{\alpha-1} - 2 \cdot 4^\alpha.$$

Let

$$g(x) = (x+2)^\alpha + \alpha x(x+2)^{\alpha-1}.$$

We get

$$g'(x) = \alpha(x+2)^{\alpha-2}(x(\alpha+1)+4) < 0.$$

So, $g(x)$ is strictly decreasing for $x \geq 2$, thus implying $g(x) \leq 4^\alpha + 2\alpha 4^{\alpha-1}$. Consequently,

$$f'(x) \leq 3^\alpha - 4^\alpha + 2\alpha 4^{\alpha-1} = 4^\alpha \left(\left(\frac{3}{4} \right)^\alpha + \frac{\alpha}{2} - 1 \right).$$

Considering the function $h(x) = \frac{x}{2} + (\frac{3}{4})^x$, we get $h''(x) = (ln(\frac{3}{4}))^2 (\frac{3}{4})^x > 0$, hence $h(x)$ is strictly convex. Since $h(-1) = 5/6 < 1$ and $h(0) = 1$, $h(x)$ being strictly convex on $[-1, 0)$, it follows that $h(x) < 1$ on this interval, or $f'(x) < 0$ for every $-1 \leq \alpha < 0$, hence $f(x)$ is strictly decreasing for $x \geq 2$.

It follows that for $3 < \frac{n+2}{2} \leq \triangle \leq n-1$ we have $\chi_\alpha(G) < f(\triangle) < f(3) < f(2)$ and for $3 \leq \triangle \leq \frac{n+1}{2}$ we obtain $\chi_\alpha(G) \leq f(\triangle) \leq f(3) < f(2)$. It follows that C_n is the unique n-vertex unicyclic graph with maximum general sum-connectivity index, equal to $f(2)$. Also the n-vertex unicyclic graphs with maximum degree $\triangle = 3$ and general sum-connectivity index $f(3)$ are the n-vertex graphs with the second maximum general sum-connectivity index. By Theorem 3.2.1, these graphs consist of a cycle C_l of an arbitrary length l, $3 \leq l \leq n-2$ and a path of length at least two attached to a vertex of C_l. $\square$

Chapter 4

Graphs With Fixed Number of Pendent Vertices and Minimal First Zagreb Index

Goubko proved that for trees with n_1 pendent vertices, $M_1 \geq 9\,n_1 - 16$. In this chapter, we showed how this result can be extended to hold for any connected graph with cyclomatic number $\gamma \geq 0$. In addition, graphs with n vertices, n_1 pendent vertices, cyclomatic number γ, and minimal M_1 are characterized. Explicit expressions for minimal M_1 are given for $\gamma = 0, 1, 2$, which directly can be extended for $\gamma > 2$.

4.1 Goubko's Theorem and its Generalization

Recently, Goubko [26] discovered an interesting property of n_1-trees, namely that any n_1-tree T obeys the inequality $M_1(T) \geq 9\,n_1 - 16$, irrespective the number of its vertices (see also [30, 31, 35]). In this section, we showed that Goubko's theorem can be directly extended to any n_1-graph with a fixed value of cyclomatic number.

If the number of vertices of degree k will be denoted by n_k. Then, evidently,

$$\sum_{k\geq 1} n_k = n \tag{4.1.1}$$

$$\sum_{k\geq 1} k\, n_k = 2m \tag{4.1.2}$$

and

$$\sum_{k\geq 1} k^2\, n_k = M_1(G) \tag{4.1.3}$$

Theorem 4.1.1. *Let G be a connected graph with n_1 pendent vertices and cyclomatic number γ. Then*

$$M_1(G) \geq 9\, n_1 + 16(\gamma - 1)\ . \tag{4.1.4}$$

Equality in (4.1.4) holds if and only if all non-pendent vertices of G are of degree 4, provided such graphs exist.

Proof. Multiply Eq. (4.1.1) by 16, multiply Eq. (4.1.2) by -8, and add these to Eq. (4.1.3). This yields

$$\sum_{k\geq 1} (k^2 + 16 - 8k) n_k = M_1 + 16(n - m) = M_1(G) - 16(\gamma - 1)$$

i.e.,

$$\begin{aligned} M_1(G) &= 16(\gamma - 1) + \sum_{k\geq 1} (k-4)^2\, n_k \\ &= 16(\gamma - 1) + 9\, n_1 + \sum_{k\geq 2} (k-4)^2\, n_k\ . \end{aligned} \tag{4.1.5}$$

Theorem 4.1.1 is an immediate consequence of Eq. (4.1.5). □

Corollary 4.1.2. *If graphs, specified in Theorem 4.1.1, for which the equality $M_1 = 9n_1 - 16(\gamma - 1)$ holds, do not exist, then*

$$M_1(G) \geq 9\, n_1 + 16(\gamma - 1) + 1\ . \tag{4.1.6}$$

Equality in (4.1.6) holds if and only if one non-pendent vertex of G is of degree 3 and all other non-pendent vertices are of degree 4, and/or one non-pendent vertex of G is of degree 5 and all other non-pendent vertices are of degree 4, provided such graphs exist.

The original result of Goubko is just the special case of Theorem 4.1.1 and Corollary 4.1.2 for $\gamma = 0$.

Although Eq. (4.1.4) in Goubko's theorem 4.1.1 provides an elegant and simple structural condition for graphs with minimal first Zagreb indices, it is restricted to graphs with very special number of vertices. Thus, Goubko's theorem determines the n_1-trees and n_1-unicyclic graphs with minimal first Zagreb index only if $n = (3/2)n_1 - 1$ and $n = (3/2)n_1$, respectively, and requires that n_1 be even.

In what follows we show how this limitation can be circumvented. For this we need an auxiliary result [12, 74].

4.2 (n, n_1)-Trees with Minimal First Zagreb Index

Let $i_1, i_2, \ldots, i_n$ be integers. We say that these integers are *almost equal* if

$$\max\Big\{i_1, i_2, \ldots, i_n\Big\} - \min\Big\{i_1, i_2, \ldots, i_n\Big\} \leq 1 \ .$$

Lemma 4.2.1. *[12, 74] The first Zagreb index of a graph G will be minimal if the degrees of its non-pendent vertices are almost equal.*

Proof. Let u and v be any two vertices of the graph G. Let $\deg(u) = a$ and $\deg(v) = b$, such that $a - b = 2k$ or $2k + 1$, where k is non-negative integer. If G' is a graph obtained from G so that $\deg(u) = a - k$, $\deg(v) = b + k$ whereas the degrees of all other vertices in G' are same as in G, then

$$\begin{aligned} M_1(G) - M_1(G') &= a^2 + b^2 - \left[(a-k)^2 + (b+k)^2\right] \\ &= 2k(a-b-k) = \begin{cases} 2k^2 & \text{if } a-b=2k \\ 2k(k+1) & \text{if } a-b=2k+1 \end{cases} \end{aligned}$$

implying $M_1(G) - M_1(G') \geq 0$, and that this difference is minimal for $k = 0$, i.e., if the degrees of u and v are almost equal. □

A graph with n vertices and n_1 pendent vertices will be said to be an (n, n_1)-graph. In the subsequent sections we characterize (n, n_1)-graphs with a given cyclomatic number, having minimal first Zagreb index. We begin with the case $\gamma = 0$.

Theorem 4.2.1. *Let T be a tree of order n with n_1 pendent vertices. Then*

$$M_1(T) \geq 4n - 6 + (n + n_1 - 4)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor - (n-n_1)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor^2 . \tag{4.2.1}$$

Equality in (4.2.1) is attained if and only if T consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor - n_1 + 2$ vertices of degree $t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n - 2 - (n-n_1)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor$ vertices of degree $t+1$.

Proof. Suppose that the tree T has minimal Zagreb index. Then by Lemma 4.2.1 it has n_t $(0 < n_t \leq n - n_1)$ non-pendent vertices of degree t and $n_{t+1} = n - n_1 - n_t$ non-pendent vertices of degree $t+1$. Then,

$$M_1(T) = n_1 + n_t\, t^2 + n_{t+1}\,(t+1)^2 .$$

The parameters t, n_t, and n_{t+1} are calculated from the conditions

$$n_1 + n_t + n_{t+1} = n \tag{4.2.2}$$

$$n_1 + t\, n_t + (t+1) n_{t+1} = 2m = 2(n-1) \tag{4.2.3}$$

which yield

$$t(n-n_1) - n_t = n-2 \qquad \text{i.e.,} \qquad t = \frac{n-2}{n-n_1} + \frac{n_t}{n-n_1} \; .$$

Since t is a positive integer, we get

$$t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1$$

which substituted back into Eqs. (4.2.2) and (4.2.3) leads to

$$\begin{aligned} n_t &= (n-n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor - n_1 + 2 \\ n_{t+1} &= n-2-(n-n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor \end{aligned}$$

as required. □

(n, n_1)-Trees with minimal first Zagreb index, of the form specified in Theorem 4.2.1, exist for any value of n and n_1, provided $n > n_1 \geq 2$.

4.3 Unicyclic and Bicyclic (n, n_1)-Graphs with Minimal First Zagreb Index

If $\gamma > 0$ the considerations are fully analogous. Instead of Eq. (4.2.3) one has to use

$$n_1 + t\,n_t + (t+1)n_{t+1} = 2m = 2(n-1+\gamma) \; .$$

Without proof we state the results for $\gamma = 1$ and $\gamma = 2$.

Theorem 4.3.1. *Let U be a unicyclic (n, n_1)-graph. Then*

$$M_1(U) \geq 4n + (n+n_1) \left\lfloor \frac{n}{n-n_1} \right\rfloor - (n-n_1) \left\lfloor \frac{n}{n-n_1} \right\rfloor^2 . \tag{4.3.1}$$

Equality in (4.3.1) is attained if and only if U consists of n_1 pendent vertices, $n_t = (n-n_1) \left\lfloor \frac{n}{n-n_1} \right\rfloor - n_1$ vertices of degree $t = \left\lfloor \frac{n}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n - (n-n_1) \left\lfloor \frac{n}{n-n_1} \right\rfloor$ vertices of degree $t+1$.

Unicyclic (n, n_1)-graphs with minimal first Zagreb index, of the form specified in Theorem 4.3.1, exist for any value of n and n_1, provided $n \geq 3$ and $n_1 \geq 0$.

Theorem 4.3.2. *[74] Let B be a bicyclic (n, n_1)-graph. Then*

$$M_1(B) \geq 4n + 6 + (n + n_1 + 4) \left\lfloor \frac{n+2}{n-n_1} \right\rfloor - (n - n_1) \left\lfloor \frac{n+2}{n-n_1} \right\rfloor^2 . \tag{4.3.2}$$

Equality in (4.3.2) is attained if and only if B consists of n_1 pendent vertices, $n_t = (n - n_1) \left\lfloor \frac{n+2}{n-n_1} \right\rfloor - n_1 - 2$ vertices of degree $t = \left\lfloor \frac{n+2}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n + 2 - (n - n_1) \left\lfloor \frac{n+2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Bicyclic (n, n_1)-graphs with minimal first Zagreb index, of the form specified in Theorem 4.3.2, exist for any value of n and n_1, provided $n \geq 4$ and $n_1 \geq 0$.

Also for any value of γ greater than 2, structural characterizations of γ-cyclic (n, n_1)-graphs with minimal first Zagreb index can be achieved in a fully analogous manner.

Chapter 5

First Reformulated Zagreb Index and Some Graph Operations

This chapter delt with some exact expressions for the first reformulated Zagreb index of graph operations containing cartesian product, composition, join, corona product, splice, link and chain of graphs. We apply these results to some graphs to chemical and general interest, such as C_4 nanotubes and nanotori, hypercube and prism graph.

5.1 Auxiliary Lemmas

This section describes some useful lemmas which are straightforward from definitions. For more details see [4, 17, 40, 56].

Lemma 5.1.1. *Let G and H be graphs. Then we have:*
(a) $|V(G\Box H)| = |V(G[H])| = |V(G)||V(H)|; |V(G \circ H)| = |V(H)|(|V(G)| + 1);$
$|V(G + H)| = |V(G)| + |V(H)|;$
$|E(G\Box H)| = |E(G)||V(H)| + |V(G)||E(H)|;$
$|E(G + H)| = |E(G)| + |E(H)| + |V(G)||V(H)|;$
$|E(G[H])| = |E(G)||V(H)|^2 + |E(H)||V(G)|.$
(b) The cartesian product, join and composition of graphs are associative and all of them are commutative except from composition.
(c) $d_{G\Box H}((a, c),(b, d)) = d_G(a, b) + d_H(c, d).$

(d)

$$d_{G+H}(u,v)=\begin{cases}0 & u=v\\ 1 & uv\in E(G)\ or\ uv\in E(H)\ or\\ & (u\in V(G)\ \&\ v\in V(H))\\ 2 & otherwise.\end{cases}$$

(e)

$$d_{G[H]}((a,b),(c,d))=\begin{cases}d_G(a,c) & a\neq c\\ d_H(b,d) & a=c\ \&\ d_G(a)=0,\\ \min\{d_H(b,d),2\} & a=c\ \&\ d_G(a)\neq 0.\end{cases}$$

(f)

$$d_{G\square H}((a,b))=d_G(a)+d_H(b).$$

(g)

$$d_{G[H]}((a,b))=|V(H)|d_G(a)+d_H(b).$$

(h)

$$d_{G+H}(a)=\begin{cases}d_G(a)+|V(H)|; & a\in V(G)\\ d_H(a)+|V(G)|; & a\in V(H).\end{cases}$$

(i)

$$d_{G_1\circ G_2}(v)=\begin{cases}d_{G_1}(v)+|V(G_2)|; & v\in V(G_1)\\ d_{G_2}(v)+1 \quad ; & v\ belongs\ to\ a\ copy\ of\ G_2.\end{cases}$$

Lemma 5.1.2. *Suppose that G_1 and G_2 are graphs. Then:*

(a)

$$d_{(G_1.G_2;v_1,v_2)}(u)=\begin{cases}d_{G_i}(u) & if\ u\in V(G_i)\ and\ u\neq v_i\ (i=1,2)\\ d_{G_1}(v_1)+d_{G_2}(v_2) & if\ u=v_i,\ i=1,2.\end{cases}$$

(b)

$$d_{(G_1\sim G_2;v_1,v_2)}(u)=\begin{cases}d_{G_i}(u) & if\ u\in V(G_i)\ and\ u\neq v_i\ (i=1,2)\\ d_{G_i}(v_i)+1 & if\ u=v_i,\ i=1,2.\end{cases}$$

Lemma 5.1.3. *Consider a chain graph $G=(G_1,G_1,\cdots,G_n;v_1,v_2,\cdots,v_n)$. We have*

$$d_G(u)=\begin{cases}d_{G_i}(u) \quad ; & u\in V(G_i)\quad and\ u\neq v_i, 1\leq i\leq n\\ d_{G_i}(u)+1; & u=v_i,\ i=1,n\\ d_{G_i}(u)+2; & u=v_i,\ 2\leq i\leq n-1.\end{cases}$$

Lemma 5.1.4. *[48] Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$, $E_i = E(G_i)$, $1 \leq i \leq n$, and $V = V\left(\square_{i=1}^{n} G_i\right)$. Then*

$$M_1\left(\mathop{\square}_{i=1}^{n} G_i\right) = |V| \sum_{i=1}^{n} \frac{M_1(G_i)}{|V_i|} + 4|V| \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \frac{|E_i|\,|E_j|}{|V_i|\,|V_j|}.$$

In particular,

$$M_1(G^n) = n|V(G)|^{n-2}\left(M_1(G)\,|V(G)| + 4(n-1)\,|E(G)|^2\right).$$

5.2 Explicit formulas

In this section, we derived expression for the first reformulated Zagreb index of each of the composite graphs introduced above. Those expressions include the first reformulated Zagreb indices of the components, the number of their vertices and edges, and in some expressions also their first Zagreb indices and S_u.

Theorem 5.2.1. *Let G and H be graphs. Then*

$$\begin{aligned} EM_1(G \square H) =& 12\,|E_H|\,M_1(G) + 12\,|E_G|\,M_1(H) + |V_H|\,EM_1(G) \\ &+ |V_G|\,EM_1(H) - 32\,|E_G|\,|E_H|. \end{aligned}$$

Proof.

$$EM_1(G \square H) = \sum_{((a,b),(c,d)) \in E(G \square H)} \left(d_{G \square H}(a,b) + d_{G \square H}(c,d) - 2\right)^2.$$

By Lemma 5.1.1(b, f) this expression equals

$$\begin{aligned} &\sum_{a \in V(G)} \sum_{bd \in E(H)} (2d_G(a) + d_H(b) + d_H(d) - 2)^2 \\ &+ \sum_{ac \in E(G)} \sum_{b \in V(H)} (d_G(a) + d_G(c) + 2d_H(b) - 2)^2 \end{aligned}$$

$$= \sum_{a\in V(G)} \sum_{bd\in E(H)} ((d_H(b) + d_H(d) - 2)^2 + 4d_G(a)^2$$
$$+ 4d_G(a)(d_H(b) + d_H(d) - 2)) + \sum_{ac\in E(G)} \sum_{b\in V(H)} ((d_G(a) + d_G(c) - 2)^2$$
$$+ 4d_H(b)^2 + 4d_H(b)(d_G(a) + d_G(c) - 2))$$
$$=12\,|E_H|\,M_1(G) + 12\,|E_G|\,M_1(H) + |V_H|\,EM_1\,(G) + |V_G|\,EM_1\,(H)$$
$$- 32\,|E_G|\,|E_H|.$$

□

Corollary 5.2.2. *Let $G_1,\ldots,G_n$ be graphs with $V_i = V(G_i)$, $E_i = E(G_i)$,$1 \leq i \leq n$, and $V = V\left(\square_{i=1}^n G_i\right)$. Then*

$$EM_1\left(\mathop{\square}_{i=1}^{n} G_i\right) = 12\,|V| \sum_{\substack{i,j=1\\ i\neq j}}^{n} M_1\,(G_i)\,\frac{|E_j|}{|V_i|\,|V_j|} + |V| \sum_{i=1}^{n} \frac{EM_1\,(G_i)}{|V_i|} +$$
$$+ 96\,|V| \sum_{\substack{i,j,k=1\\ i<j<k}}^{n} \frac{|E_i|\,|E_j|\,|E_k|}{|V_i|\,|V_j|\,|V_k|} - 32\,|V| \sum_{\substack{i,j=1\\ i<j}}^{n} \frac{|E_i|\,|E_j|}{|V_i|\,|V_j|}.$$

In particular, for $G = (V, E)$ we have

$$EM_1\,(G^n) = 12n\,(n-1)\,|V|^{n-2}\,|E|\,M_1\,(G) + n|V|^{n-1} EM_1\,(G) +$$
$$+ 16n\,(n-1)\,(n-2)\,|V|^{n-3}|E|^3 - 16n\,(n-1)\,|V|^{n-2}|E|^2\,.$$

Proof. By denoting $V = V(\square_{i=1}^n G_i)$, from Lemma 5.1.1($a$), using an inductive argument, we get $|E(\square_{i=1}^n G_i)| = |V| \sum_{i=1}^n \frac{|E_i|}{|V_i|}$ since $|V| = \prod_{i=1}^n |V_i|$.
For $n = 2$ the statement is true by Theorem [5.2.1]. Let $n \geq 2$ and suppose that the formula is true for n graphs. By Theorem [5.2.1] and the induction hypothesis we get

$$EM_1\left(\mathop{\square}_{i=1}^{n+1} G_i\right) = EM_1\left(\mathop{\square}_{i=1}^{n} G_i \square G_{n+1}\right)$$
$$= 12\,|E_{n+1}|\,M_1\left(\mathop{\square}_{i=1}^{n} G_i\right) + 12\left|E\left(\mathop{\square}_{i=1}^{n} G_i\right)\right| M_1\,(G_{n+1}) +$$
$$+ |V_{n+1}|\,EM_1\left(\mathop{\square}_{i=1}^{n} G_i\right) + |V|\,EM_1\,(G_{n+1}) - 32\left|E\left(\mathop{\square}_{i=1}^{n} G_i\right)\right| |E_{n+1}|\,.$$

By Lemma(5.1.4) this is equal to

$$12\left|E_{n+1}\right|(|V|\sum_{i=1}^{n}\frac{M_1(G_i)}{|V_i|}+8|V|\sum_{\substack{i,j=1\\i<j}}^{n}\frac{|E_i|\,|E_j|}{|V_i|\,|V_j|})+12|V|\,M_1(G_{n+1})\sum_{i=1}^{n}\frac{|E_i|}{|V_i|}$$

$$+\left|V_{n+1}\right|(12|V|\sum_{\substack{i,j=1\\i\neq j}}^{n}M_1(G_i)\frac{|E_j|}{|V_i|\,|V_j|}+|V|\sum_{i=1}^{n}\frac{EM_1(G_i)}{|V_i|}+96|V|\sum_{\substack{i,j,k=1\\i<j<k}}^{n}\frac{|E_i|\,|E_j|\,|E_k|}{|V_i|\,|V_j|\,|V_k|}-$$

$$-32|V|\sum_{\substack{i,j=1\\i<j}}^{n}\frac{|E_i|\,|E_j|}{|V_i|\,|V_j|})+|V|\,EM_1\left(G_{n+1}\right)-32|V|\left|E_{n+1}\right|\sum_{i=1}^{n}\frac{|E_i|}{|V_i|}$$

$$=12\left(\left|E_{n+1}\right||V|\sum_{i=1}^{n}\frac{M_1\left(G_i\right)}{|V_i|}+|V|\,M_1\left(G_{n+1}\right)\sum_{i=1}^{n}\frac{|E_i|}{|V_i|}+|V|\left|V_{n+1}\right|\sum_{\substack{i,j=1\\i\neq j}}^{n}\frac{M_1\left(G_i\right)|E_j|}{|V_i|\,|V_j|}\right)+$$

$$+\left(|V|\left|V_{n+1}\right|\sum_{i=1}^{n}\frac{EM_1\left(G_i\right)}{|V_i|}+|V|\,EM_1\left(G_{n+1}\right)\right)+$$

$$+96\left(|V|\left|E_{n+1}\right|\sum_{\substack{i,j=1\\i<j}}^{n}\frac{|E_i|\,|E_j|}{|V_i|\,|V_j|}+|V|\left|V_{n+1}\right|\sum_{\substack{i,j,k=1\\i<j<k}}^{n}\frac{|E_i|\,|E_j|\,|E_k|}{|V_i|\,|V_j|\,|V_k|}\right)-$$

$$-32\left(|V|\left|V_{n+1}\right|\sum_{\substack{i,j=1\\i<j}}^{n}\frac{|E_i|\,|E_j|}{|V_i|\,|V_j|}+|V|\left|E_{n+1}\right|\sum_{i=1}^{n}\frac{|E_i|}{|V_i|}\right).$$

By denoting $W=V(\Box_{i=1}^{n+1}G_i)$ we have $|W|=|V||V_{n+1}|$. We can conclude that

$$EM_1\left(\mathop{\Box}_{i=1}^{n+1}G_i\right)=12|W|\sum_{\substack{i,j=1\\i\neq j}}^{n+1}M_1\left(G_i\right)\tfrac{|E_j|}{|V_i||V_j|}+|W|\sum_{i=1}^{n+1}\tfrac{EM_1(G_i)}{|V_i|}$$
$$+96|W|\sum_{\substack{i,j,k=1\\i<j<k}}^{n+1}\tfrac{|E_i||E_j||E_k|}{|V_i||V_j||V_k|}-32|W|\sum_{\substack{i,j=1\\i<j}}^{n+1}\tfrac{|E_i||E_j|}{|V_i||V_j|}.$$

The second part is a direct consequence of the above equation. $\square$

Theorem 5.2.3. *Let $G_1,G_2,\ldots,G_n$ be graphs with $V_i=V(G_i),E_i=E(G_i),1\leq i\leq n,G=G_1+G_2+\cdots+G_n$ and $V=V(G)$. Then*

$$EM_1(G) = \sum_{i=1}^{n} \left(EM_1(G_i) + 4M_1(G_i)(|V| - |V_i|) + 4|E_i| \left((|V| - |V_i| - 1)^2 - 1 \right) \right)$$

$$+ \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \Big(|V_i| M_1(G_j) + |V_j| M_1(G_i) + 8|E_i||E_j| + 4(|E_i||V_j| + |E_j||V_i|)$$

$$\cdot (2|V| - |V_i| - |V_j| - 2) + |V_i||V_j|(2|V| - |V_i| - |V_j| - 2)^2 \Big).$$

In particular, for $H = (V, E)$ we get

$$\begin{aligned} EM_1(nH) = & n(EM_1(H) + 4(n-1)|V|M_1(H) + \\ & + 4|E| \left(((n-1)|V| - 1)^2 - 1 \right) + \\ & + \frac{1}{2} n(n-1)(2|V| M_1(H) + 8|E|^2 + 16|V||E|(n-1)|V| - 1) + \\ & + 4|V|^2((n-1)|V| - 1)^2). \end{aligned}$$

Proof. There are two type of edges in $G_1 + G_2 + \cdots + G_n$. Both of the ends of a first type edge belong to G_i, for some i. An edge of second type connects a vertex of G_i to a vertex of $G_j, i \neq j$. So by Lemma 5.1.1(i) and this fact that $G \cong G_i + (G_1 + \cdots + G_{i-1} + G_{i+1} + \cdots + G_n), d_G(v) = d_{G_i}(v) + |V| - |V_i|$, for each $v \in V_i$. Thus

$$EM_1(G) = \sum_{ab \in E(G)} (d(a) + d(b) - 2)^2$$

$$= \sum_{i=1}^{n} \sum_{uv \in E(G_i)} (d_{G_i}(u) + |V| - |V_i| + d_{G_i}(v) + |V| - |V_i| - 2)^2 +$$

$$+ \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \sum_{u \in V(G_i)} \sum_{v \in V(G_j)} \left(d_{G_i}(u) + |V| - |V_i| + d_{G_j}(v) + |V| - |V_j| - 2 \right)^2$$

$$= \sum_{i=1}^{n} \sum_{uv \in E(G_i)} (d_{G_i}(u) + d_{G_i}(V) - 2 + 2|V| - 2|V_i|)^2$$

$$+ \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \sum_{u \in V(G_i)} \sum_{v \in V(G_j)} \left(d_{G_i}(u) + d_{G_j}(v) + 2|V| - |V_i| - |V_j| - 2 \right)^2$$

$$
\begin{aligned}
=&\sum_{i=1}^{n}\sum_{uv\in E(G_i)}\Big((d_{G_i}(u)+d_{G_i}(v)-2)^2+4|V|^2+4|V_i|^2+\\
&+4(|V|-|V_i|)(d_{G_i}(u)+d_{G_i}(v)-2)-8|V||V_i|\Big)\\
&+\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{n}\sum_{u\in V(G_i)}\sum_{v\in V(G_j)}\Big(d_{G_i}(u)^2+d_{G_j}(v)^2+(2\left|V\right|-\left|V_i\right|-\left|V_j\right|-2)^2\\
&+2(d_{G_i}(u)+d_{G_j}(v))(2\left|V\right|-\left|V_i\right|-\left|V_j\right|-2)+2d_{G_i}(u)d_{G_j}(v)\Big)\\
=&\sum_{i=1}^{n}(EM_1(G_i)+4M_1(G_i)(|V|-|V_i|)+4\left|E_i\right|((|V|-|V_i|-1)^2-1))
\end{aligned}
$$

$$
+\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{n}\Big(\left|V_i\right|M_1(G_j)+\left|V_j\right|M_1(G_i)+8\left|E_i\right|\left|E_j\right|+4(\left|E_i\right|\left|V_j\right|+\left|E_j\right|\left|V_i\right|)(2\left|V\right|-\left|V_i\right|-\left|V_j\right|-2)+
$$

$$
+\left|V_i\right|\left|V_j\right|(2\left|V\right|-\left|V_i\right|-\left|V_j\right|-2)^2\Big).
$$

The second part is a direct consequence of the above equation. □

Theorem 5.2.4. *Let* $G=(V_G,E_G)$ *and* $H=(V_H,E_H)$ *be graphs. Then*

$$
\begin{aligned}
EM_1\left(G[H]\right)=&|V_H|^4EM_1\left(G\right)+\left|V_G\right|EM_1\left(H\right)+10\left|V_H\right|\left|E_G\right|M_1\left(H\right)\\
&+4|V_H|^2M_1\left(G\right)\left(|V_H|^2-\left|V_H\right|+3\left|E_H\right|\right)+8\left|E_G\right|\left|E_H\right|^2-32\left|V_H\right|\left|E_G\right|\left|E_H\right|\\
&-4|V_H|^2\left|E_G\right|\left(|V_H|^2-1\right).
\end{aligned}
$$

Proof. By Lemma 5.1.1(e,g) we deduce

$$
EM_1\left(G[H]\right)=\sum_{((a,c),(b,d))\in E(G[H])}\left(d_{G[H]}\left((a,c)\right)+d_{G[H]}\left((b,d)\right)-2\right)^2
$$

$$
\begin{aligned}
=&\sum_{w\in V(G)}\sum_{uv\in E_H}(\left|V_H\right|d_G\left(w\right)+d_H\left(u\right)+\left|V_H\right|d_G\left(w\right)+d_H\left(v\right)-2)^2+\\
&+\sum_{ab\in E(G)}\sum_{u\in V(H)}\sum_{v\in V(H)}(\left|V_H\right|d_G\left(a\right)+d_H\left(u\right)+\left|V_H\right|d_G\left(b\right)+d_H\left(v\right)-2)^2
\end{aligned}
$$

$$= \sum_{w\in V(G)} \sum_{uv\in E(H)} \left(d_H(u) + d_H(v) - 2 + 2|V_H|\, d_G(w)\right)^2 +$$

$$+ \sum_{ab\in E(G)} \sum_{u\in V(H)} \sum_{v\in V(H)} \left(|V_H|\left(d_G(a) + d_G(b) - 2\right) + d_H(u) + d_H(v) + 2|V_H| - 2\right)^2$$

$$= \sum_{w\in V(G)} \sum_{uv\in E(H)} ((d_H(u) + d_H(v) - 2)^2 + 4|V_H|^2 d_G(w)^2 +$$

$$+ 2(d_H(u) + d_H(v) - 2)(2|V_H|d_G(w))) +$$

$$+ \sum_{ab\in E(G)} \sum_{u\in V(H)} \sum_{v\in V(H)} \Big(|V_H|^2 (d_G(a) + d_G(b) - 2)^2 + (d_H(u) + d_H(v) + 2|V_H| - 2)^2 +$$

$$+ 2|V_H|\left(d_G(a) + d_G(b) - 2\right)\left(d_H(u) + d_H(v) + 2|V_H| - 2\right)\Big).$$

Since

$$\sum_{u\in V_H} \sum_{v\in V_H} (d_H(u) + d_H(v)) = 4|V_H||E_H|,$$

after some calculations we deduce that the last sum equals

$$|V_G|\, EM_1(H) + 4|V_H|^2\, |E_H|\, M_1(G) + 4|V_H|\left(2|E_G|\, M_1(H) - 4|E_G|\,|E_H|\right) +$$
$$+ |V_H|^4 EM_1(G) + 2|V_H|\,|E_G|\, M_1(H) + 4|V_H|^2 M_1(G)\left(|V_H|^2 - |V_H| + 2|E_H|\right) -$$
$$- 4|V_H|^2\, |E_G|\left(|V_H|^2 - 1\right) + 8|E_G|\,|E_H|^2 - 16|V_H|\,|E_G|\,|E_H|.$$

□

Theorem 5.2.5. *Let $G = (V_G, E_G)$ and $H = (V_H, E_H)$ be two graphs. Then*

$$\begin{aligned} EM_1(G\circ H) =& EM_1(G) + |V_G|\, EM_1(H) + 8|V_H|^2|E_G| + |V_G|(5M_1(H) - 8|E_H|) \\ & + |V_H|\left(5M_1(G) - 12|E_G|\right) + |V_G|\,|V_H|\left(|V_H| - 1\right)^2 + \\ & + 4|E_H|\left(|V_G|\,|V_H| + 2|E_G|\right). \end{aligned}$$

Proof.

$$EM_1(G\circ H) = \sum_{ab\in E(G\circ H)} \left(d_{G\circ H}(a) + d_{G\circ H}(b) - 2\right)^2.$$

By Lemma 5.1.1(i) this equals

$$\sum_{ac\in E(G)} \left(d_G(a)+|V_H|+d_G(c)+|V_H|-2\right)^2+$$

$$+\sum_{a\in V(G)}\sum_{b\in V(H)} \left(d_G(a)+|V_H|+d_H(b)+1-2\right)^2+$$

$$+\sum_{a\in V(G)}\sum_{bd\in E(H)} \left(d_H(b)+1+d_H(d)+1-2\right)^2$$

$$=\sum_{ac\in E(G)} \left(d_G(a)+d_G(c)-2+2|V_H|\right)^2+$$

$$+\sum_{a\in V(G)}\sum_{b\in V(H)} \left(d_G(a)+d_H(b)+|V_H|-1\right)^2+\sum_{a\in V(G)}\sum_{bd\in E(H)} \left(d_H(b)+d_H(d)\right)^2$$

$$=\sum_{ac\in E(G)} ((d_G(a)+d_G(c)-2)^2+4|V_H|^2+4|V_H|(d_G(a)+d_G(c)-2))+$$

$$+\sum_{a\in V(G)}\sum_{b\in V(H)} \Big(d_G(a)^2+d_H(b)^2+|V_H|^2+1+2d_G(a)\,d_H(b)+$$

$$+2|V_H|d_G(a)-2d_G(a)+2|V_H|\,d_H(b)-2d_H(b)-2|V_H|\Big)+$$

$$+\sum_{a\in V(G)}\sum_{bd\in E(H)} \left((d_H(b)+d_H(d)-2)^2+4+4\left(d_H(b)+d_H(d)-2\right)\right)$$

$$\begin{aligned}=&EM_1(G)+|V_G|\,EM_1(H)+8|V_H|^2|E_G|+|V_G|(5M_1(H)-8|E_H|)+\\&+|V_H|\left(5M_1(G)-12|E_G|\right)+|V_G|\,|V_H|\left(|V_H|-1\right)^2+\\&+4|E_H|\left(|V_G|\,|V_H|+2|E_G|\right).\end{aligned}$$

□

Theorem 5.2.6. *Let $G=(G_1.G_2;v_1,v_2)$ be a splice graph such that $d_{G_1}(v_1)=s$ and $d_{G_2}(v_2)=t$. Then*

$$EM_1(G)=EM_1(G_1)+EM_2(G_2)+3st\,(s+t)+2\,(sS_{v_2}+tS_{v_1})-8st.$$

Proof. Clearly,

$$\begin{aligned}E(G)=&\left(E(G_1)\setminus\{v_1v_i: i=1,2,\cdots,s\}\right)\bigcup\left(E(G_2)\setminus\{v_2u_i: i=1,2,\cdots,t\}\right)\\&\bigcup\{v_{12}v_i: i=1,2,\cdots,s\}\bigcup\{v_{12}u_i: i=1,2,\cdots,t\},\end{aligned}$$

where v_{12} is the new vertex obtained by the identification of v_1 and v_2 in G.

$$EM_1(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v) - 2)^2.$$

By Lemma 5.1.2(a) this is equal to

$$\sum_{uv\in E(G_1)\setminus\{v_1v_i:i=1,2,\cdots,s\}} \left(d_{G_1}(u) + d_{G_1}(v) - 2\right)^2$$

$$+ \sum_{uv\in E(G_2)\setminus\{v_2u_i:i=1,2,\cdots,t\}} \left(d_{G_2}(u) + d_{G_2}(v) - 2\right)^2$$

$$+ \sum_{i=1}^{s} \left(d_{(G_1.G_2;v_1,v_2)}(v_{12}) + d_{G_1}(v_i) - 2\right)^2 + \sum_{i=1}^{t} \left(d_{(G_1.G_2;v_1,v_2)}(v_{12}) + d_{G_2}(u_i) - 2\right)^2$$

$$= \sum_{uv\in E(G_1)\setminus\{v_1v_i:i=1,2,\cdots,s\}} \left(d_{G_1}(u) + d_{G_1}(v) - 2\right)^2$$

$$+ \sum_{uv\in E(G_2)\setminus\{v_2u_i:i=1,2,\cdots,t\}} \left(d_{G_2}(u) + d_{G_2}(v) - 2\right)^2$$

$$+ \sum_{i=1}^{s} \left(d_{G_1}(v_1) + d_{G_2}(v_2) + d_{G_1}(v_i) - 2\right)^2 + \sum_{i=1}^{t} \left(d_{G_1}(v_1) + d_{G_2}(v_2) + d_{G_2}(u_i) - 2\right)^2$$

$$= \sum_{uv\in E(G_1)\setminus\{v_1v_i:i=1,2,\cdots,s\}} \left(d_{G_1}(u) + d_{G_1}(v) - 2\right)^2$$

$$+ \sum_{uv\in E(G_2)\setminus\{v_2u_i:i=1,2,\cdots,t\}} \left(d_{G_2}(u) + d_{G_2}(v) - 2\right)^2$$

$$+ \sum_{i=1}^{s} \left(\left(d_{G_1}(v_1) + d_{G_1}(v_i) - 2\right)^2 + d_{G_2}(v_2)^2 + 2\left(d_{G_1}(v_1) + d_{G_1}(v_i) - 2\right) d_{G_2}(v_2)\right) +$$

$$+ \sum_{i=1}^{t} \left(\left(d_{G_2}(v_2) + d_{G_2}(u_i) - 2\right)^2 + d_{G_1}(v_1)^2 + 2\left(d_{G_2}(v_2) + d_{G_2}(u_i) - 2\right) d_{G_1}(v_1)\right)$$

$$= EM_1(G_1) + EM_1(G_2) + st^2 + 2s^2t + 2t\sum_{i=1}^{s} d_{G_1}(v_i) - 4st + s^2t + 2st^2 +$$

$$+ 2s\sum_{i=i}^{t} d_{G_2}(u_i) - 4st$$

$$= EM_1(G_1) + EM_1(G_2) + 3st(s+t) + 2\left(sS_{v_2} + tS_{v_1}\right) - 8st.$$

□

Theorem 5.2.7. *Let $G = (G_1 \sim G_2; v_1, v_2)$ be a link graph such that $d_{G_1}(v_1) = s$ and $d_{G_2}(v_2) = t$. Then*

$$EM_1(G) = EM_1(G_1) + EM_1(G_2) + 2(S_{v_1} + S_{v_2}) + 2(s^2 + t^2)$$

$$+(s+t)^2 - 3\,(s+t)\,.$$

Proof. Clearly,

$$E\,(G) = E(G_1) \cup E(G_2) \cup \{v_1v_2\}.$$

Using similar notations as above and by Lemma 5.1.2(b) we have

$$EM_1\,(G) = \sum_{uv \in E(G)} \left(d_G\,(u) + d_G\,(v) - 2\right)^2$$

$$= \sum_{uv \in E(G_1) \setminus \{v_1v_i : i=1,2,\cdots,s\}} \left(d_{G_1}\,(u) + d_{G_1}\,(v) - 2\right)^2$$

$$+ \sum_{uv \in E(G_2) \setminus \{v_2u_i : i=1,2,\cdots,t\}} \left(d_{G_2}\,(u) + d_{G_2}\,(v) - 2\right)^2 +$$

$$+ \sum_{i=1}^{s} \Big(d_{(G_1 \sim G_2; v_1, v_2)}\,(v_1) + d_{(G_1 \sim G_2; v_1, v_2)}\,(v_i) - 2\Big)^2$$

$$+ \sum_{i=1}^{t} \Big(d_{(G_1 \sim G_2; v_1, v_2)}\,(v_2) + d_{(G_1 \sim G_2; v_1, v_2)}\,(u_i) - 2\Big)^2$$

$$+ \Big(d_{(G_1 \sim G_2; v_1, v_2)}\,(v_1) + d_{(G_1 \sim G_2; v_1, v_2)}\,(v_2) - 2\Big)^2$$

$$= \sum_{uv \in E(G_1) \setminus \{v_1v_i : i=1,2,\cdots,s\}} \left(d_{G_1}\,(u) + d_{G_1}\,(v) - 2\right)^2$$

$$+ \sum_{uv \in E(G_2) \setminus \{v_2u_i : i=1,2,\cdots,t\}} \left(d_{G_2}\,(u) + d_{G_2}\,(v) - 2\right)^2$$

$$+\sum_{i=1}^{s}\left(d_{G_1}\left(v_1\right)+1+d_{G_1}\left(v_i\right)-2\right)^2+\sum_{i=1}^{t}\left(d_{G_2}\left(v_2\right)+1+d_{G_2}\left(u_i\right)-2\right)^2+$$
$$+\left(d_{G_1}\left(v_1\right)+1+d_{G_2}\left(v_2\right)+1-2\right)^2$$
$$=EM_1\left(G_1\right)+EM_1\left(G_2\right)+\sum_{i=1}^{s}\left(2\left(d_{G_1}\left(v_1\right)+d_{G_1}\left(v_i\right)-2\right)+1\right)+$$
$$+\sum_{i=1}^{t}\left(2\left(d_{G_2}\left(v_2\right)+d_{G_2}\left(u_i\right)-2\right)+1\right)+\left(s+t\right)^2$$
$$=EM_1(G_1)+EM_1(G_2)+2(S_{v_1}+S_{v_2})+2(s^2+t^2)+(s+t)^2-3\left(s+t\right).$$

□

Theorem 5.2.8. *Suppose that $G=(G_1,G_2,\cdots,G_n;v_1,v_2,\cdots,v_n)$, where $n\geq 3$ is a chain graph and $d_{G_i}(v_i)=t_i$ for $1\leq i\leq n$. Then*

$$EM_1(G)=\sum_{i=1}^{n}EM_1(G_i)+2t_1^2+2t_n^2-3t_1-3t_n+4\sum_{i=2}^{n-1}t_i^2-4\sum_{i=2}^{n-1}t_i+(t_1+t_2+1)^2+$$
$$+(t_{n-1}+t_n+1)^2+\sum_{i=2}^{n-2}(t_i+t_{i+1}+2)^2+2S_{v_1}+2S_{v_n}+4\sum_{i=2}^{n-1}S_{v_i},$$

where $S_{v_i}=\sum_{u\in N_{G_i}(v_i)}d_{G_i}(u)$.

Proof. Using similar notations we deduce:

$$E(G)=\bigcup_{i=1}^{n}E(G_i)\cup\bigcup_{i=1}^{n-1}\{v_iv_{i+1}\}$$

and

$$EM_1\left(G\right)=\sum_{uv\in E(G)}\left(d_G\left(u\right)+d_G\left(v\right)-2\right)^2$$
$$=\sum_{i=1}^{n}\sum_{uv\in E(G_i);u,v\neq v_i}(d_G(u)+d_G(v)-2)^2+\sum_{i=1}^{n}\sum_{v_iu\in E(G_i)}(d_G(v_i)+d_G(u)-2)^2$$
$$+\sum_{i=1}^{n-1}(d_G(v_i)+d_G(v_{i+1})-2)^2$$

$$
\begin{aligned}
&= \sum_{i=1}^{n} \sum_{uv \in E(G_i); u,v \neq v_i} (d_{G_i}(u) + d_{G_i}(v) - 2)^2 + \sum_{v_1 u \in E(G_1)} (t_1 + d_{G_1}(u) - 2 + 1)^2 + \\
&+ \sum_{v_n u \in E(G_n)} (t_n + d_{G_n}(u) - 2 + 1)^2 + \sum_{i=2}^{n-1} \sum_{v_i u \in E(G_i)} (t_i + d_{G_i}(u) - 2 + 2)^2 + \\
&+ (t_1 + t_2 + 1)^2 + (t_n + t_{n-1} + 1)^2 + \sum_{i=2}^{n-2} (t_i + t_{i+1} + 2)^2 \\
&= \sum_{i=1}^{n} EM_1(G_i) + t_1 + 2t_1^2 + 2S_{v_1} - 4t_1 + t_n + 2t_n^2 + 2S_{v_n} - 4t_n + \\
&+ \sum_{i=2}^{n-1} \sum_{v_i u \in E(G_i)} (4 + 4(t_i + d_{G_i}(u) - 2)) + (t_1 + t_2 + 1)^2 + (t_n + t_{n-1} + 1)^2 + \\
&+ \sum_{i=1}^{n-2} (t_i + t_{i+1} + 2)^2.
\end{aligned}
$$

Since

$$
\sum_{i=2}^{n-1} \sum_{v_i u \in E(G_i)} (4 + 4(t_i + d_{G_i}(u) - 2)) = -4 \sum_{i=2}^{n-1} t_i + 4 \sum_{i=2}^{n-1} t_i^2 + 4 \sum_{i=2}^{n-1} S_{v_i},
$$

the result follows. □

5.3 Applications

Now we apply the derived results on some families of graphs of chemical and general interest.

Consider the graph G whose vertices are N-tuples $c_1 c_2 \cdots c_N$ with $c_i \in \{0, 1, \cdots, n_i - 1\}, n_i \geq 2$ and two vertices are adjacent if the corresponding tuples differ in exactly one place. Such type of graph is called *Hamming* graph. It is known that a graph G is a Hamming graph if and only if it can be written in the form $G = \square_{i=1}^{N} K_{n_i}$. By using the Corollary 5.2.2 we can easily compute its fist reformulated Zagreb index.

Corollary 5.3.1. *We have*

$$EM_1(G) = EM_1(\mathop{\square}_{i=1}^{N} K_{n_i}) = 2\prod_{i=1}^{N} n_i\Big(3\sum_{\substack{i,j=1\\ i\neq j}}^{N}(n_i-1)^2(n_j-1) + \sum_{i=1}^{N}(n_i-1)(n_i-2)^2$$
$$+6\sum_{\substack{i,j,k=1\\ i<j<k}}^{N}(n_i-1)(n_j-1)(n_k-1) - 4\sum_{\substack{i,j=1\\ i<j}}^{N}(n_i-1)(n_j-1)\Big).$$

Proof. By Corollary (5.2.2) we have:

$$\begin{aligned} EM_1(G) =& 12|V|\sum_{\substack{i,j=1\\ i\neq j}}^{N} M_1(K_{n_i})\frac{|E_{n_j}|}{|V_{n_i}||V_{n_j}|} + |V|\sum_{i=1}^{N}\frac{EM_1(K_{n_i})}{|V_{n_i}|} + \\ &+96|V|\sum_{\substack{i,j,k=1\\ i<j<k}}^{N}\frac{|E_{n_i}||E_{n_j}||E_{n_k}|}{|V_{n_i}||V_{n_j}||V_{n_k}|} - 32|V|\sum_{\substack{i,j=1\\ i<j}}^{N}\frac{|E_{n_i}||E_{n_j}|}{|V_{n_i}||V_{n_j}|} \\ =& 2\prod_{i=1}^{N} n_i\Big(3\sum_{\substack{i,j=1\\ i\neq j}}^{N}(n_i-1)^2(n_j-1) + \sum_{i=1}^{N}(n_i-1)(n_i-2)^2 + \\ &+6\sum_{\substack{i,j,k=1\\ i<j<k}}^{N}(n_i-1)(n_j-1)(n_k-1) - 4\sum_{\substack{i,j=1\\ i<j}}^{N}(n_i-1)(n_j-1)\Big), \end{aligned}$$

since $M_1(K_{n_i}) = n_i(n_i-1)^2$ and $EM_1(K_{n_i}) = 2n_i(n_i-1)(n_i-2)^2$. □

C_4 *Nanotube* is the Cartesian product of path and cycle, $P_m \square C_n$.

Corollary 5.3.2.

$$EM_1(P_m \square C_n) = \begin{cases} 72mn - 98n & ;\ m,n \geq 3 \\ 48n & ; m = 2, n \geq 3. \end{cases}$$

A special case of C_4 Nanotube is *prism graph* $P_2 \square C_n$. We get $EM_1(P_2 \square C_n) = 48n$ for $n \geq 3$.

Next example is the *rectangular grid* obtained by Cartesian product of two paths, $P_q \square P_r$.

Corollary 5.3.3.

$$EM_1\left(P_q\square P_r\right)=\begin{cases}72qr-98\left(q+r\right)+112; & q,r\geq 3\\ 48r-84 & ;q=2,r\geq 3\\ 16 & ;q=r=2.\end{cases}$$

For *square grid*, $P_q\square P_q$, we have a simpler expression.

Corollary 5.3.4.

$$EM_1\left(P_q\square P_q\right)=72q^2-196q+112.$$

By setting $q=2$ we obtain a *ladder graph* $L_r=P_2\square P_r$.

Corollary 5.3.5.

$$EM_1\left(P_2\square P_r\right)=\begin{cases}48r-84; & r\geq 3\\ 16 & ;r=2\end{cases}$$

An *open fence* is a graph obtained by composition of P_n with K_2.

Corollary 5.3.6.

$$EM_1\left(K_2[P_n]\right)=4n^4+16n^3-4n^2-36n-12\ for\ n\geq 3.$$

Closed fence is the graph obtained by composing C_n with K_2.

Corollary 5.3.7.

$$EM_1\left(K_2[C_n]\right)=4n\left(n^3+4n^2+5n+2\right)\ for\ n\geq 3.$$

By definition, the *complete n-partite graph* is the join of n empty graphs $G_1,G_2,\ldots,G_n$ with $m_1,m_2,\ldots,m_n$ vertices, respectively. It is denoted by $K_{m_1,m_2,\cdots,m_n}$. By Theorem(5.2.3) we get:

Corollary 5.3.8.

$$EM_1\left(K_{m_1,m_2,\cdots,m_n}\right)=\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{n}\left|V_i\right|\left|V_j\right|\left(2\left|V\right|-\left|V_i\right|-\left|V_j\right|-2\right)^2.$$

Fan graph is the join of P_n and K_1.

Corollary 5.3.9.

$$EM_1\left(P_n+K_1\right)=n^3+2n^2+13n-32\ for\ n\geq 3.$$

When we join C_n with K_1 we obtain the *wheel graph.*

Corollary 5.3.10.

$$EM_1\left(C_n+K_1\right)=n^3+2n^2+17n\ for\ n\geq 3.$$

Chapter 6

Distance Based Topological Indices and Double Graph

In this chapter, we first derived closed-form formulas for some distance based topological indices for double graphs $D[G]$ in terms of G. Finally, these formulas are applied for several special kinds of graphs, such as, the complete graph, the path and the cycle.

6.1 Some Lemmas

Let $G(V, E)$ be a simple graph and $G'(V', E')$ be its distinct copy. Let $D[G]$ be the double graph of G and $V(D[G]) = V(G) \cup V(G')$, where $V(G) = \{x_1, x_2, \ldots, x_n\}$ and $V(G') = \{y_1, y_2, \ldots, y_n\}$ and y_i is the corresponding vertex of x_i in $V(G')$.

Lemma 6.1.1. *For the above defined double graph $D[G]$*

$$d_{D[G]}(x_i, x_j) = d_G(x_i, x_j) \quad ; i, j = 1, \ldots, n.$$

Proof. Clearly, $G \subset D[G]$. Let $\{x_i, x_j\} \subseteq V(G) \subset V(D[G])$ then $d_{D[G]}(x_i, x_j) \leq d_G(x_i, x_j)$. Suppose $l = d_{D[G]}(x_i, x_j) < d_G(x_i, x_j) = m$ and a shortest path in $D[G]$ from x_i to x_j is $x_i v_1 v_2 \cdots v_{l-1} x_j$. If $l = 1$ then the property is obvious. Suppose $l \geq 2$. Since $l < m$, there exists some $v_k \in V(G')$. As v_{k-1} and v_{k+1} are adjacent to v_k, by definition of the double graph v_{k-1} and v_{k+1} are adjacent to x_k(corresponding vertex of v_k in $V(G)$). Now we have obtained a path $x_i v_1 v_2 \ldots x_k \cdots v_{l-1} x_j$. In this way we can find a path $x_i x_1 x_2 \dots x_k \cdots x_{l-1} x_j$ in G of length l, which is a contradiction. It follows that $d_{D[G]}(x_i, x_j) = d_G(x_i, x_j)$. Similarly, $d_{D[G]}(y_i, y_j) = d_G(y_i, y_j)$. □

Lemma 6.1.2. *For the double graph $D[G]$*

$$d_{D[G]}(x_i, y_j) = d_G(x_i, x_j) \ \ ; i, j = 1, \dots, n.$$

Proof. Let $x_i \in V(G)$ and $y_j \in V(G')$. Suppose $l = d_{D[G]}(x_i, y_j) < d_G(x_i, x_j) = m$ and a shortest path in $D[G]$ is $x_i v_1 v_2 \cdots v_{l-1} y_j$. If $l = 1$ the property is true. Let $l \geq 2$. It follows that there exists some $v_k \in V(G')$. Since v_{k-1} and v_{k+1} are adjacent to v_k, by construction v_{k-1} and v_{k+1} are adjacent to x_k(corresponding vertex of v_k in $V(G)$). We have obtained a path $x_i v_1 v_2 \dots x_k \dots v_{l-1} y_j$ in $D[G]$, which implies the existence of a path $x_i x_1 x_2 \dots x_k \dots x_{l-1} x_j$ in G of length l, a contradiction. If $l = d_{D[G]}(x_i, y_j) > d_G(x_i, x_j) = m$ we get a similar contradiction. Consequently, $d_{D[G]}(x_i, y_j) = d_G(x_i, x_j)$. □

The following results are obvious from the construction of the double graph.

Lemma 6.1.3. *We have*

$$d_{D[G]}(x_i, y_i) = 2 \ \ ; i = 1, \dots, n.$$

Lemma 6.1.4. *For the double graph $D[G]$*

$$d_{D[G]}(x_i) = d_{D[G]}(y_i) = 2 d_G(x_i) \ \ ; i = 1, \dots, n.$$

Lemma 6.1.5. *The eccentricities of the vertices of the double graph $D[G]$ are*

$$\begin{aligned} ecc_{D[G]}(x_i) &= ecc_{D[G]}(y_i) = ecc_G(x_i) \ \ if \ \ ecc_G(x_i) \geq 2 \ \ ; i = 1, \dots, n \\ ecc_{D[G]}(x_i) &= ecc_{D[G]}(y_i) = 2 \qquad\qquad if \ \ ecc_G(x_i) = 1 \ \ ; i = 1, \dots, n. \end{aligned}$$

6.2 Main Results

Theorem 6.2.1. *Let G be a simple graph with n vertices. Then the Wiener index of $D[G]$ is given by*

$$W(D[G]) = 4W(G) + 2n.$$

Proof. The Wiener index of $D[G]$ is

$$W(D[G]) = \sum_{1 \leq i < j \leq n} d_{D[G]}(v_i, v_j)$$

$$= \sum_{1 \leq i < j \leq n} d_{D[G]}(x_i, x_j) + \sum_{1 \leq i < j \leq n} d_{D[G]}(y_i, y_j) + \sum_{\substack{i,j=1,\dots,n \\ i \neq j}} d_{D[G]}(x_i, y_j) +$$

$$+\sum_{i=1,\ldots,n} d_{D[G]}\left(x_i, y_i\right).$$

By Lemmas 6.1.1 $-$ 6.1.3 we deduce

$$\begin{aligned} W\left(D\left[G\right]\right) &= \sum_{1\leq i<j\leq n} d_G\left(x_i, x_j\right) + \sum_{1\leq i<j\leq n} d_G\left(x_i, x_j\right) + \sum_{\substack{i,j=1,\ldots,n \\ i\neq j}} d_G\left(x_i, x_j\right) + 2n \\ &= W(G) + W(G) + 2W(G) + 2n \\ &= 4W\left(G\right) + 2n. \end{aligned}$$

□

A well known property of the Wiener index of trees implies the following corollary.

Corollary 6.2.2. *Suppose T_n is a tree with n vertices. Then*

$$W\left(D\left[S_n\right]\right) \leq W\left(D\left[T_n\right]\right) \leq W\left(D\left[P_n\right]\right).$$

Theorem 6.2.3. *Let G be a simple graph with n vertices. Then the Harary index of $D[G]$ is given by*

$$H\left(D[G]\right) = 4H(G) + \frac{n}{2}.$$

Proof. The Harary index of $D[G]$ is

$$H(D[G]) = \sum_{1\leq i<j\leq n} \frac{1}{d_{D[G]}(v_i, v_j)}$$

$$= \sum_{1\leq i<j\leq n} \frac{1}{d_{D[G]}\left(x_i, x_j\right)} + \sum_{1\leq i<j\leq n} \frac{1}{d_{D[G]}\left(y_i, y_j\right)} + \sum_{\substack{i,j=1,\ldots,n \\ i\neq j}} \frac{1}{d_{D[G]}\left(x_i, y_j\right)} +$$

$$+\sum_{i=1,\ldots,n} \frac{1}{d_{D[G]}\left(x_i, y_i\right)}.$$

By Lemmas 6.1.1 $-$ 6.1.3 we have

$$\begin{aligned} H\left(D\left[G\right]\right) &= \sum_{1\leq i<j\leq n} \frac{1}{d_G\left(x_i, x_j\right)} + \sum_{1\leq i<j\leq n} \frac{1}{d_G\left(x_i, x_j\right)} + \sum_{\substack{i,j=1,\ldots,n \\ i\neq j}} \frac{1}{d_G\left(x_i, x_j\right)} + \frac{n}{2} \\ &= H(G) + H(G) + 2H(G) + \frac{n}{2} \\ &= 4H\left(G\right) + \frac{n}{2}. \end{aligned}$$

□

Corollary 6.2.4. *Let T_n be a tree with n vertices. Then*

$$H\left(D\left[P_n\right]\right) \leq H\left(D\left[T_n\right]\right) \leq H\left(D\left[S_n\right]\right).$$

Theorem 6.2.5. *Let G be a simple graph with m edges. Then the additively weighted Harary index of $D[G]$ is given by*

$$H_A\left(D\left[G\right]\right) = 8H_A\left(G\right) + 4m.$$

Proof. The additively Harary index of $D[G]$ is

$$\begin{aligned}
H_A(D[G]) &= \sum_{1\leq i<j\leq n} \frac{d_{D[G]}(v_i) + d_{D[G]}(v_j)}{d_{D[G]}(v_i, v_j)} \\
&= \sum_{1\leq i<j\leq n} \frac{d_{D[G]}\left(x_i\right) + d_{D[G]}\left(x_j\right)}{d_{D[G]}\left(x_i, x_j\right)} + \sum_{1\leq i<j\leq n} \frac{d_{D[G]}\left(y_i\right) + d_{D[G]}\left(y_j\right)}{d_{D[G]}\left(y_i, y_j\right)} + \\
&+ \sum_{\substack{i,j=1,\ldots,n \\ i\neq j}} \frac{d_{D[G]}\left(x_i\right) + d_{D[G]}\left(y_j\right)}{d_{D[G]}\left(x_i, y_j\right)} + + \sum_{i=1,\ldots,n} \frac{d_{D[G]}\left(x_i\right) + d_{D[G]}\left(y_i\right)}{d_{D[G]}\left(x_i, y_i\right)}.
\end{aligned}$$

By Lemmas 6.1.1 − 6.1.4 the last expression is equal to

$$\begin{aligned}
&\sum_{1\leq i<j\leq n} \frac{2d_G\left(x_i\right) + 2d_G\left(x_j\right)}{d_G\left(x_i, x_j\right)} + \sum_{1\leq i<j\leq n} \frac{2d_G\left(x_i\right) + 2d_G\left(x_j\right)}{d_G\left(x_i, x_j\right)} + \sum_{\substack{i,j=1,\ldots,n \\ i\neq j}} \frac{2d_G\left(x_i\right) + 2d_G\left(x_j\right)}{d_G\left(x_i, x_j\right)} + \\
&+ \sum_{x_i\in V(G)} \frac{2d_G\left(x_i\right) + 2d_G\left(x_i\right)}{2} \\
&= 2H_A\left(G\right) + 2H_A\left(G\right) + 4H_A\left(G\right) + 2\sum_{x_i\in V(G)} d_G\left(x_i\right) \\
&= 8H_A\left(G\right) + 4m.
\end{aligned}$$

□

Corollary 6.2.6. *Suppose T_n and U_n be tree and unicyclic graphs, respectively, with n vertices. Then*

$$H_A\left(D[T_n]\right) = 8H_A\left(T_n\right) + 4\left(n-1\right).$$
$$H_A\left(D[U_n]\right) = 8H_A\left(U_n\right) + 4n.$$

Corollary 6.2.7. *Suppose T_n is a tree with n vertices. Then*

$$H_A\left(D\left[P_n\right]\right) \leq H_A\left(D\left[T_n\right]\right) \leq H_A\left(D\left[S_n\right]\right).$$

Theorem 6.2.8. *Let G be a simple graph. The multiplicative weighted Harary index of $D[G]$ is given by*

$$H_M\left(D\left[G\right]\right) = 16H_M\left(G\right) + 2\sum_{x_i\in V(G)} d_G(x_i)^2.$$

Proof. The multiplicative Harary index of $D[G]$ is

$$H_M(D[G]) = \sum_{1\le i<j\le n} \frac{d_{D[G]}(v_i)d_{D[G]}(v_j)}{d_{D[G]}(v_i,v_j)}$$

$$= \sum_{1\le i<j\le n} \frac{d_{D[G]}\left(x_i\right)d_{D[G]}\left(x_j\right)}{d_{D[G]}\left(x_i,x_j\right)} + \sum_{1\le i<j\le n} \frac{d_{D[G]}\left(y_i\right)d_{D[G]}\left(y_j\right)}{d_{D[G]}\left(y_i,y_j\right)} + \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{d_{D[G]}\left(x_i\right)d_{D[G]}\left(y_j\right)}{d_{D[G]}\left(x_i,y_j\right)} +$$

$$+ \sum_{i=1,\ldots,n} \frac{d_{D[G]}\left(x_i\right)d_{D[G]}\left(y_i\right)}{d_{D[G]}\left(x_i,y_i\right)}.$$

By Lemmas $6.1.1 - 6.1.4$ this expression equals

$$\sum_{1\le i<j\le n} \frac{2d_G\left(x_i\right)2d_G\left(x_j\right)}{d_G\left(x_i,x_j\right)} + \sum_{1\le i<j\le n} \frac{2d_G\left(x_i\right)2d_G\left(x_j\right)}{d_G\left(x_i,x_j\right)} + \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{2d_G\left(x_i\right)2d_G\left(x_j\right)}{d_G\left(x_i,x_j\right)} +$$

$$+ \sum_{x_i\in V(G)} \frac{2d_G\left(x_i\right)2d_G\left(x_i\right)}{2}$$

$$= 4H_M\left(G\right) + 4H_M\left(G\right) + 8H_M\left(G\right) + 2\sum_{x_i\in V(G)} d_G(x_i)^2$$

$$= 16H_M(G) + 2\sum_{x_i\in V(G)} d_G(x_i)^2.$$

□

Corollary 6.2.9. *Suppose P_n, S_n, C_n and K_n be the path, star cyclic and complete graphs with n vertices. Then*

$$\begin{aligned}
H_M\left(D\left[P_n\right]\right) &= 16H_M\left(P_n\right) + 8n - 12\\
H_M\left(D\left[S_n\right]\right) &= 16H_M\left(S_n\right) + 2n\left(n-1\right)\\
H_M\left(D\left[C_n\right]\right) &= 16H_M\left(C_n\right) + 8n\\
H_M\left(D\left[K_n\right]\right) &= 16H_M\left(K_n\right) + 2n(n-1)^2.
\end{aligned}$$

Theorem 6.2.10. *Suppose G is a graph of order n, having k vertices v such that $ecc(v) = 1$ (or equivalently, $d_G(v) = n-1$). The eccentric connectivity index of $D[G]$ is given by*

$$\zeta^c\left(D\left[G\right]\right) = 4\zeta^c\left(G\right) + 4k(n-1).$$

Proof.

$$\zeta^c\left(D\left[G\right]\right) = \sum_{i=1}^{n} d_{D[G]}(x_i)ecc_{D[G]}(x_i) + \sum_{i=1}^{n} d_{D[G]}(y_i)ecc_{D[G]}(y_i).$$

By Lemmas 6.1.4 and 6.1.5 we have

$$\zeta^c\left(D\left[G\right]\right) = 2\sum_{i|ecc(x_i)\geq 2} d_G(x_i)ecc_G(x_i) + 4\sum_{i|ecc_G(x_i)=1} d_G(x_i) + 2\sum_{i|ecc_G(x_i)\geq 2} d_G(x_i)ecc_G(x_i)$$

$$+4\sum_{i|ecc_G(x_i)=1} d_G(x_i) = 4\zeta^c\left(G\right) + 4\sum_{i|ecc_G(x_i)=1} d_G(x_i) = 4\zeta^c\left(G\right) + 4k(n-1).$$

□

Theorem 6.2.11. *Let G be a simple graph having k vertices with $ecc_G(v) = 1$. The total eccentricity index of $D[G]$ is given by*

$$\zeta\left(D\left[G\right]\right) = 2\zeta\left(G\right) + 2k.$$

Proof.

$$\zeta\left(D\left[G\right]\right) = \sum_{i=1}^{n} ecc_{D[G]}(x_i) + \sum_{i=1}^{n} ecc_{D[G]}(y_i).$$

By Lemma 6.1.5 we have

$$\zeta(D[G]) = 2\left(\sum_{i|ecc_G(x_i)\geq 2} ecc_G(x_i) + \sum_{i|ecc_G(x_i)=1} 2\right) = 2\zeta\left(G\right) + 2k.$$

□

Corollary 6.2.12. *For the star and the complete graph we have:*

$$\zeta\left(D\left[S_n\right]\right) = 2\zeta\left(S_n\right) + 2;$$

$$\zeta\left(D\left[K_n\right]\right) = 2\zeta\left(K_n\right) + 2n.$$

Chapter 7

Concluding Remarks and Possible Directions for Future work

In chapters 2 and 3, we studied the general sum-connectivity index and zeroth-order general Randić index of graphs with some given parameters. In chapter 2, we found that in the class of trees of order n and independence number s, the spur $S_{n,s}$ is the unique graph maximizing zeroth-order general Randić for $\alpha > 1$ and general sum-connectivity index for $\alpha \geq 1$. Although, this property does not hold for general Randić index if $\alpha \geq 2$. In chapter 3, we found the maximum value for the general sum-connectivity index of n-vertex trees for $-1.7036 \leq \alpha < 0$ and of n-vertex unicyclic graphs for $-1 \leq \alpha < 0$ respectively, with fixed maximum degree $\triangle$. We also characterized the corresponding extremal graphs, as well as the n-vertex unicyclic graphs with the second maximum general sum-connectivity index for $n \geq 4$.

Possible future work in this direction is to find the minimum sum-connectivity index of trees and general graphs with given order n and independence number s, then try to extend these results for the general sum-connectivity index. One can study the behavior of general sum connectivity index for $\alpha > 0$ in the classes of $T(n, \triangle)$ and $U(n, \triangle)$ also the minimum of these indices for graphs with fixed maximum degree $\triangle$ can be discuss.

Goubko proved that for trees with n_1 pendent vertices, $M_1 \geq 9n_1 - 16$. In chapter

4, we extended this result for any connected graph with cyclomatic number $\gamma \geq 0$. In addition, graphs with n vertices, n_1 pendent vertices, cyclomatic number γ and minimal M_1 are characterized. One possible direction for future work is of course to find similar results for the second Zagreb index M_2.

In chapter 5, we dealt with some exact expressions for the first reformulated Zagreb index of some graph operations containing cartesian product, composition, join, corona product, splice, link and chain of graphs. Then we applied the results to some graphs to chemical and general interest, such as C_4 nanotubes and nanotori, hypercube and prism graph etc.

Many operations of chemical interest were not included here, such as, tensor product, disjunction, symmetric difference, strong product of graphs. Derivation of explicit formulas for such graphs will not be much difficult.

In chapter 6, we first derived closed-form formulas for Wiener index, Harary index and eccentric connectivity index for double graphs $D[G]$ in terms of these parameters for G. Then, these formulas were applied to many special kinds of graphs.

We discussed only few indices, but one can study closed-form formulas for other indices of double graphs.

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