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Preface

In the recent years, the mathematical–chemistry literature is flooded by countless graph–based topological indices, proposed to serve as molecular structure descriptors.

Topological indices have attracted much attention of chemical and mathematical researchers, especially those focussing on graph theory, from all over the world. Nowadays many interesting results and lot of open problems on it have been reported in literature. In most cases, the mathematical investigation of these indices consist of finding lower and upper bounds for them, and characterizing the graphs for which these inequalities become equalities. Again, the number of results obtained along these lines, and the number of respective publications, is so large that no human can satisfactorily follow them and recognize what is significant and what is not.

In order to help colleagues to find their way through the data jungle, we decided to devote one book in our "*Mathematical Chemistry Monographs*" series to bounds on topological indices and the related extremal graphs. To this end, in the Summer of 2016 we invited a number of colleagues to contribute chapters to our book. The scholars invited were among those who are currently active and who publish in this field of chemical graph theory. Their response was beyond anything what we could have expected.

Thus, instead of a single "*Mathematical Chemistry Monograph*", we had to produce three volumes, that is:

- Mathematical Chemistry Monograph No. 19:
  Bounds in Chemical Graph Theory – Basics
  Faculty of Science & University, Kragujevac, 2017
- Mathematical Chemistry Monograph No. 20:
  Bounds in Chemical Graph Theory – Mainstreams
  Faculty of Science & University, Kragujevac, 2017
- Mathematical Chemistry Monograph No. 21:
  Bounds in Chemical Graph Theory – Advances
  Faculty of Science & University, Kragujevac, 2017

The present book is the "*Mathematical Chemistry Monograph*" No. 21, completed in February 2017.

Editors:

Ivan Gutman
Boris Furtula
Kinkar Ch. Das
Emina I. Milovanović
Igor Ž. Milovanović

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Nordhaus–Gaddum Type Results in Chemical Graph Theory*

Yaping Mao

Department of Mathematics, Qinghai Normal University, Xining, Qinghai 810008, P. R. China
maoyaping@ymail.com

Abstract

Let $\mathcal{G}(n)$ denote the class of simple graphs of order n $(n \geq 2)$ and $\mathcal{G}(n,m)$ the subclass of $\mathcal{G}(n)$ in which every graph has n vertices and m edges. Give a graph parameter $f(G)$ and a positive integer n, the *Nordhaus–Gaddum Problem* is to determine sharp bounds for $f(G) + f(\overline{G})$ and $f(G) \cdot f(\overline{G})$, as G ranges over the class $\mathcal{G}(n)$ or $\mathcal{G}(n,m)$, and characterize the extremal graphs, i.e., graphs that achieve the bounds. A further problem is to determine the set of all integer pairs (x,y) such that $f(G) = x$ and $f(\overline{G}) = y$ for some graph G of order n. We refer to this latter problem as the *Realizability Problem*. In their paper, Nordhaus and Gaddum [121] determined bounds for $\chi(G) + \chi(\overline{G})$ and $\chi(G) \cdot \chi(\overline{G})$, where $\chi(G)$ denotes the chromatic number of graph G. The characterization of the corresponding extremal graphs and the realizability problem were resolved by Finck [52]. Nordhaus–Gaddum type relations have received wide attention; see the survey [7] by Aouchiche and Hansen. Let $k \geq 2$ be an integer. A *k-decomposition* $(G_1, G_2, \ldots, G_k)$ of a graph G is a partition of its edge set to form k spanning subgraph $G_1, G_2, \ldots, G_k$. That is, each G_i has the same vertices as G, and every edge of G belongs to exactly one of $G_1, G_2, \ldots, G_k$. For a graph parameter f, a positive integer k, and a graph G, the *Generalized Nordhaus–Gaddum Problem* is to determine sharp bounds for $\left\{\sum_{i=1}^{k} f(G_i) : (G_1, G_2, \ldots, G_k) \text{ is a decomposition of } G\right\}$ and $\left\{\prod_{i=1}^{k} f(G_i) : (G_1, G_2, \ldots, G_k) \text{ is a decomposition of } G\right\}$. In this chapter we summarize the known results on the (generalized-) Nordhaus–Gaddum type results in chemical graph theory.

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1. Distance–based parameters

All graphs in this chapter are undirected, finite and simple. We refer to [11] for graph theoretical notation and terminology not described here. For a graph G, let $V(G)$, $E(G)$, $e(G)$, $\overline{G}$ and $L(G)$ denote the set of vertices, the set of edges, the size, the complement, and the line graph of G, respectively. Distance is one of the basic concepts of graph theory [12]. If G is a connected graph and $u, v \in V(G)$, then the *distance* $d(u,v)$ between u and v is the length of a shortest path connecting u and v. If v is a vertex of a connected graph G, then the *eccentricity* $e(v)$ of v is defined by $e(v) = \max\{d(u,v) \,|\, u \in V(G)\}$. Furthermore, the *radius* $rad(G)$ and *diameter* $diam(G)$ of G are defined by $rad(G) = \min\{e(v) \,|\, v \in V(G)\}$ and $diam(G) = \max\{e(v) \,|\, v \in V(G)\}$. These last two concepts are related by the inequalities $rad(G) \leq diam(G) \leq 2rad(G)$. Goddard and Oellermann gave a survey paper on this subject [55].

In this section, we assume that G and $\overline{G}$ are both connected. In the sequel, the set of neighbors of a vertex v in a graph G is denoted by $N_G(v)$. Let $N_G[v] = N_G(v) \cup \{v\}$. For any subset X of $V(G)$, let $G[X]$ denote the subgraph induced by X, and $E[X]$ the edge set of $G[X]$; similarly, for any subset F of $E(G)$, let $G[F]$ denote the subgraph induced by F. We use $G - X$ to denote the subgraph of G obtained by removing all the vertices of X together with the edges incident with them from G; similarly, we use $G \setminus F$ to denote the subgraph of G obtained by removing all the edges of F from G. If $X = \{v\}$ and $F = \{e\}$, we simply write $G - v$ and $G \setminus e$ for $G - \{v\}$ and $G \setminus \{e\}$, respectively. For two subsets X and Y of $V(G)$ we denote by $E_G[X, Y]$ the set of edges of G with one end in X and the other end in Y. If $X = \{x\}$, we simply write $E_G[x, Y]$ for $E_G[\{x\}, Y]$.

The *path* of order n is denoted by P_n, and the *star* of order n is denoted by S_n. A *complete graph* is a graph in which every pair of vertices are adjacent, and a complete graph on n vertices is denoted by K_n. A graph is *bipartite* if its vertex set can be partitioned into two subsets X and Y so that every edge has one end in X and the other end in Y; such a partition (X, Y) is called a *bipartition* of the graph, and X and Y its parts. If each vertex in X is adjacent to every vertex in Y, then G is called a *complete bipartite graph*. Let $K_{s,t}$ denote a complete bipartite graph the cardinalities of whose two parts are s, t, respectively. A *path* on n vertices is denoted by P_n, and a *cycle* on n vertices is denoted by C_n. A connected graph without any cycles is called a *tree*. A *forest* is a graph whose every component is a tree. A *subtree* of a graph is a subgraph of the graph which is a tree. If this subtree is a spanning subgraph, it is called a *spanning tree* of the graph.

The *degree* of a vertex v in a graph G, denoted by $d_G(v)$, is the number of edges of G incident with

v. A vertex of degree zero is called an *isolated vertex*. We denote by $\delta(G)$ and $\Delta(G)$ the minimum and maximum degrees of the vertices of G. A graph G is called *k-regular* if $d_G(v) = k$ for every $v \in V(G)$. A 3-regular graph is called a *cubic graph*. The *distance* between two vertices u and v in a connected graph G, denoted by $d_G(u, v)$, is the length of a shortest path between them in G. The *eccentricity* of a vertex v is $ecc(v) := \max_{x \in V(G)} d(v, x)$. The *diameter* of G is $diam(G) := \max_{x \in V(G)} ecc(x)$.

Two graphs are called *disjoint* if they have no vertex in common, and *edge–disjoint* if they have no edge in common. The *union* $G \cup H$ of two graphs G and H is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. If G and H are disjoint, we refer to their union as a *disjoint union*. It can be seen that every graph may be expressed uniquely (up to order) as a disjoint union of connected graphs, and these graphs are called the *connected components*, or simply *components*, and we denote the number of components of a graph G by $\omega(G)$. If G is the disjoint union of k copies of a graph H, we simply write $G = kH$. The *join* $G \vee H$ of two disjoint graphs G and H is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{uv \,|\, u \in V(G), v \in V(H)\}$.

The following Table 1.1 shows the authors contributing the Nordhaus–Gaddum problem for distance–based parameters.

Distance-based Parameters	Authors contributing N-G Problem
Wiener index	Zhang and Wu [144]
	Das and Gutman [26]
	Li, Wu, Yang, and An [100]
Wiener-type invariant	Hamzeh, Hossein–Zadeh, and Ashrafi [74]
Wiener polarity index	Zhang and Hu [143]
	Hua and Das [83]
Hyper-Wiener index	Zhang, Wu, and An [145]
	Su, Xiong, Sun, and Li [129]
Reverse Wiener Index	Cai and Zhou [13]
Reciprocal reverse Wiener index	Zhou, Yang, and Trinajstić [164]
Reciprocal complementary Wiener index	Zhou, Cai, and Trinajstić [155]
Steiner Wiener index	Mao, Wang, Gutman, and Li [113]
Harary index	Zhou, Cai, and Trinajstić [154]
	Das, Zhou, and Trinajstić [37]
Szeged index	Das and Gutman [27]
Vertex PI index	Das and Gutman [29]
Co-PI index	Su, Xiong, and Xu [131]
Second geometric-arithmetic index	Das, Gutman, and Furtula [32]
Third geometric-arithmetic index	Das, Gutman, and Furtula [31]
Eccentric distance sum	Hua, Zhang, and Xu [84]

Table 1.1. Distance–based parameters

1.1 Wiener index

The *Wiener index* is defined as the sum of ordinary distances of all pairs of vertices of the underlying graph, i.e., as

$$W(G) = \sum_{u,v \in V(G)} d(u,v)$$

and its mathematical theory is nowadays well elaborated. For details see the surveys [38, 141].

1.1.1 Norhaus–Gaddum type results

A tree is called a *double star* $S_{p,q}$ if it is obtained from S_p and S_q by connecting the center of S_p with that of S_q. Since the Wiener index is connected with the distance of vertices, the diameter is important for us to study the index. The following facts might be found in some graph theory textbook.

Lemma 1.1. [11] *Let G be a connected graph with the connected complement. Then*

(1) *if* $diam(G) > 3$*, then* $diam(\overline{G}) = 2$*;*

(2) *if* $diam(G) = 3$*, then* $\overline{G}$ *has a spanning subgraph which ia s double star.*

Proof. (1) is an easy exercise. To prove (2), we take two vertices u, v in G such that $d_G(u, v) = 3$. Then, $w \notin N_G(u) \cap N_G(v)$ for any vertex $w \in V(G)\backslash\{u, v\}$, which means $w \in N_{\overline{G}}(u) \cup N_{\overline{G}}(v)$ in $\overline{G}$. Therefore, $\overline{G}$ contains a spanning double star whose two centers are u and v. ■

Entringer, Jackson, and Snyder [44] obtained the following result for trees.

Lemma 1.2. [44] *Among all trees with* n *vertices,* P_n *is the unique extremal structure with the largest Wiener index.*

Note that P_4 is the unique graph of order 4 whose complement is connected, and $\overline{P}_4 \cong P_4$. So, $W(P_4) + W(\overline{P}_4) = 2W(P_4) = 20$. Next, we calculate the value of $W(P_n) + W(\overline{P}_n)$ for $n \geq 5$. Let $P_n = v_1v_2\cdots v_n$. Then $d_{P_n}(v_i, v_{i+k}) = k$ for $i = 1, 2, \cdots, n-k$ and those pairs of vertices are all the pairs with distance k in P_n. Therefore,

$$W(P_n) = \sum_{i=1}^{n-1} i(n-i) = n\sum_{i=1}^{n-1} i - \sum_{i=1}^{n-1} i^2 = \frac{n^3-n}{6}.$$

On the other hand, since $diam(\overline{P}_n) = 2$, it follows that $W(\overline{P}_n) = e(\overline{P}_n) + 2e(P_n) = [\binom{n}{2} - (n-1)] + 2(n-1) = \frac{n^2}{2} + \frac{n}{2} - 1$. Hence, $W(P_n) + W(\overline{P}_n) = \frac{n^3-n}{6} + \frac{n^2}{2} + \frac{n}{2} - 1 = \frac{n^3+3n^2+2n-6}{6}$.

Lemma 1.3. [144] *Let* $G \in \mathcal{G}(n)$ $(n \geq 5)$ *be a graph. If* $diam(\overline{G}) = 2$*, then*

$$W(G) + W(\overline{G}) \leq W(P_n) + W(\overline{P}_n).$$

Proof. Let T be a spanning tree of G. Then $\overline{G}$ ia a spanning subgraph of $\overline{T}$ has diameter 2. Therefore, $W(G) + W(\overline{G}) - W(\overline{T}) = W(G) + (e(\overline{T}) - e(\overline{G})) = W(G) + (e(G) - e(T)) \leq W(T) \leq W(P_n)$ by Lemma 1.2. ■

In [144], Zhang and Wu studied the Nordhaus–Gaddum problem for the Wiener index.

Theorem 1.1. [144] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected graph. Then*

$$3\binom{n}{2} \leq W(G) + W(\overline{G}) \leq \frac{1}{6}(n^3 + 3n^2 + 2n - 6)\,. \tag{1}$$

Proof. The lower bound is immediate from

$$W(G) + W(\overline{G}) \geq (e(G) + 2e(\overline{G})) + (e(\overline{G}) + 2e(G)) = 3\binom{n}{2}.$$

For the upper bound, it remains to consider the case $diam(G) = diam(\overline{G}) = 3$ in view of Lemmas 1.1 and 1.3. Let s_i be the number of pair of vertices with distance i in G, for $i = 1, 2, 3$, and $\overline{s}_i$ be that in $\overline{G}$. Then $W(G)+W(\overline{G}) = \sum_{i=1}^{3} i(s_i+\overline{s}_i) = s_1+\overline{s}_1+2(s_2+\overline{s}_2+s_3+\overline{s}_3)+s_3+\overline{s}_3 = 3\binom{n}{2}+s_3+\overline{s}_3$. By Lemma 1.1, let S_{p_1,q_1} be spanning subgraph of G and S_{p_2,q_2} be that of $\overline{G}$, where $p_i + q_j = n$ for $j = 1, 2$. Hence, $s_3 \leq (p_1 - 1)(q_1 - 1) = p_1q_1 - n + 1$ and $\overline{s}_3 \leq p_2q_2 - n + 1$. Since $p_iq_i \leq g(n)$ for $i = 1$ and 2, where $g(n) = \frac{n^2}{4}$ if n is even, and otherwise $\frac{n^2-1}{4}$, we have $s_3 \leq g(n) - n + 1$ and $\overline{s}_3 \leq g(n) - n + 1$, and thus $W(G) + W(\overline{G}) \leq 3\binom{n}{2} + 2(g(n) - n + 1)$. One can easy to check that $3\binom{n}{2} + 2(g(n) - n + 1) \leq \frac{n^3+3n^2+2n-6}{6}$ if $n \geq 5$. This completes the proof. ■

Note that bounds are sharp. Obviously. the upper bound can be obtained on the graph P_n. To see the lower bound is best possible,we construct a sequence of graphs. Let G_n be a graph of order n,which is obtained from C_5 by replacing a vertex of C_5 by complete graph of order $n - 4$. It is easy to see that $diam(G_n) = diam(\overline{G}_n) = 2$ and so $W(G_n) + W(\overline{G}_n) = 3\binom{n}{2}$.

1.1.2 Norhaus–Gaddum type results in terms of diameter, size and order

Denote by G^* a graph of diameter d ($3 \leq d \leq 4$ and $|V(G^*)| \geq d + 2$), having the following property. Let P_{d+1} be a $(d + 1)$-vertex path contained in G^*. Then for any vertex $v_i \in V(G^*) \setminus V(P_{d+1})$ and for any vertex $v_j \in V(G^*)$, $j \neq i$, it should be either $d_{G^*}(v_i, v_j) = 1$ or $d_{G^*}(v_i, v_j) = 2$. In Table 1.2 are depicted two examples of G^*-type graphs.

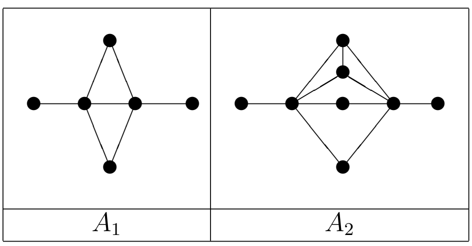

Table 1.2 Two graphs of G^* type.

Das and Gutman [26] gave lower and upper bounds for the Wiener index in terms of the number of vertices n, the number of edges m, and the diameter d.

Lemma 1.4. [26] *Let $G \in \mathcal{G}(n, m)$ $(n \geq 2)$ be a connected graph with diameter d. Then*

$$W(G) \geq \frac{1}{6}(d - 2)(d - 1) + n(n - 1) - m, \tag{2}$$

and

$$W(G) \leq \frac{1}{2}n(n-1)d - \frac{1}{3}(d-2)(d-1) - (d-1)m, \tag{3}$$

Equality in (2) holds if and only if G is a graph of diameter at most 2 or $G \cong P_n$ or G is isomorphic to some G^*. Equality in (3) holds if and only if G is a graph of diameter at most 2 or $G \cong P_n$.

By the above bound, they obtained a lower bound for $W(G) + W(\overline{G})$.

Theorem 1.2. [26] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph with diameter d. Then*

$$W(G) + W(\overline{G}) \geq \frac{3n(n-1)}{2} + \frac{1}{6}(d-2)(d-1)d, \tag{4}$$

with equality holding in (4) if and only if G is a graph of diameter 2 or $G \cong P_n$ or G is isomorphic to some G^* and $\overline{G}$ is a graph of diameter 2.

Proof. Using (2) from Lemma 1.4, we arrive at

$$W(G) + W(\overline{G}) \geq 2n(n-1) - (m + \overline{m}) + \frac{1}{6}(d-2)(d-1)d + \frac{1}{6}(\overline{d}-2)(\overline{d}-1)\overline{d}, \tag{5}$$

where $\overline{m}$ and $\overline{d}$ are, respectively, the number of edges and diameter of $\overline{G}$. Since $(m + \overline{m}) = \frac{n(n-1)}{2}$, $(\overline{d}-2)(\overline{d}-1)\overline{d} \geq 0$, we get (4) from (5).

Suppose now that equality holds in (4). Then all inequalities in the above argument must be equalities. Then from equality in (5) we conclude that G is a graph of diameter 2 or $G \cong P_n$ or G is isomorphic to some G^*, and $\overline{G}$ is a graph of diameter 2 or $G \cong P_n$ or G is isomorphic to some G^*, from equality holds in (4), we get $\overline{d} \leq 2$. Hence G is a graph of diameter 2 or $G \cong P_n$ or G is isomorphic to some G^* and $\overline{G}$ is a graph of diameter 2.

Conversely, let G be a graph of diameter 2 and let $\overline{G}$ be a graph of diameter 2. So $d = \overline{d} = 2$, and thus

$$W(G) + W(\overline{G}) = n(n-1) - m + n(n-1) - \overline{m} = \frac{3}{2}n(n-1)$$

as $m + \overline{m} = \frac{n(n-1)}{2}$.

Let $G \cong P_n$ and let $\overline{G}$ be a graph of diameter 2. For $\overline{d} = 2$ and $d = 3$,

$$W(G) + W(\overline{G}) = n(n-1) - m + 1 + n(n-1) - \overline{m} = \frac{3}{2}n(n-1) + 1$$

whereas for $\overline{d} = 2$ and $d = 4$,

$$W(G) + W(\overline{G}) = n(n-1) - m + 4 + n(n-1) - \overline{m} = \frac{3}{2}n(n-1) + 4.$$

Hence the theorem. ■

Remark 1.1. [26] *One can easily check that our lower bound in (4) on $W(G) + W(\overline{G})$ is always better than (1) as $(d-2)(d-1)d \geq 0$.*

An upper bound for $W(G) + W(\overline{G})$ in terms of the number of vertices n, and diameters d, $\bar{d}$ of G and $\overline{G}$, respectively, is also obtained.

Theorem 1.3. [26] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph with a connected $\overline{G}$. If $k = \max\{d, \bar{d}\}$, then*

$$W(G) + W(\overline{G}) \leq \frac{n(n-1)}{2}(k+1) - \frac{1}{3}(k-2)(k-1)k, \tag{6}$$

where d and $\bar{d}$ are the diameters of G and $\overline{G}$, respectively. Moreover, equality holds if and only if both G and $\overline{G}$ have diameter 2.

Proof. We start by (3). Since G and $\overline{G}$ are connected, it follows that $d, \bar{d} \geq 2$. Without loss of generality, we can assume that $d \geq \bar{d}$. So we have $k = d$. Let $\overline{m}$ be the number of edges of $\overline{G}$. Then

$$\begin{aligned} W(G) + W(\overline{G}) &\leq \frac{n(n-1)(d+\bar{d})}{2} - \frac{(d-2)(d-1)d}{3} - \frac{(\bar{d}-2)(\bar{d}-1)\bar{d}}{3} \\ &\quad - (d-1)m - (\bar{d}-1)\overline{m} \qquad (7) \\ &= \frac{n(n-1)(d+\bar{d}+1)}{2} - \frac{(d-2)(d-1)d}{3} - \frac{(\bar{d}-2)(\bar{d}-1)\bar{d}}{3} \\ &\quad - dm - \bar{d}\left(\frac{n(n-1)}{2} - m\right) \quad \text{as } m + \overline{m} = \frac{n(n-1)}{2}, \\ &= \frac{n(n-1)(d+1)}{2} - \frac{(d-2)(d-1)d}{3} - \frac{(\bar{d}-2)(\bar{d}-1)\bar{d}}{3} - m(d-\bar{d}) \\ &\leq \frac{n(n-1)(k+1)}{2} - \frac{(k-2)(k-1)k}{3} \quad \text{as } k = d \text{ and } d \geq \bar{d}. \qquad (8) \end{aligned}$$

Now supposed that the equality in (6). Then (7) and (8) hold. From (7), we conclude that G is a graph of diameter at most 2 or $G \cong P_n$ and that $\overline{G}$ is a graph of diameter at most 2 or $G \cong P_n$. From (8), we must have $k = d = \bar{d}$ and $\bar{d} \leq 2$. Hence both G and $\overline{G}$ have diameter 2.

Conversely, one can easily see that the equality in (6) if G and $\overline{G}$ have diameter 2. ■

Remark 1.2. [26] *For $k \leq \frac{n}{3}$, we have*

$$\frac{n^3 + 3n^2 + 2n - 6}{6} \geq \frac{n(n-1)(k+1)}{2}.$$

From this we conclude that the upper bound (6) is always better than the upper bound (1), provided $k \leq \frac{n}{3}$.

Remark 1.3. [26] *The lower and upper bounds given by (4) and (6), respectively, are equal when both G and $\overline{G}$ have diameter 2.*

1.1.3 Generalized Norhaus–Gaddum type results

Theorem 1.1 indicates that for any $n \geq 5$ and 2-decomposition (G_1, G_2) of K_n, if G_1 and G_2 are connected, then $3\binom{n}{2} \leq W(G) + W(\overline{G}) \leq \frac{1}{6}(n^3 + 3n^2 + 2n - 6)$.

Later, Li, Wu, Yang, and An [100] turned their attention to the generalized Nordhaus–Gaddum problem.

The following result, due to Erdös, Pach, Pollack, and Tuza, is crucial.

Lemma 1.5. [45] *For a connected graph $G \in \mathcal{G}(n)$,*

$$diam(G) \le \frac{3n}{\delta(G)+1} - 1.$$

Lemma 1.6. [100] *Let $G \in \mathcal{G}(n)$ be a simple graph. If $\delta(G) \ge n/2$, then $diam(G) \le 2$.*

In [44], Entringer, Jackson, and Snyder got the following result.

Lemma 1.7. [44] *For a connected graph $G \in \mathcal{G}(n)$, $W(G) \le \frac{n^3-n}{6}$, with equality if and only if $G \cong P_n$.*

For a fixed positive integer n, define a function

$$f(x_1, x_2) = \sum_{i=1}^{2} \left(\frac{x_i(n - x_i + 2)^2}{2} + \frac{(n - x_i + 2)^3}{2} \right).$$

Lemma 1.8. [100] *Let G_1 and G_2 be two connected graphs with the same vertex set and $E(G_1) \cap E(G_2) = \emptyset$. If $\Delta(G_1) + \Delta(G_2) \ge c$ for some positive real number c, then*

$$W(G_1) + W(G_2) < 2n^2 + f\left(\frac{c}{2}, \frac{c}{2}\right).$$

For two positive integers n, d with $n > d$, $T_{n,d}$ denotes the graph obtained from identifying a leaf of the star $K_{1,d}$ with that of P_{n-d}. It is trivial to see that $\Delta(T_{n,d}) = d$ if $d \ge 2$, and the order of $T_{n,d}$ is n, and that if $d = 2$, $T_{n,d} \cong P_n$. By an easy calculation, $W(T_{n,d})$ is equal to

$$(d-1)(d-2) + \frac{(d-1)(n-d+1)(n-d+2)}{2} + \frac{(n-d+1)^3 - (n-d+1)}{6}.$$

For convenience, set $g(n, d) = W(T_{n,d})$ in squeal. Observe that $g(n, d) \ge g(n, d + 1)$ whenever $2 \le d < n - 1$.

Lemma 1.9. [100] *For a connected graph $G \in \mathcal{G}(n)$ and $\Delta(G) \ge d \ge 2$, $W(G) \le g(n, d)$, with equality if and only if $G \cong T_{n,d}$.*

Li, Wu, Yang, and An [100] obtained the Nordhaus–Gaddum-type results for Wiener index of graphs when decomposing into three parts.

Theorem 1.4. [100] *Let K_n be the complete graph of order n. Assume that (G_1, G_2, G_3) is a 3-decomposition of K_n such that G_i is connected for each $i = 1, 2, 3$. Then for any sufficiently large n,*

$$5\binom{n}{2} \le \sum_{i=1}^{3} W(G_i) \le \frac{n^3-n}{3} + \binom{n}{2} + 2(n-1).$$

Proof. We only give the proof of the upper bound. Let us consider the following cases.

Case 1. $\delta(G_i) \ge 18$ and $\delta(G_j) \ge 18$ for some two distinct $i, j \in \{1, 2, 3\}$.

By Lemma 1.5, we have $diam(G_i) \le \frac{3n}{\delta(G_i)+1} \le \frac{3n}{19}$ and $diam(G_j) \le \frac{3n}{\delta(G_j)+1} \le \frac{3n}{19}$, and hence $W(G_i) \le \frac{1}{2}n(n-1) \times \frac{3n}{19}$, $W(G_j) \le \frac{1}{2}n(n-1) \times \frac{3n}{19}$. Hence, for any $n \ge \Delta(G) + 1 \ge 19$, we have

$$\sum_{i=1}^{3} W(G_i) < 2 \times \frac{1}{2}n(n-1) \times \frac{3n}{19} + \frac{n^3-n}{6} < \frac{n^3-n}{3}.$$

Case 2. There is exactly one G_i with $\delta(G_i) \geq 18$.

Without loss of generality, we assume that $\max\{\delta(G_1), \delta(G_2\} \leq 18$ and $\delta(G_3) \geq 18$. If $\delta(G_3) \geq \frac{n}{2}$, then it follows from Lemma 1.6 that $diam(G_3) = 2$. Then

$$\begin{aligned} \sum_{i=1}^{3} W(G_i) &= W(G_1) + W(G_2) + 2\binom{n}{2} - e(G_3) \\ &\leq W(G_1) + W(G_2) + 2\binom{n}{2} + e(G_1) + e(G_2) \\ &\leq W(P_n) + W(P_n) + 2\binom{n}{2} + e(P_n) + e(P_n) \\ &\leq \frac{n^3 - n}{3} + \binom{n}{2} + 2(n-1). \end{aligned}$$

The above second inequality follows from the observation below and Lemma 1.7. If one of G_1 and G_2, say G_1, contains a cycle, then $G_1 - e_1$ is connected (where e_1 is an edge on the cycle) and $W(G_1 - e_1) > W(G_1)$, and thus

$$W(G_1) + e(G_1) \leq W(G_1 - e_1) + e(G_1 - e_1).$$

If $\frac{n}{5} \leq \delta(G_3) < \frac{n}{2}$, then it follows from Lemma 1.5 that $diam(G_3) \leq \frac{3n}{\frac{n}{5}+1} \leq 15$. On the other hand, $\Delta(G_1) + \Delta(G_2) \geq n - 1 - \delta(G_3) > \frac{n}{2} - 1$, and hence $\Delta(G_1) + \Delta(G_2) \geq \frac{n-1}{2}$. By Lemma 1.8, we have

$$\begin{aligned} W(G_1) + W(G_2) &< 2n^2 + f\left(\frac{n-1}{4}, \frac{n-1}{4}\right) \\ &\leq 2n^2 + 2 \times \left(\frac{1}{2} \cdot \frac{n}{4} \cdot \left(\frac{3n}{4}\right)^2 + \frac{1}{6} \cdot \left(\frac{3n}{4}\right)^3 + o(n^3)\right) = \frac{9}{32}n^3 + o(n^3). \end{aligned}$$

Hence, for large enough n,

$$\sum_{i=1}^{3} W(G_i) \leq \frac{9}{32}n^3 + o(n^3) + \binom{n}{2} \times 15 < \frac{n^3 - n}{3}.$$

If $18 \leq \delta(G_3) < \frac{n}{5}$, then $\Delta(G_1) + \Delta(G_2) \geq n - \lfloor \frac{n}{5} \rfloor - 1$, and since $f(\frac{2n}{5}, \frac{2n}{5}) = (\frac{1}{2} \cdot \frac{2n}{5}(\frac{3n}{5})^2 + \frac{1}{6} \cdot (\frac{3n}{5})^3 + o(n^3)) \times 2 = \frac{27}{125}n^3$, by Lemma 1.8, we have

$$W((G_1) + W((G_2) < 2n^2 + f\left(\frac{2n}{5}, \frac{2n}{5}\right) = \frac{27}{125}n^3 + o(n^3).$$

Hence, for large enough n,

$$\begin{aligned} \sum_{i=1}^{3} W(G_i) &< 2n^2 + f\left(\frac{2n}{5}, \frac{2n}{5}\right) + W(G_3) \leq \frac{27}{125}n^3 + o(n^3) + \binom{n}{2} \times \frac{3n}{19} \\ &\leq \frac{27}{125}n^3 + o(n^3) + \frac{3}{38}n^3 < \frac{n^3 - n}{3}. \end{aligned}$$

Case 3. $\max\{\delta(G_1), \delta(G_2), \delta(G_3)\} \leq 17$.

Without loss of generality, we suppose $\Delta(G_1) \geq \Delta(G_2) \geq \Delta(G_3)$. Then

$$\begin{aligned}\Delta(G_1)+\Delta(G_2) &\geq n-1-\delta(G_3) \geq n-18,\\ \Delta(G_2)+\Delta(G_3) &\geq n-1-\delta(G_1) \geq n-18,\end{aligned}$$

and $\Delta(G_1) \geq \Delta(G_2) \geq \frac{n}{2}-9$.

If $\Delta(G_3) \geq \frac{n}{2}$, then it follows from Lemma 1.9 that

$$\begin{aligned}W(G_i) &\leq W(T_{n,\Delta(G_i)}) = g(n,\Delta(G_i)) < n^2 + \frac{\frac{n}{2}(n-\frac{n}{2}+2)^2}{2} + \frac{(n-\frac{n}{2}+2)^3}{6}\\ &= \frac{1}{12}n^3 + o(n^3).\end{aligned}$$

So, for large enough n,

$$\sum_{i=1}^{3} W(G_i) \leq 3W(T_{n,\Delta(G_i)}) \leq \frac{1}{4}n^3 + o(n^3) < \frac{n^3-n}{3}.$$

If $\frac{n}{5} \leq \Delta(G_3) < \frac{n}{2}$, then it follows from Lemma 1.9 that

$$\sum_{i=1}^{3} W(G_i) \leq \sum_{i=1}^{3} W(T_{n,\Delta(G_i)}) \leq 2W(T_{n,\lfloor\frac{n}{2}-9\rfloor}) + W(T_{n,\lfloor\frac{n}{5}\rfloor}) < 0.318n^3 + o(n^3) < \frac{n^3-n}{3}.$$

Suppose $\Delta(G_3) < \frac{n}{5}$. Let v_1 be a vertex of G_1 with $d_{G_1}(v_1) = \delta(G_1)$. Then

$$n-1 = d_{G_1}(v_1) + d_{G_2}(v_1) + d_{G_3}(v_1) \leq d_{G_1}(v_1) + d_{G_2}(v_1) + \Delta(G_3),$$

and thus

$$d_{G_2}(v_1) \geq n-1-\Delta(G_3) - d_{G_1}(v_1) > \frac{4n}{5} - 18,$$

so $\Delta(G_1) \geq \Delta(G_2) \geq d_{G_2}(v_1) > \frac{4n}{5} - 18$.

From Lemma 1.9, for large enough n, we have

$$\sum_{i=1}^{3} W(G_i) \leq \sum_{i=1}^{3} W(T_{n,\Delta(G_i)}) \leq 2W(T_{n,\lfloor\frac{4n}{5}-18\rfloor}) + W(P_n) < \frac{13}{375}n^3 + \frac{n^3-n}{6} + o(n^3) < \frac{n^3-n}{3}.$$

The proof is now complete. ■

1.2 Hyper–Wiener index

The *hyper-Wiener index* WW is one of the distance-based graph invariants [126]

$$WW = WW(G) = \frac{1}{2}W(G) + \frac{1}{2}W_2(G),$$

where $W_2(G) = \sum_{\{u,v\}\in V(G)} d_G(u,v)^2$.

1.2.1 Norhaus–Gaddum type results

Zhang, Wu, and An [145] showed that

Theorem 1.5. [145] *Let $G \in \mathcal{G}(n)$ be a connected graph. Then for any sufficiently large n, we have*

$$4\binom{n}{2} \leq WW(G) + WW(\overline{G}) \leq 2\binom{n+4}{4}.$$

The lower and the upper bounds are sharp.

1.2.2 Generalized Norhaus–Gaddum type results

In [129], Su, Xiong, Sun, and Li presented the following result.

Theorem 1.6. [129] *Let (G_1, G_2, G_3) be a 3-decomposition of K_n such that each cell G_i is connected. Then for any $n \geq 70$, we have*

$$7\binom{n}{2} \leq WW(G_1) + WW(G_2) + WW(G_3) \leq 2\binom{n+2}{4} + \binom{n}{2} + 4(n-1),$$

with right equality if and only $G_1 = G_2 = P_n$, and with left equality if and only $diam(G_1) = diam(G_2) = 2$.

To complete the proof, we need the following auxiliary results.

Lemma 1.10. [129] *Let (G_1, G_2, G_3) be a 3-decomposition of K_n such that each cell G_i is connected. Then there exists at most one cell G_i with $\delta(G_i) \geq \frac{n}{2}$.*

Lemma 1.11. [129] *Let G be a connected non-complete graph and e be its non-cut-edge. Then*

$$WW(G-e) + 2e(G-e) \geq WW(G) + 2e(G).$$

Lemma 1.12. [68] *Let T be a tree with order n. Then $WW(S_n) \leq WW(T) \leq WW(P_n)$.*

Lemma 1.13. [109] *Let G' be a connected spanning subgraph of G. Then $WW(G) \leq WW(G')$.*

Let $G_{n,d}$ denote the graph with order n and diameter $d \geq 2$, and $e_i(G)$ the number of pairs of vertices whose distance is i for $1 \leq i \leq d$ in G, thus $e_1(G)$ is the number of edges of G.

Lemma 1.14. [129] *$WW(G_{n,d}) \geq WW(G_{n,2})$ holds for $d \geq 2$.*

Lemma 1.15. [129] *Let (G_1, G_2, G_3) be a 3-decomposition of K_n such that each cell G_i is connected. Then $\Delta(G_i) + \Delta(G_j) \geq n - 1 - \delta(G_k)$.*

Lemma 1.16. [129] *Let G_1 and G_2 be two connected edge-disjoint graphs with the same order n. If $\Delta(G_1) + \Delta(G_2) \geq c$ for some positive real number c, then $WW(G_1) + WW(G_2) < 3n^2 + \frac{1}{2}\sigma(\frac{c}{2}, \frac{c}{2})$, where $\sigma(x_1, x_2) = \sum_{i=1}^{2}[\frac{x_i(n-x_i+2)^2}{2} + \frac{(n-x_i+2)^3}{6} + \frac{x_i(n-x_i+2)^3}{3} + \frac{(n-x_i+2)^4}{12}]$.*

A *splice* $\binom{G_1:G_2}{a_1:a_2}$ of two connected graphs G_1 and G_2 is a graph obtained by identifying the vertices $a_1 \in V_1$ and $a_2 \in V_2$.

Let n and d be two integers with $n > d$, we denote $T_{n,d} = \binom{K_{1,d}:P_{n-d}}{b_1:b_2}$ the graph obtained from identifying a leaf b_1 of the star $K_{1,d}$ with a leaf b_2 of the path P_{n-d}. It is trivial to see that the graph $T_{n,d}$ has maximum degree d and order n. In particular, $T_{n,d} = P_n$ when $d = 2$.

Lemma 1.17. [129] *Let $G \in \mathcal{G}(n)$ be a connected graph with $\Delta(G) \geq d \geq 2$. Then $WW(G) \leq \Phi(n,d)$, with equality if and only if $G = T_{n,d}$, where $\Phi(n,d) = \frac{1}{2}W(T_{n,d}) + \frac{1}{2}W_2(T_{n,d})$ for $2 \leq d \leq n-1$.*

We are now in a position to give the proof of Theorem 1.6.

Proof of Theorem 1.6: Let us firstly prove the upper bound. For sake of simplicity, let

$$\mathcal{P}(n) = 2\binom{n+2}{4} + \binom{n}{2} + 4(n-1) = \frac{n^4 + 2n^3 + 5n^2 + 40n - 48}{12}.$$

We distinguish the following three cases:

Case 1. There exist at least two cells of $\{G_1, G_2, G_3\}$, say G_1, G_2. such that $\delta(G_i) \geq 11$ for $i \in \{1, 2\}$.

By Lemma 1.5, $diam(G_i) \leq \frac{3n}{\delta(G_i)+1} \leq \frac{n}{4}$, and then

$$WW(G_i) = \frac{1}{2}W(G_i) + \frac{1}{2}W_2(G_i) \leq \frac{1}{2} \cdot \binom{n}{2} \cdot \frac{n}{4} + \frac{1}{2} \cdot \binom{n}{2} \cdot \frac{n^2}{16} = \frac{1}{64}n^4 + \frac{3}{64}n^3 - \frac{1}{16}n^2.$$

Hence, for any $n \geq \Delta(G) + 1 \geq 12$, we have

$$\begin{aligned} WW(G_1) + WW(G_2) + WW(G_3) &\leq \frac{7}{96}n^4 + \frac{17}{96}n^3 - \frac{1}{6}n^2 - \frac{1}{12}n \\ &< \frac{n^4 + 2n^3 + 5n^2 + 40n - 48}{12} = \mathcal{P}(n). \end{aligned}$$

Case 2. There is exactly one cell of $\{G_1, G_2, G_3\}$, say G_3, such that $\delta(G_3) \geq 11$.

We consider the following two subcases.

Subcase 2.1. $\delta(G_3) \geq \frac{n}{2}$.

By Lemmas 1.6 and 1.10, we have $diam(G_3) \leq 2$. Then it is obvious that

$$\begin{aligned} WW(G_1) + WW(G_2) &+ WW(G_3) = WW(G_1) + WW(G_2) + \frac{1}{2}W(G_3) + \frac{1}{2}W_2(G_3) \\ &= WW(G_1) + WW(G_2) + 3\binom{n}{2} - 2e(G_3) \\ &= WW(G_1) + WW(G_2) + \binom{n}{2} + 2e(G_1) + 2e(G_2). \end{aligned}$$

Let $\mathcal{Q}(n, G_1, G_2)$ be the last expression in the above equation. Let T_i be a spanning tree of G_i. Then T_i can be obtained from G_i by deleting $t = m - n + 1$ edges in order, say $e_{i,1}, e_{i,2}, \cdots, e_{i,t}$, of graph G_i outside of T_i for $i = 1, 2$. By applying Lemma 1.11 to G_i, for $1 \leq l \leq t$ we have

$$WW(G_1 - e_{1,l}) + 2e(G_1 - e_{1,l}) \geq WW(G_1) + 2e(G_1)$$

and

$$WW(G_2 - e_{2,l}) + 2e(G_2 - e_{2,l}) \geq WW(G_2) + 2e(G_2).$$

Thus by Lemmas 1.11 and 1.12, we have

$$\begin{aligned}
\mathcal{Q}(n \mid G_1, G_2) &\leq [WW(G_1 - e_{11}) + 2e(G_1)] + [WW(G_2 - e_{21}) + 2e(G_2)] + \binom{n}{2} \\
&\leq \cdots\cdots \\
&\leq [WW(T_1) + 2(n-1)] + [WW(T_2) + 2(n-1)] + \binom{n}{2} \\
&\leq [WW(P_n) + 2(n-1)] + [WW(P_n) + 2(n-1)] + \binom{n}{2} \\
&= 2WW(P_n) + \binom{n}{2} + 4(n-1) = \mathcal{P}(n).
\end{aligned}$$

Subcase 2.2. $11 \leq \delta(G_3) < \frac{n}{2}$.

By Lemma 1.15, we have $\Delta(G_1) + \Delta(G_2) \geq \frac{n-1}{2}$, thus by Lemma 1.16,

$$\begin{aligned}
WW(G_1) + WW(G_2) &< 3n^2 + \frac{1}{2}\sigma\left(\frac{n-1}{4}, \frac{n-1}{4}\right) \\
&= 3n^2 + \frac{1}{6}\left(\frac{3}{2}n + \frac{3}{2}\right)\left(\frac{3}{4}n + \frac{9}{4}\right)^2 + \frac{1}{12}\left(\frac{7}{4}n + \frac{5}{4}\right)\left(\frac{3}{4}n + \frac{9}{4}\right)^3 \\
&= \frac{1}{12} \cdot \frac{189}{256}n^4 + \frac{576}{64}n^3 + \frac{2315}{64}n^2 + \frac{1701}{384}n + \frac{7533}{3072}.
\end{aligned}$$

On the other hand, $WW(G_3) = \frac{1}{64}n^4 + o(n^4)$, since $diam(G_3) \leq \frac{3n}{\delta(G_3)+1} \leq \frac{n}{4}$. Hence, for $n > 10$, we have

$$\begin{aligned}
WW(G_1) + WW(G_2) &+ WW(G_3) \\
&< \left(\frac{1}{12} \cdot \frac{189}{256} + \frac{1}{64}\right)n^4 + \frac{576}{64}n^3 + \frac{2315}{64}n^2 + \frac{1701}{384}n + \frac{7533}{3072} \\
&= \frac{1}{12} \cdot \frac{237}{256}n^4 + \frac{576}{64}n^3 + \frac{2315}{64}n^2 + \frac{1701}{384}n + \frac{7533}{3072} \\
&< \frac{n^4 + 2n^3 + 5n^2 + 40n - 48}{12} = \mathcal{P}(n).
\end{aligned}$$

Case 3. $\delta(G_i) < 11$ for $i = 1, 2, 3$.

Without loss of generality, suppose $\Delta(G_1) \geq \Delta(G_2) \geq \Delta(G_3)$. By Lemma 1.15, $\Delta(G_1) \geq \frac{n}{2} - 6$. We have the following possibilities.

Subcase 3.1. $\Delta(G_3) \geq \frac{n}{2} - 6$.

By Lemma 1.17, for $n > 36$ we have

$$\begin{aligned} WW(G_1)+WW(G_2)+WW(G_3) &\leq WW(T_{n,\Delta(G_1)})+WW(T_{n,\Delta(G_2)})+WW(T_{n,\Delta(G_3)}) \\ &= \Phi(T_{n,\Delta(G_1)})+\Phi(T_{n,\Delta(G_2)})+\Phi(T_{n,\Delta(G_3)}) \\ &\leq 3\left(\frac{5}{384}n^4+\frac{7}{12}n^3+\frac{69}{8}n^2-\frac{20}{3}n-\frac{1148}{3}\right) \\ &< \frac{n^4+2n^3+5n^2+40n-48}{12}=\mathcal{P}(n), \end{aligned}$$

since

$$\begin{aligned} WW(G_i) &\leq \Phi(T_{n,\Delta(G_i)})=\frac{1}{2}\Phi_1(T_{n,\Delta(G_i)})+\frac{1}{2}\Phi_2(T_{n,\Delta(G_i)}) \\ &\leq \frac{1}{2}\left(n^2+\frac{(\frac{n}{2}-6)(n-\frac{n}{2}+8)^2}{2}+\frac{(n-\frac{n}{2}+8)^3}{6}\right) \\ &\quad +\frac{1}{2}\left(2n^2+\frac{(\frac{n}{2}-6)(n-\frac{n}{2}+8)^3}{3}+\frac{(n-\frac{n}{2}+8)^4}{12}\right) \\ &= \frac{5}{384}n^4+\frac{7}{12}n^3+\frac{69}{8}n^2-\frac{20}{3}n-\frac{1148}{3}. \end{aligned}$$

Subcase 3.2. $\Delta(G_2) \geq \frac{n}{2}-6 > \Delta(G_3) \geq 10$.

By Lemma 1.17, we have

$$\begin{aligned} WW(T_{n,10}) &\leq \frac{1}{2}\Phi_1(n,10)+\frac{1}{2}\Phi_2(n,10) \\ &= \frac{1}{2}\left(9\cdot 8+\frac{9(n-9)(n-8)}{2}+\frac{(n-9)^3-(n-9)}{6}\right) \\ &\quad +\frac{1}{2}\left(2\cdot 9\cdot 8+\frac{9(n-9)(n-8)(2n-17)}{6}+\frac{(n-10)(n-8)(n-9)^2}{12}\right) \\ &= \frac{1}{24}n^4-\frac{4}{3}n^3+\frac{383}{24}n^2-\frac{1233}{12}n+378. \end{aligned}$$

Hence, for $n > 36$ we have

$$\begin{aligned} &WW(G_1)+WW(G_2)+WW(G_3) \\ \leq\ & WW(T_{n,\Delta(G_1)})+WW(T_{n,\Delta(G_2)})+WW(T_{n,\Delta(G_3)}) \\ \leq\ & 2WW(T_{n,\lfloor\frac{n}{2}-6\rfloor})+WW(T_{n,10}) \\ <\ & 2\left(\frac{5}{384}n^4+\frac{7}{12}n^3+\frac{69}{8}n^2-\frac{20}{3}n-\frac{1148}{3}\right) \\ &+\left(\frac{1}{24}n^4-\frac{4}{3}n^3+\frac{383}{24}n^2-\frac{1233}{12}n+378\right) \\ =\ & \frac{1}{12}\cdot\frac{13}{16}n^4-\frac{1}{6}n^3+\frac{797}{24}n^2-\frac{1393}{12}n-\frac{1162}{3} \\ <\ & \frac{n^4+2n^3+5n^2+40n-48}{12}=\mathcal{P}(n). \end{aligned}$$

Subcase 3.3. $\Delta(G_2) \geq \frac{n}{2} - 6 \geq 10 > \Delta(G_3)$.

By Lemma 1.17, for $n \geq 70$ we have

$$\begin{aligned}
WW(G_1) + WW(G_2) + WW(G_3) &\leq WW(T_{n,\Delta(G_1)}) + WW(T_{n,\Delta(G_2)}) + WW(P_n) \\
&\leq 2WW(T_{n,\lfloor \frac{n}{2} - 6 \rfloor}) + WW(P_n) \\
&= 2\left(\frac{5}{384}n^4 + \frac{7}{12}n^3 + \frac{69}{8}n^2 - \frac{20}{5}n - \frac{1148}{3}\right) \\
&\quad + \left(\frac{1}{24}n^4 + \frac{1}{12}n^3 - \frac{1}{24}n^2 - \frac{1}{12}n\right) \\
&= \frac{1}{12} \cdot \frac{13}{16}n^4 + \frac{5}{4}n^3 + \frac{413}{24}n^2 - \frac{161}{12}n \\
&< \frac{n^4 + 2n^3 + 5n^2 + 40n - 48}{12} = \mathcal{P}(n).
\end{aligned}$$

Subcase 3.4. $\Delta(G_1) \geq \frac{n}{2} - 6 > \Delta(G_2)$.

It is obvious that $\Delta(G_2) + \Delta(G_3) < n - 12$. By Lemma 1.15, we have $\Delta(G_2) + \Delta(G_3) \geq n - 1 - \delta(G_1) > n - 12$. Thus $\Delta(G_2) + \Delta(G_3) = n - 12$, hence $\Delta(G_1) \geq \frac{n}{2} - 6 > \Delta(G_2) \geq \frac{n}{2} - 6$. By the same arguments as Subcases 3.1 and 3.2, the proof can be obtained.

Finally, we consider the lower bound. By Lemma 1.14, we have

$$WW(G_1) + WW(G_2) + WW(G_3) \geq 9\binom{n}{2} - 2[e(G_1) + e(G_2) + e(G_3)] = 7\binom{n}{2}.$$

This completes the proof of Theorem 1.6, as desired. ■

The key contribution of their paper is the following. They introduced the concept of k-decomposition for a graph, and then presented the Nordhaus–Gaddum-type inequality of a 3-decomposition of K_n for the hyper-Wiener index. However, exploring the corresponding Nordhaus–Gaddum-type inequality of a k-decomposition is still an open problem for $k \geq 4$. We leaved those questions for future research.

Conjecture 1.1. [129] *Let $(G_1, G_2, \cdots, G_k)$ be a k-decomposition of K_n such that each cell G_i is connected. Then for any sufficiently large n with respect to k, we have*

$$(3k-2)\binom{n}{2} \leq WW(G_1) + WW(G_2) + \cdots + WW(G_k) \leq (k-1)\binom{n+2}{4} + \binom{n}{2} + 2(k-1)(n-1).$$

The lower and upper bounds are sharp.

If Conjecture 1.1 holds, we can extend Theorem 1.5 for arbitrarily large k. The upper bound is attained when $G_1 = G_2 = \cdots = G_{k-1} = P_n$, since if $\binom{n}{2} - (k-1)(n-1) \geq \frac{1}{2}n\delta(G_k) \geq \frac{n^2}{4}$, i.e.,

$k \leq \frac{n}{4}$, then by Lemma 1.6 we have $diam(G_k) = 2$ for any sufficiently large n. Hence

$$\begin{aligned}
& WW(G_1) + WW(G_2) + \cdots + WW(G_k) \\
= \; & WW(G_1) + WW(G_2) + \cdots + WW(G_{k-1}) + 3\binom{n}{2} - 2e(G_k) \\
= \; & [WW(G_1) + 2e(G_1)] + [WW(G_2) + 2e(G_2)] + \cdots + [WW(G_{k-1}) + 2e(G_{k-1})] + \binom{n}{2} \\
= \; & (k-1)WW(P_n) + 2(k-1)(n-1) + \binom{n}{2}.
\end{aligned}$$

The lower bound is trivial and is attained by any k-decomposition $(G_1, G_2, \cdots, G_k)$ of K_n with $diam(G_i) = 2$ for $i = 1, 2, \cdots, k$, this is because $WW(G_i) = 3\binom{n}{2} - 2e(G_i)$ and $\sum_{i=1}^{k} e(G_i)\binom{n}{2}$.

1.3 Wiener–type invariant

Let $d(G, k)$ be the number of pairs of vertices of G that are at distance k, and λ be a real number. Then

$$W_\lambda(G) = \sum_{k=1}^{d} d(G, k)k^\lambda,$$

where $d = diam(G)$ denotes the diameter of the graph G is called the *Wiener type invariant* of G associated to real number λ, see [61, 92] for details.

Hamzeh, Hossein-Zadeh, and Ashrafi [74] first derived a lower bound of $W_\lambda(G)$ for an incomplete connected graph.

Lemma 1.18. [74] *Let $G \in \mathcal{G}(n)$ $(n \geq 3)$ be an incomplete connected graph. Then*

$$W_\lambda(G) \geq (1 - 2^\lambda)|E(G)| + 2^\lambda \binom{n}{2}$$

with equality if and only if $diam(G) = 2$.

Next, they obtained the following Nordhaus–Gaddum-type result for Wiener-type invariant.

Theorem 1.7. [74] *Let $G \in \mathcal{G}(n)$ $(n \geq 3)$ be a connected incomplete graph with a connected complement $\overline{G}$. Then*

$$W_\lambda(G) + W_\lambda(\overline{G}) \geq \binom{n}{2}(1 + 2^\lambda)$$

with equality if and only if $diam(G) = diam(\overline{G}) = 2$.

Proof. From Lemma 1.18, we have

$$\begin{aligned}
W_\lambda(G) + W_\lambda(\overline{G}) \; & \geq \; (1 - 2^\lambda)|E(G)| + 2^\lambda \binom{n}{2} + (1 - 2^\lambda)|E(\overline{G})| + 2^\lambda \binom{n}{2} \\
& = \; (1 - 2^\lambda)(|E(G)| + |E(\overline{G})|) + 2^{\lambda+1} \binom{n}{2} \\
& = \; (1 - 2^\lambda)\binom{n}{2} + 2^{\lambda+1}\binom{n}{2} = \binom{n}{2}(1 + 2^\lambda),
\end{aligned}$$

as desired. ■

Proposition 1.1. [74] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected graph such that $diam(G) = diam(\overline{G}) = 3$. Then*

$$W_\lambda(G) + W_\lambda(\overline{G}) < \binom{n}{2}(1 + 3^\lambda).$$

Proof. Suppose $t_k = d(G, k)$ and $\bar{t}_k = d(\overline{G}, k)$. It is clear that $t_2 + t_3 = \bar{t}_1$, $\bar{t}_2 + \bar{t}_3 = t_1$ and $t_1 + \bar{t}_1 = \binom{n}{2}$. Then

$$\begin{aligned} W_\lambda(G) + W_\lambda(\overline{G}) &= \sum_{k=1}^{3}(t_k + \bar{t}_k)k^\lambda = (t_1 + \bar{t}_1) + 2^\lambda(t_2 + \bar{t}_2) + 3^\lambda(t_3 + \bar{t}_3) \\ &< \binom{n}{2} + 3^\lambda(t_2 + \bar{t}_2 + t_3 + \bar{t}_3) = \binom{n}{2}(1 + 3^\lambda), \end{aligned}$$

proving the proposition. ■

1.4 Wiener polarity index

The *Wiener polarity index* $W_p(G)$ is defined as

$$W_p(G) = |\{(u, v) \mid d_G(u, v) = 3,\ u, v \in V(G)\}|,$$

which is the number of unordered pairs of vertices u, v of G such that $d_G(u, v) = 3$. Inorganic compounds, say paraffin, the W_p is the number of pairs of carbon atoms separated by three carbon-carbon bonds. Wiener [137] used a linear formula of W and W_p to calculate the boiling points t_B of the paraffins, i.e.,

$$t_B = aW + bW_p + c,$$

where a, b, and c are constants for a given isomeric group.

1.4.1 Nordhaus–Gaddum–type inequalities in $\mathcal{G}(n)$

Zhang and Hu [143] presented the Nordhaus–Gaddum–type inequality of a graph G and its complement $\overline{G}$ in the case both $diam(G) = 3$ and $diam(\overline{G}) = 3$.

The following two facts are useful which can be found in graph theory textbook.

Lemma 1.19. [11] *Let G be a graph. If $diam(G) > 3$, then $diam(\overline{G}) < 3$.*

Note that $W_p(G) = 0$ for any G with $diam(G) \leq 2$. By Lemma 1.19, we always have $W_p(G) = 0$ or $W_p(\overline{G}) = 0$ when either $diam(G) \neq 3$ and $diam(\overline{G}) \neq 3$. Therefore, the authors first considered the case both $diam(G) = 3$ and $diam(\overline{G}) = 3$.

Lemma 1.20. [143] *If G be a graph with $diam(G) = 3$, then $\overline{G}$ contains a spanning double star whose two centers are u and v, where u and v are two vertices of G such that $d_G(u, v) = 3$.*

Proof. We consider two vertices u and v in G such that $d_G(u,v) = 3$. Then, $w \notin N_G(v) \cap N_G(u)$ for any vertex $w \in V(G)\backslash\{u,v\}$, and hence $w \in N_{\overline{G}}(v) \cup N_{\overline{G}}(u)$, as desired. ∎

Before proceeding, they introduced two sets. Let

$$S = \{v \in V(S_p) \,|\, \exists\, u \in V(S_q), d_G(u,v) = 3\},$$

and

$$T = \{u \in V(S_q) \,|\, \exists\, v \in V(S_p), d_G(v,u) = 3\},$$

where G is a graph having a spanning double star $S_{p,q}$.

Lemma 1.21. [143] *Let G be a graph with $diam(G) = 3$, $diam(\overline{G}) = 3$, and u, v be two arbitrary vertices of G. If $d_{\overline{G}}(u,v) = 3$, then neither u nor v is an end vertex of a diametrical path of G.*

Proof. Since $diam(\overline{G}) = 3$, it follows from Lemma 1.20 that G contains a double star $S_{p,q}$ indeed. Now we only need to demonstrate that $d_{\overline{G}}(u,v) \leq 2$ for any vertex $v \in S \cup T$ and for any vertex $u \in V(G)\backslash\{v\}$. If $d_G(u,v) = 2, 3$, then $d_{\overline{G}}(v,u) = 1$. If $d_G(v,u) = 1$, then there exists a vertex u_0 on distance 3 from v, since $v \in S \cup T$. By Lemma 1.20, we have $uu_0 \in E(\overline{G})$, and hence $d_{\overline{G}}(u,v) \leq 2$. ∎

For the sake of convenient, they gave two kinds of graphs.

- Denote by G^* the graph of order $n \geq 5$ obtained from a path P_4 by joining $n-4$ isolated vertices to each internal vertex of the path P_4 such that $V(G^*)\backslash V(P_4)$ is a clique.
- Let $S^*_{p,q}$,be a graph containing a double-star $S_{p,q}$ such that any two vertices both in $V(S_p)$ or those both in $V(S_q)$ may be adjacent.

From the definition of the Wiener polarity index, one can easily obtain

$$W_p(G^*) = 1,\ W_p(\overline{G}^*) = 1;$$

and

$$W_p(S^*_{p,q}) = (p-1)(q-1),\ W_p(\overline{S}^*_{p,q}) = 1.$$

Zhang and Hu gave the Nordhaus–Gaddum–type inequality for the Wiener polarity index for the main case:

Theorem 1.8. [143] *Let $G \in \mathcal{G}(n)$ $(n \geq 4)$ be a graph, and $\overline{G}$ be its complement. If $diam(G) = diam(\overline{G}) = 3$, then*

$$2 \leq W_p(G) + W_p(\overline{G}) \leq \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor - n + 2. \tag{9}$$

Moreover, the lower bound holds if and only if $G \cong P_4$ or G is isomorphic to some G^* ; the upper bound occurs if and only if G is isomorphic to some $S^*_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ or $\overline{G}$ is isomorphic to some $S^*_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Proof. Let $|S| = s$, $|T| = t$. Without loss of generality, we assume that $s \geq t \geq 1$. Therefore,

$$W_p(G) \leq st. \tag{10}$$

Note that equality in (10) holds if and only if $d_G(v,u) = 3$ for any vertex $v \in S$ and for any vertex $u \in T$. Suppose $v_0 \in S$, $u_0 \in T$ satisfying $d_G(v_0,u_0) = 3$, by the proof of Lemma 1.20, we have $w \in N_{\overline{G}}(v_0) \cap N_{\overline{G}}(u_0)$ for any vertex $w \in V(G) \setminus \{v_0, u_0\}$. Let

$$N_1 = \{w \in V \setminus (S \cup T) \,|\, wv_0 \notin E(G),\ wu_0 \in E(G)\}, |N_1| = n_1,$$

and

$$N_2 = \{w \in V \setminus (S \cup T) \,|\, wv_0 \in E(G),\ wu_0 \notin E(G)\}, |N_2| = n_2.$$

Obviously, $n_1 \geq 1$, $n_2 \geq 1$ and $n_1 + n_2 + s + t \leq n$. Without loss of generality, we assume that $n_1 \geq n_2$. By Lemma 1.21, we arrive at

$$W_p(\overline{G}) \leq n_1 n_2, \tag{11}$$

and the equality in (11) happens if and only if they are nonadjacent in $\overline{G}$ for any vertex in N_1 and for vertex in N_2.

Firstly, we consider the lower bound. It is obvious since $diam(G) = 3$ and $diam(\overline{G}) = 3$. By the inequality (10) and (11), the lower bound is obtained if and only if $W_p(G) = W_p(\overline{G}) = 1$, namely, $n_1 = n_2 = s = t = 1$. For $n = 4$, note that P_4 is the unique graph of order 4, whose complement also has has diameter 3, and that $\overline{P}_4 \cong P_4$. Thus, $W_p(P_4) + W_p(\overline{P}_4) = 2$. Otherwise, $n \geq 5$. Let P_4 be a path contained in graph G. Since $n_1 = n_2 = s = t = 1$, it follows that the remaining $n-4$ vertices are dajacent to each internal vertex of the path P_4. Therefore, G is isomorphic to some G^*.

Conversely, one can easily see that the lower bound holds for the path P_4 when $n = 4$ or for a graph G^*. Then we prove the upper bound. Using the inequality (10) and (11), we conclude

$$\begin{aligned} W_p(G) + W_p(\overline{G}) &\leq st + n_1 n_2 \leq st + \left\lceil \frac{n-s-t}{2} \right\rceil \left\lfloor \frac{n-s-t}{2} \right\rfloor \\ &= \begin{cases} st + \frac{n^2}{4} - \frac{n(s+t)}{2} + \frac{(s+t)^2}{4} & \text{if } n-s-t \text{ is even;} \\ st + \frac{n^2}{4} - \frac{n(s+t)}{2} + \frac{(s+t)^2}{4} - \frac{1}{4} & \text{if } n-s-t \text{ is odd.} \end{cases} \end{aligned}$$

Note that s and t are positive integers. Applying the average inequality, $st \leq \frac{(s+t)^2}{4}$ if $s+t$ is even, and $st \leq \frac{(s+t)^2}{4} - \frac{1}{4}$ if $s+t$ is odd. Therefore,

$$W_p(G) + W_p(\overline{G}) \leq \begin{cases} \frac{n^2}{4} - \frac{n(s+t)}{2} + \frac{(s+t)^2}{2} + 0 & \text{if } n \text{ is even and } s+t \text{ is even;} \\ \frac{n^2}{4} - \frac{n(s+t)}{2} + \frac{(s+t)^2}{2} - \frac{1}{2} & \text{if } n \text{ is even and } s+t \text{ is odd;} \\ \frac{n^2}{4} - \frac{n(s+t)}{2} + \frac{(s+t)^2}{2} - \frac{1}{4} & \text{if } n \text{ is odd.} \end{cases}$$

Let $f(x) = \frac{n^2}{4} - \frac{nx}{2} + \frac{x^2}{2}$ for $2 \leq x \leq n-2$. It is easy to see that the maximum of $f(x)$ is achieved at $x = 2$ or $x = n-2$. Simple calculation shows that $f(x) \leq f(2) = f(n-2)$. So,

$$\begin{aligned} W_p(G) + W_p(\overline{G}) &\leq \begin{cases} \frac{n^2}{4} - n + 2 & \text{if } n \text{ is even;} \\ \frac{n^2}{4} - n + \frac{7}{4} & \text{if } n \text{ is odd;} \end{cases} \\ &= \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor - n + 2. \end{aligned}$$

Now we consider the graphs which obtain the upper bound. If the upper bound holds, then all the inequalities discussed above must be equalities. Hence (i) $n_1 = n_2 = 1, s = \lceil \frac{n-2}{2} \rceil$, and $t = \lfloor \frac{n-2}{2} \rfloor$ or (ii) $s = t = 1, n_1 = \lceil \frac{n-2}{2} \rceil$ and $n_2 = \lfloor \frac{n-2}{2} \rfloor$. Meanwhile, it is $d_G(v, u) = 3$ for any vertex $v \in S$ and for any vertex $u \in T$, and they are nonadjacent in $\overline{G}$ for any vertex in N_1 and for any vertex in N_2. Those imply that G is isomorphic to some $S^*_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$, or $\overline{G}$ is isomorphic to some $S^*_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Conversely, simple calculation shows that the upper bound holds in Theorem 1.8 if G is isomorphic to some $S^*_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ or $\overline{G}$ is isomorphic to some $S^*_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. ■

Remark 1.4. [143] *The lower and upper bounds given in Theorem 1.8 are equal when* $n = 4$.

Zhang and Hu [143] studied the Nordhaus–Gaddum-type inequality for any connected graph G with a connected complement $\overline{G}$.

Theorem 1.9. [143] *Let* $G \in \mathcal{G}(n)$ $(n \geq 4)$ *be a connected graph, and* $\overline{G}$ *be its connected complement. If* $d = 3$ *and* $\overline{d} = 3$*, then*

$$2 \leq W_p(G) + W_p(\overline{G}) \leq \begin{cases} \lceil \frac{n}{2} \rceil \lfloor \frac{n}{2} \rfloor - n + 2, & \text{if } n \leq 8 \\ \left\lfloor \frac{(n-3)^2}{3} \right\rfloor, & \text{if } n \geq 9. \end{cases}$$

for any unicyclic graph of order n.

1.4.2 Nordhaus–Gaddum–type inequalities in $\mathcal{G}(n, m)$

Let H_{n-4} be any graph of order $n-4$. Denote by G^{**} the graph of order $n \geq 5$ obtained from a path P_4 by joining each vertex of H_{n-4} to each internal vertex of the path P_4 such that $V(G^{**}) \setminus V(P_4) = V(H_{n-4})$.

In [83], Hua and Das had the following remark.

Remark 1.5. [83] *In Theorem 1.8, the lower bound occurs in (9) if and only if* $G \cong P_4$ *or* G *is isomorphic to some* G^**. But the extremal graphs in this characterization is not clear. It should be the following:*

The lower bound occurs in (9) if and only if $G \cong P_4$ *or* $G \cong G^{**}$*.*

In general, the lower bound on $W_p(G) + W_p(\overline{G})$ *is the following [143]:*

$$W_p(G) + W_p(\overline{G}) \geq 0$$

with equality if and only if both $d = 2$ *and* $\overline{d} = 2$*.*

Hua and Das first gave a lower bound on $W_p(G) + W_p(\overline{G})$:

Theorem 1.10. [83] *Let* G *be a connected graph with a connected complement* $\overline{G}$*. Then*

$$W_p(G) + W_p(\overline{G}) \geq d + \overline{d} - 4, \tag{12}$$

where d *and* $\overline{d}$ *are the diameter of* G *and* $\overline{G}$*, respectively. Moreover, the equality holds in (12) if and only if* $G \cong P_n$ *or* $G \cong G^{**}$ *or* $d = \overline{d} = 2$*.*

Proof. Since both G and $\overline{G}$ are connected, we have $d \geq 2$ and $\overline{d} \geq 2$. Let us consider a diametral path $P_{d+1} : v_1 v_2 \ldots, v_{d+1}$ in G. Then one can easily see that $W_p(G) \geq W_p(P_{d+1}) = d - 2$. Similarly, we have $W_p(\overline{G}) \geq \overline{d} - 2$. Therefore we get the required result in (12). The first part of the proof is done.

For $d \geq 4$, $W_p(G) = d - 2$ if and only if $G \cong P_n$. For $d = 3$, $W_p(G) = d - 2$ if and only if $G \cong P_4$ or $G \cong G^{**}$. For $d = 2$, we have $W_p(G) = d - 2$. Hence the equality holds in (12) if and only if $G \cong P_n$ or $G \cong G^{**}$ or $d = \overline{d} = 2$. ■

Remark 1.6. [83] *In Theorem 1.10, the lower bound on $W_p(G) + W_p(\overline{G})$ is given by means of d and $\overline{d}$. Since G and $\overline{G}$ are connected, we have $d \geq 2$ and $\overline{d} \geq 2$. Hence we can conclude that our lower bound in (12) is always better than the lower bound in $W_p(G) + W_p(\overline{G}) \geq 0$.*

Liu and Liu [108] obtained an upper bound on $W_p(G)$ in terms of the first Zagreb index (M_1), the second Zagreb index (M_2) and the number of edges:

Lemma 1.22. [108]

$$W_p(G) \leq M_2(G) - M_1(G) + m, \tag{13}$$

with equality holding if and only if G is either acyclic or if its girth is greater than 6.

Denote by $K^*_{2,n-2}$, a connected graph of order n, which is obtained from the complete bipartite graph $K_{2,n-2}$ by joining an edge between two vertices of degree $n-2$. Let $Ki_{n,n-1}$ denote a kite graph obtained from the complete graph K_{n-1} and an isolated vertex by adding one pendant edge. Still we do not have any upper bound on $W_p(G) + W_p(\overline{G})$ for any graph.

Next, Hua and Das gave an upper bound on $W_p(G) + W_p(\overline{G})$:

Theorem 1.11. [83] *Let $G \in \mathcal{G}(n, m)$ be a connected graph with a connected complement $\overline{G}$.Then*

$$\begin{aligned} W_p(G) + W_p(\overline{G}) &< \frac{n(n-1)(n-2)^2}{2} + 2m^2 + \left(n - \frac{3}{2}\right)\left[\frac{2(m-\Delta)^2}{n-2} - \Delta(n-\Delta)\right] \\ &- \frac{m}{2}(4n^2 - 19n + 17) - 2\left[\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)(\Delta_2-\delta)^2}{(n-1)^2}\right], \end{aligned}$$

where Δ_1 Δ_2 and δ are the maximum degree, the second maximum degree and the minimum degree in G, respectively.

Proof. By (13), we have

$$W_p(G) + W_p(\overline{G}) < M_2(G) + M_2(\overline{G}) - M_1(G) + M_1(\overline{G}) + m + \overline{m},$$

where $\overline{m}$ is the number of edges in $\overline{G}$.

By Theorem 2.10 in [35], we have

$$M_1(G) + M_1(\overline{G}) \geq n(n-1)^2 - 4m(n-1) + 2\left[\Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)(\Delta_2-\delta)^2}{(n-1)^2}\right]$$

with equality if and only if G is a regular graph or G is isomorphic a graph of order n such that $\Delta_2 = d_G(v_2) = d_G(v_3) = \ldots = d_G(v_n) = \delta \neq \Delta$. By Theorem 3.4 in [35], we have

$$M_2(G)+M_2(\overline{G}) \leq \frac{n(n-1)^3}{2}+2m^2+\left(n-\frac{3}{2}\right)\left[(n+1)m-\Delta(n-\Delta)+\frac{2(m-\Delta)^2}{n-2}\right]-3m(n-1)^2$$

with equality if and only if $G \cong K^*_{2,n-2}$ or $G \cong K_n$ or $Ki_{n,n-1}$.

According to the fact $2m+2\overline{m} = n(n-1)$, in conjunction with the above results, we get the required result. This completes the proof. ■

1.5 Reverse Wiener index

Let G be a connected (molecular) graph with the vertex-set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The *distance matrix* D of G is an $n \times n$ matrix (d_{ij}) such that d_{ij} is just the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G.

The *reverse distance matrix* or the *reverse Wiener matrix* of the graph G is an $n \times n$ matrix (r_{ij}) such that

$$r_{ij} = \begin{cases} d - d_{ij} & \text{if } i \neq j, \\ 0 & \text{otherwise,} \end{cases}$$

where d is the diameter of G.

Parallel to the definition of the Wiener index $W(G) = \sum_{i<j} d_{ij}$ using distance matrix, Balaban, Mills, Ivanciuc, and Basak [9] defined the *reverse Wiener index* $RW(G)$ of a connected graph G of order n as

$$RW(G) = \sum_{i<j} r_{ij} = \frac{n(n-1)diam(G)}{2} - W(G).$$

Nordhaus–Gaddum inequalities for RW were proved by Cai and Zhou [13] in 2008.

Theorem 1.12. [13] *Let $G \in \mathcal{G}(n)$ $(n \geq 6)$ be a graph with a connected $\overline{G}$. Then*

$$\frac{n(n-1)}{2} \leq RW(G) + RW(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6},$$

with left equality if and only if G and $\overline{G}$ have diameter 2 and with right equality if and only if $G = P_n$ or $\overline{P_n}$.

For simplicity, let $m(G)$ and $diam(G)$ be respectively the number of edges and the diameter of the graph G.

Lemma 1.23. [13] *Let $G \in \mathcal{G}(n)$ $(n \geq 6)$ be a graph. If $diam(G) = diam(\overline{G}) = 3$, then*

$$RW(G) + RW(\overline{G}) < \frac{(n-1)(n-2)(2n+3)}{6}.$$

Proof. Since $diam(G) = diam(\overline{G}) = 3$, it follows that $W(G) + W(\overline{G}) > m(G) + 2m(\overline{G}) + m(\overline{G}) + 2m(G) = \frac{3}{2}n(n-1)$, and hence

$$\begin{aligned} RW(G) + RW(\overline{G}) &= \frac{1}{2}n(n-1)\cdot 6 - [W(G) + W(\overline{G})] \\ &< 3n(n-1) - \frac{3}{2}n(n-1) \\ &< \frac{(n-1)(n-2)(2n+3)}{6}. \end{aligned}$$

The last inequality holds because $n \geq 6$. ■

Lemma 1.24. [13] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph. Then*

$$0 \leq RW(G) \leq \frac{n(n-1)(n-2)}{3}$$

with left equality if and only if $G = K_n$, and with right equality if and only if $G = P_n$.

Lemma 1.25. [13] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a graph. If $diam(\overline{G}) = 2$, then*

$$RW(G) + RW(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$$

with equality if and only if $G \cong P_n$.

Proof. Let $d = diam(G)$. By Lemma 1.24, $RW(G) \leq RW(P_n)$ with equality if and only if $G = P_n$. Since $n \geq 5$, we have $diam(\overline{G}) = diam(\overline{P}_n) = 2$, and so $RW(G) = m(\overline{G}) \leq \frac{n(n-1)}{2} - (n-1) = m(\overline{P}_n) = RW(\overline{P}_n)$ with equality if and only if G is a tree whose complement has diameter 2. Note that

$$\begin{aligned} RW(P_n) + RW(\overline{P}_n) &= \frac{n(n-1)(n-2)}{3} + \frac{n(n-1)}{2} - (n-1) \\ &= \frac{(n-1)(n-2)(2n+3)}{6}. \end{aligned}$$

The result follows easily. ■

Remark 1.7. [13] (i) *There is exactly one pair of connected graphs G and $\overline{G}$ with 4 vertices: P_4 and $\overline{P}_4 = P_4$. Obviously, $diam(P_4) = 3$ and $RW(P_4) + RW(\overline{P}_4) = 16$.*

(ii) *There are exactly five pair of connected graphs G and $\overline{G}$ with 5 vertices, in which three pairs satisfy $diam(G) = diam(\overline{G}) = 3$, T and $\overline{T}$, U_1 and $\overline{U}_1$, U_2 and $\overline{U}_2 = U_2$, where T be the unique tree with 5 vertices and diameter 3, U_1 is the graph formed from T by adding an edge between its two pendent vertices with a common and vertex, and U_2 is formed from the path P_5 by adding an edge between the two neighbors of its center. The values of $RW(G) + RW(\overline{G})$ for them are respectively 27, 27 and 28. The two other pairs are P_5 and $\overline{P}_5$, C_5 and $\overline{C}_5$. Note that $RW(P_5) + RW(\overline{P}_5) = 26$.*

Lemma 1.26. [13] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ be a connected graph with diameter d. Then*

$$(d-1)m \leq RW(G) \leq \frac{n(n-1)}{2}(d-2) + m$$

with either equality if and only if $d \leq 2$.

We are ready to give the proof of Theorem 1.5.

Proof of Theorem 1.12: By Lemma 1.26,

$$RW(G) + RW(\overline{G}) \geq m(G) + m(\overline{G}) = \frac{1}{2}n(n-1)$$

with equality if and only if G and $\overline{G}$ have equal diameter 2. If $diam(G) = diam(\overline{G}) = 3$, then it follows from Lemma 1.23 that $RW(G) + RW(\overline{G}) < \frac{(n-1)(n-2)(2n+3)}{6}$. If $diam(\overline{G}) = 2$, then it follows from Lemma 1.25 that $RW(G) + RW(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$ with equality if and only if $G = P_n$. Similarly, if $diam(G) = 2$, then $RW(G) + RW(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$ with equality if and only if $G = \overline{P}_n$. Note that if $diam(\overline{G}) \geq 3$ then $diam(G) \leq 3$. The result follows. ■

1.6 Reciprocal reverse Wiener index

The *reciprocal reverse Wiener matrix* of a graph G is an $n \times n$ matrix (rr_{ij}) such that

$$rr_{ij} = \frac{1}{r_{ij}} = \begin{cases} \frac{1}{d-d_{ij}} & \text{if } i \neq j \text{ and } d_{ij} < d, \\ 0 & \text{otherwise.} \end{cases}$$

Parallel to the definitions of the Wiener index $W(G) = \sum_{i<j} d_{ij}$ using distance matrix and the reverse Wiener index

$$RW(G) = \sum_{i<j} r_{ij} = \frac{1}{2}n(n-1)d - W(G)$$

using reverse Wiener matrix of the graph G, the reciprocal reverse Wiener index $RRW(G)$ of the graph G is defined as [88]

$$RRW(G) = \sum_{i<j} rr_{ij}.$$

Zhou, Yang, and Trinajstić [164] got the following Nordhaus–Gaddum–type results for reciprocal reverse Wiener index.

Theorem 1.13. [164] *Let $G \in \mathcal{G}(n)$ $(n \geq 4)$ be a graph with a connected complement $\overline{G}$. Then*

(a) $RRW(G) + RRW(\overline{G}) \leq \frac{2n^2-5n+1}{2}$ *with equality if and only if G is the graph formed from the path on 5 vertices by adding an edge between the two neighbors of its center;*

(b) *If G and $\overline{G}$ have at most $\frac{(n+1)(n-2)}{3}$ edges, then $RRW(G) + RRW(\overline{G}) \leq \frac{3n^2-3n-8}{2}$.*

1.7 Reciprocal complementary Wiener index

The *complementary distance matrix* of a graph G is an $n \times n$ matrix (c_{ij}) such that

$$c_{ij} = \begin{cases} 1 + D - d_{ij} & \text{if } i \neq j, \\ 0 & \text{otherwise,} \end{cases}$$

where D is the diameter of the graph G. The *reciprocal complementary distance matrix* of a graph G is an $n \times n$ matrix rc_{ij} such that

$$rc_{ij} = \begin{cases} \frac{1}{c_{ij}} & \text{if } i \neq j, \\ 0 & \text{otherwise.} \end{cases}$$

The Hosoya definition of the Wiener number of G, denoted by $W(G)$, is given by [80]

$$W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij} = \sum_{i<j} d_{ij}.$$

The *reciprocal complementary Wiener number* of the graph G is similarly defined as [86]

$$RCW(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} rc_{ij} = \sum_{i<j} rc_{ij}.$$

Zhou, Cai, and Trinajstić [155] obtained the following result for reciprocal complementary Wiener number.

Theorem 1.14. [155] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a graph with a connected complement $\overline{G}$. Then*

$$RCW(G) + RCW(\overline{G}) \leq \frac{3n(n-1)}{4}$$

with equality if and only if both G and $\overline{G}$ have diameter 2, whilst

$$RCW(G) + RCW(\overline{G}) \geq \begin{cases} \frac{5n(n-1)}{12} + 1 & \text{if } 5 \leq n \leq 8, \\ \frac{n^2+5n-6}{4} & \text{if } n \geq 9, \end{cases}$$

with equality if and only if $G = P_n$ or $G = \overline{P_n}$ for $n \geq 9$, and both G and $\overline{G}$ have diameter three with $d(G,3) = d(\overline{G},3) = 1$ for $5 \leq n \leq 8$, where $d(G,k)$ is the number of the unordered pairs of vertices of G that are at distance k, $k = 1, 2, \ldots, diam(G)$.

Lemma 1.27. [155] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph. Then*

$$RCW(G) \leq \frac{n(n-1)}{2}$$

with equality if and only if $G = K_n$.

Lemma 1.28. [155] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 3)$ be a noncomplete connected graph. Then*

$$RCW(G) \leq \frac{n(n-1)}{2} - \frac{m}{2}$$

with equality if and only if G has diameter 2.

There is only one connected graph P_4 on 4 vertices with the connected complement $\overline{P}_4 = P_4$. Obviously, $RCW(P_4) + RCW(\overline{P}_4) = 6$. For $n \geq 5$, the diameter of $\overline{P}_n$ is 2.

Lemma 1.29. [155] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected graph. If $\overline{G}$ has diameter 2, then*

$$RCW(G) + RCW(\overline{G}) \geq \frac{n^2+5n-6}{4}$$

with equality if and only if $G = P_n$.

Proof. By Lemma 1.27, $RCW(G) \geq n-1$ with equality if and only if $G = P_n$. Let $\overline{m}$ be the number of edges in $\overline{G}$. Then $\overline{m} \leq \frac{n(n-1)}{2} - (n-1)$. By Lemma 1.28, $RCW(\overline{G}) = \frac{n(n-1)}{2} - \frac{\overline{m}}{2} \geq \frac{n(n-1)}{2} - \frac{1}{2}[\frac{n(n-1)}{2} - (n-1)] = \frac{n(n-1)}{4} + \frac{n-1}{2}$ with equality if and only if the number of edges of G is equal to $n-1$. The result follows easily. ■

Lemma 1.30. [155] *Let $G \in \mathcal{G}(n)$ be a graph. Suppose that both G and $\overline{G}$ have diameter 3. Then*

$$RCW(G) + RCW(\overline{G}) \geq \frac{5n(n-1)}{12} + 1$$

with equality if and only if $d(G,3) = d(\overline{G},3) = 1$.

Proof. Let $t_k = d(G,k)$ and $\overline{t_k} = d(\overline{G},k)$. Obviously, $t_2 + t_3 = \bar{t}_1$, $\bar{t}_2 + \bar{t}_3 = t_1$ and $t_1 + \bar{t}_1 = \frac{n(n-1)}{2}$. Then

$$\begin{aligned} RCW(G) + RCW(\overline{G}) &= \sum_{k=1}^{3} \frac{t_k + \bar{t}_k}{4-k} = \frac{t_1 + \bar{t}_1}{3} + \frac{t_2 + t_3 + \bar{t}_2 + \bar{t}_3}{2} + \frac{t_3 + \bar{t}_3}{2} \\ &= \frac{t_1 + \bar{t}_1}{3} + \frac{t_1 + \bar{t}_1}{2} + \frac{t_3 + \bar{t}_3}{2} = \frac{5}{6}(t_1 + \bar{t}_1) + \frac{t_3 + \bar{t}_3}{2} \\ &= \frac{5n(n-1)}{12} + \frac{t_3 + \bar{t}_3}{2} \geq \frac{5n(n-1)}{12} + 1 \end{aligned}$$

with equality if and only if $t_3 = \bar{t}_3 = 1$. ■

It is easily seen that there are pairs of graphs on n vertices such that both of them have diameter three and $t_3 = \bar{t}_3 = 1$. For example, if $n = 5$, then there is exactly one pair G and $\overline{G}$: the graph formed from the path P_5 by adding an edge between the two neighbors of its center and its complement which is isomorphic to itself such that $RCW(G) + RCW(\overline{G}) = \frac{28}{3} = \frac{5n(n-1)}{12} + 1$.

Proof of Theorem 1.14: Let m and $\overline{m}$ be respectively the number of edges of G and $\overline{G}$. Then $m + \overline{m} = \frac{n(n-1)}{2}$. From Lemma 1.28,

$$RCW(G) + RCW(\overline{G}) \leq \frac{n(n-1)}{2} - \frac{m}{2} + \frac{n(n-1)}{2} - \frac{\overline{m}}{2} = n(n-1) - \frac{m + \overline{m}}{2} = \frac{3n(n-1)}{4}$$

with equality if and only if both G and $\overline{G}$ have diameter 2.

On the other hand, note that either both G and $\overline{G}$ have diameter 3 or one of them has diameter 2, and that $\frac{5n(n-1)}{12} + 1 > \frac{n^2+5n-6}{4}$ if and only if $n \geq 9$. The second part of the proposition follows from Lemmas 1.29 and 1.30.

1.8 Steiner Wiener index

The distance between two vertices u and v in a connected graph G also equals the minimum size of a connected subgraph of G containing both u and v. This observation suggests a generalization of distance. The Steiner distance of a graph, introduced by Chartrand, Oellermann, Tian and Zou [14] in 1989, is a natural generalization of the concept of classical graph distance. For a graph $G(V,E)$ and a set

$S \subseteq V(G)$ of at least two vertices, *an S-Steiner tree* or *a Steiner tree connecting S* (or simply, *an S-tree*) is a such subgraph $T(V', E')$ of G that is a tree with $S \subseteq V'$. Let G be a connected graph of order at least 2 and let S be a nonempty set of vertices of G. Then the *Steiner distance* $d_G(S)$ among the vertices of S (or simply the distance of S) is the minimum size among all connected subgraphs whose vertex sets contain S. Note that if H is a connected subgraph of G such that $S \subseteq V(H)$ and $|E(H)| = d_G(S)$, then H is a tree. Observe that $d_G(S) = \min\{e(T) \mid S \subseteq V(T)\}$, where T is subtree of G. Furthermore, if $S = \{u, v\}$, then $d_G(S)$ coincides with the classical distance between u and v.

Observation 1.1. *Let G be a graph of order n and k be an integer, $2 \le k \le n$. If $S \subseteq V(G)$ and $|S| = k$, then $k - 1 \le d_G(S) \le n - 1$.*

The *average Steiner distance* $\mu_k(G)$ of a graph G, introduced by Dankelmann, Oellermann and Swart in [20, 22], is defined as the average of the Steiner distances of all k-subsets of $V(G)$, i.e.

$$\mu_k(G) = \binom{n}{k}^{-1} \sum_{S \subseteq V(G), |S| = k} d_G(S). \tag{14}$$

Let n and k be two integers with $2 \le k \le n$. The *Steiner k-eccentricity* $e_k(v)$ of a vertex v of G is defined by $e_k(v) = \max\{d(S) \mid S \subseteq V(G), |S| = k, v \in S\}$. The *Steiner k-radius* of G is $srad_k(G) = \min\{e_k(v) \mid v \in V(G)\}$, whereas the *Steiner k-diameter* of G is $sdiam_k(G) = \max\{e_k(v) \mid v \in V(G)\}$. Note that for any vertex v of any connected graph G, $e_2(v) = e(v)$, and in addition and that $srad_2(G) = rad(G)$ and $sdiam_2(G) = diam(G)$. For more details on Steiner distance we refer to [14, 20, 22, 111].

Mao [111] obtained the following results.

Lemma 1.31. [111] *Let G be a connected graph with connected complement $\overline{G}$. If $sdiam_k(G) \ge 2k$, then $sdiam_k(\overline{G}) \le k$.*

Lemma 1.32. [111] *Let $G \in \mathcal{G}(n)$ be a connected graph. Then $sdiam_3(G) = 2$ if and only if $0 \le \Delta(\overline{G}) \le 1$.*

Lemma 1.33. [111] *Let n, k be two integers with $2 \le k \le n$, and let G be a connected graph of order n. If $sdiam_k(G) = k - 1$, then $0 \le \Delta(\overline{G}) \le k - 2$.*

Lemma 1.34. [111] *Let $G \in \mathcal{G}(n)$ be a connected graph with connected complement $\overline{G}$. Let k be an integer such that $3 \le k \le n$. Let $x = 0$ if $n \ge 2k - 2$ and $x = 1$ if $n < 2k - 2$. Then*

(i) $2k - 1 - x \le sdiam_k(G) + sdiam_k(\overline{G}) \le \max\{n + k - 1, 4k - 2\}$;

(ii) $(k - 1)(k - x) \le sdiam_k(G) \cdot sdiam_k(\overline{G}) \le \max\{k(n - 1), (2k - 1)^2\}$.

Lemma 1.35. [111] *Let $G \in \mathcal{G}(n)$ be a graph. Then $sdiam_{n-1}(G) = n - 2$ if and only if G is 2-connected.*

The following corollary is immediate from the above lemmas.

Corollary 1.1. [113] *Let G and $\overline{G}$ be connected graphs. If $sdiam_3(G) \ge 6$, then $sdiam_3(\overline{G}) = 3$.*

Proof. From Lemma 1.31, we have $sdiam_3(\overline{G}) \leq 3$. We claim that $sdiam_3(\overline{G}) = 3$. Assume, to the contrary, that $sdiam_3(\overline{G}) = 2$. From Lemma 1.33, we have $0 \leq \Delta(G) \leq 1$. Furthermore, G is not connected, which contradicts to the fact that $sdiam_3(G) \geq 6$. ■

Li, Mao, and Gutman [103] generalized the concept of Wiener index using Steiner distance, by defining the *Steiner k-Wiener index* $SW_k(G)$ of the connected graph G as

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S).$$

However, with regard to this definition, one should bear in mind (14), and the references [20, 22].

For $k = 2$, then the thus defined Steiner Wiener index coincides with the ordinary Wiener index. It is usual to consider SW_k for $2 \leq k \leq n-1$, but the above definition implies $SW_1(G) = 0$ and $SW_n(G) = n-1$. In this section, we assume that both G and $\overline{G}$ are connected.

An application in chemistry of the Steiner Wiener index is reported by Gutman, Furtula, and Li in [70]. For more details on the Steiner Wiener index, we refer to [70, 103, 104, 112].

In [103], Li, Mao, and Gutman obtained the following results, which will be needed later.

Lemma 1.36. [103] *Let T be a tree of order n, and let k be an integer such that $2 \leq k \leq n$. Then*

$$\binom{n-1}{k-1}(n-1) \leq SW_k(T) \leq (k-1)\binom{n+1}{k+1}.$$

Moreover, among all trees of order n, the star S_n minimizes the Steiner Wiener k-index whereas the path P_n maximizes the Steiner Wiener k-index.

Lemma 1.37. [103] *Let P_n be the path of order n $(n \geq 3)$, and let k be an integer such that $2 \leq k \leq n$. Then*

$$SW_k(P_n) = (k-1)\binom{n+1}{k+1}.$$

For general k, Mao, Wang, Gutman and Li [113] obtained the following result in next subsection.

Theorem 1.15. [113] *Let $G \in \mathcal{G}(n)$ and let k be an integer such that $3 \leq k \leq n$. Then:*

(1) $\binom{n}{k}(2k-2) \leq SW_k(G) + SW_k(\overline{G}) \leq \max\{n+k-1, 4k-2\}\binom{n}{k}$;

(2) $(k-1)^2\binom{n}{k}^2 \leq SW_k(G) \cdot SW_k(\overline{G}) \leq \max\{k(n-1), (2k-1)^2\}\binom{n}{k}^2$.

Moreover, the lower bounds are sharp.

For $k = n$, the following result is immediate.

Observation 1.2. [113] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

(1) $SW_n(G) + SW_n(\overline{G}) = 2n-2\,;$

(2) $SW_n(G) \cdot SW_n(\overline{G}) = (n-1)^2\,.$

For $k = n-1$, we will prove the following result in Subsection 1.8.1.

Proposition 1.2. [113] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a graph.*

(1) *If G and $\overline{G}$ are both 2-connected, then $SW_{n-1}(G) + SW_{n-1}(\overline{G}) = 2n(n-2)$ and $SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = n^2\,(n-2)^2$.*

(2) *If $\kappa(G) = 1$ and $\overline{G}$ is 2-connected, then $SW_{n-1}(G)+SW_{n-1}(\overline{G}) = 2n(n-2)+p$ and $SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = n(n-2)(n^2-2n+p)$, where p is the number of cut vertices in G.*

(3) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) \leq n-3$, and G has a cut vertex v with pendent edge uv such that $G - u$ contains a spanning complete bipartite subgraph, and $\Delta(\overline{G}) \leq n-3$ and $\overline{G}$ has a cut vertex q with pendent edge pq such that $G - p$ contains a spanning complete bipartite subgraph, then $SW_{n-1}(G) + SW_{n-1}(\overline{G}) = 2(n-1)^2$ and $SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = (n-1)^4$.*

(4) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(\overline{G}) = n-2$, $\Delta(G) \leq n-3$ and G has a cut vertex v with pendent edge uv such that $G - u$ contains a spanning complete bipartite subgraph, then*

$$SW_{n-1}(G) + SW_{n-1}(\overline{G}) = 2(n-1)^2 \quad \textit{or} \quad SW_{n-1}(G) + SW_{n-1}(\overline{G}) = 2(n-1)^2 + 1$$

and

$$SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = (n-1)^4 \quad \textit{or} \quad SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = (n-1)^2\,(n^2-2n+2)\,.$$

(5) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) = \Delta(\overline{G}) = n-2$, then*

$$2(n-1)^2 \leq SW_{n-1}(G) + SW_{n-1}(\overline{G}) \leq 2(n-1)^2 + 2$$

and

$$(n-1)^4 \leq SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) \leq (n^2-2n+2)^2\,.$$

In Subsection 1.8.2, they focused our attention on the case $k = 3$. For $k = 3$ and $n \geq 10$, from Theorem 1.15, we have

$$4\binom{n}{3} \leq SW_3(G) + SW_3(\overline{G}) \leq (n+2)\binom{n}{3}$$

and

$$4\binom{n}{3}^2 \leq SW_3(G) \cdot SW_3(\overline{G}) \leq 3(n-1)\binom{n}{3}^2.$$

They improved these bounds and proved the following result.

Theorem 1.16. [113] *Let $G \in \mathcal{G}(n)$ $(n \geq 4)$ be a graph. Then*

(1)

$$5\binom{n}{3} \leq SW_3(G) + SW_3(\overline{G})$$

$$\leq \begin{cases} 7\binom{n}{3} - 3n + 8 & \text{if } n = 6,7, \text{ and } sdiam_3(G) = 5 \\ & \text{or } n = 6,7, \text{ and } sdiam_3(\overline{G}) = 5 \\ 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{1}{2}(7n^2 - 35n + 48) & \text{otherwise.} \end{cases}$$

(2)

$$
\begin{aligned}
& 6\binom{n}{3}^2 + (n-2)\binom{n}{3} - (n-2)^2 \\
\leq\ & SW_3(G) \cdot SW_3(\overline{G}) \\
\leq\ & \begin{cases} \frac{1}{4}\left[7\binom{n}{3} - 3n + 8\right]^2 & \text{if } n = 6,7, \text{ and } sdiam_3(G) = 5 \\ & \text{or } n = 6,7, \text{ and } sdiam_3(\overline{G}) = 5 \\ \left[\binom{n+1}{4} + \binom{n-3}{3} + \frac{1}{4}\left(7n^2 - 35n + 48\right)\right]^2 & \text{otherwise.} \end{cases}
\end{aligned}
$$

Moreover, the bounds are sharp.

1.8.1 Results pertaining to general *k*

The following lemmas and corollaries will be used later.

Lemma 1.38. [113] *Let T be a tree of order n, and let k be an integer such that $3 \leq k \leq n$. Then there exist at least $(n-k+1)$ subsets of $V(T)$ for which the Steiner k-distance is equal to $k-1$.*

Proof. We verify this lemma by induction on n. If $n = k$, then there exists at least one subset of $V(T)$ such that the Steiner n-distance is $n-1$ since T is a spanning tree. Suppose the assertion is true for n. We then show that the assertion is true for $n+1$. In this case, T is a tree of order $n+1$. Choose a leaf of this tree, say v. Then $T - v$ is a tree of order n. By the induction hypothesis, $T - v$ contains $(n-k+1)$ subsets of $V(T)$ whose Steiner k-distance is equal to $k-1$. Choose $k-1$ vertices in $V(T) - v$ such that the subgraph induced by these $k-1$ vertices and v is a subtree of order k. Then the Steiner k-distance of these $k-1$ vertices and v is exactly $k-1$. So there exist at least $(n-k+2)$ subsets of $V(T)$ whose Steiner k-distance is $k-1$. ■

The following result is immediate.

Corollary 1.2. [113] *Let $G \in \mathcal{G}(n)$ be a connected graph, and let k be an integer such that $3 \leq k \leq n$. Then there exist at least $(n-k+1)$ subsets of $V(G)$ whose Steiner k-distance is $k-1$.*

Similarly to the proof of Lemma 1.38, we can derive the following result.

Lemma 1.39. [113] *Let T be a tree of order n, and let k be an integer such that $3 \leq k \leq n-1$. Then there exist at least $(n-k)$ subsets of $V(T)$ whose Steiner k-distance is k.*

We are now prepared to prove Theorem 1.15.

Proof of Theorem 1.15: Proof of part (1):

For any $S \subseteq V(G)$ and $|S| = k$, from the definition of Steiner diameter and Lemma 1.34, we have

$d_G(S) + d_{\overline{G}}(S) \leq \max\{n+k-1, 4k-2\}$. Then

$$\begin{aligned} SW_k(G) + SW_k(\overline{G}) &= \sum_{S\subseteq V(G)} d_G(S) + \sum_{S\subseteq V(\overline{G})} d_{\overline{G}}(S) = \sum_{S\subseteq V(G)} [d_G(S) + d_{\overline{G}}(S)] \\ &\leq \max\{n+k-1, 4k-2\}\binom{n}{k}. \end{aligned}$$

By the same reason, Lemma 1.34 implies $SW_k(G) + SW_k(\overline{G}) \geq \binom{n}{k}(2k-2)$. If $n \geq 2k-2$, then from Lemma 1.34 it follows that $SW_k(G) + SW_k(\overline{G}) \geq \binom{n}{k}(2k-1)$. ■

Proof of part (2):

For any $S' \subseteq V(G)$, $|S'| = k$ and any $S'' \subseteq V(\overline{G})$, $|S''| = k$, from the definition of Steiner diameter and Lemma 1.36, we have $d_G(S') \cdot d_{\overline{G}}(S'') \leq \max\{k(n-1), (2k-1)^2\}$. Then

$$\begin{aligned} SW_k(G) \cdot SW_k(\overline{G}) &= \sum_{S'\subseteq V(G)} d_G(S') \cdot \sum_{S''\subseteq V(\overline{G})} d_{\overline{G}}(S'') = \sum_{S'\subseteq V(G),\, S''\subseteq V(\overline{G})} d_G(S') \cdot d_{\overline{G}}(S'') \\ &\leq \max\{k(n-1), (2k-1)^2\}\binom{n}{k}^2. \end{aligned}$$

For any $S' \subseteq V(G)$, $|S'| = k$ and any $S'' \subseteq V(\overline{G})$, $|S''| = k$, from the definition of Steiner diameter and Lemma 1.35, we have $d_G(S') \cdot d_{\overline{G}}(S'') \geq (k-1)^2$. Then

$$\begin{aligned} SW_k(G) \cdot SW_k(\overline{G}) &= \sum_{S'\subseteq V(G)} d_G(S') \cdot \sum_{S''\subseteq V(\overline{G})} d_{\overline{G}}(S'') \\ &= \sum_{S'\subseteq V(G),\, S''\subseteq V(\overline{G})} d_G(S') \cdot d_{\overline{G}}(S'') \geq (k-1)^2\binom{n}{k}^2 \end{aligned}$$

as desired. ■

Akiyama and Harary [1] characterized the graphs for which both G and $\overline{G}$ are connected.

Lemma 1.40. [1] *Let $G \in \mathcal{G}(n)$ be graph with maximal vertex degree $\Delta(G)$. Then $\kappa(G) = \kappa(\overline{G}) = 1$ if and only if G satisfies the following conditions.*

(i) $\kappa(G) = 1$ *and* $\Delta(G) = n-2$*;*

(ii) $\kappa(G) = 1$, $\Delta(G) \leq n-3$*, and G has a cut vertex v with pendent edge uv, such that $G-u$ contains a spanning complete bipartite subgraph.*

We now in a position to give the proof of Proposition 1.2.

Proof of Proposition 1.2.

(1): From Lemma 1.35, if G and $\overline{G}$ are both connected, then $d_G(S) = n-2$ and $d_{\overline{G}}(S) = n-2$ for any $S \subseteq V(G)$ and $|S| = n-1$. Therefore, $SW_{n-1}(G) + SW_{n-1}(\overline{G}) = 2n(n-2)$ and $SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = n^2\,(n-2)^2$.

(2): Since $\overline{G}$ is 2-connected, it follows that $d_{\overline{G}}(S) = n-2$ for any $S \subseteq V(G)$ and $|S| = n-1$, and hence $SW_{n-1}(\overline{G}) = n(n-2)$. Note that $\kappa(G) = 1$ and there are exactly p cut vertices in G. For any $S \subseteq V(G)$ and $|S| = n-1$, if the unique vertex in $V(G) \setminus S$ is a cut vertex, then $d_G(S) = n-1$. If the unique vertex in $V(G) \setminus S$ is not a cut vertex, then $d_G(S) = n-2$. Therefore, we have $SW_{n-1}(G) = p(n-1) + (n-p)(n-2) = n(n-2) + p$, and hence $SW_{n-1}(G) + SW_{n-1}(\overline{G}) = 2n(n-2) + p$ and $SW_{n-1}(G) \cdot SW_{n-1}(\overline{G}) = n(n-2)(n^2 - 2n + p)$, where p is the number of cut vertices in G.

$(3), (4), (5)$: We have $\kappa(G) = \kappa(\overline{G}) = 1$. By condition (i) of Lemma 1.40, since $\Delta(G) = n-2$, there is a vertex of degree $n-2$, say x. Let the set of first neighbors of x be $N_G(x) = \{y_1, y_2, \ldots, y_{n-2}\}$. Let $V(G) \setminus (\{x\} \cup N_G(x)) = \{z\}$. Since $zx \notin E(G)$, there must exist a vertex in $N_G(x)$, say y_1, such that $yy_1 \in E(G)$, since G is connected. Since x, y_1 may be the cut vertices in G, it follows that there are one or two cut vertices in G. So $SW_{n-1}(G) = (n-1) + (n-1)(n-2) = (n-1)^2$ or $SW_{n-1}(G) = n + (n-1)(n-2) = (n-1)^2 + 1$.

By condition (ii) of Lemma 1.40, since $\Delta(G) \leq n-3$ and G has a cut vertex v with pendent edge uv such that $G - u$ contains a spanning complete bipartite subgraph, it follows that v is the unique cut vertex. So $SW_{n-1}(G) = n + (n-1)(n-2) = (n-1)^2 + 1$. From this argument, $(3), (4), (5)$ are true. ■

1.8.2 The case $k = 3$

We first need the following lemma.

Lemma 1.41. [113] *Let G be a connected graph. If $sdiam_3(G) = 5$, then $sdiam_3(\overline{G}) \leq 4$.*

Proof. For any $S \subseteq V(\overline{G})$ and $|S| = 3$, we let $S = \{u_1, u_2, u_3\}$. If $d_G(S) \geq 3$, then $\overline{G}[S]$ is connected, and hence $d_{\overline{G}}(S) = 2$, as desired. So we now assume that $d_G(S) = 2$. Clearly, $G[S]$ is connected, and hence $G[S] \cong K_3$ or $G[S] \cong P_3$. We only show the case that $G[S] \cong K_3$. The proof of $G[S] \cong P_3$ is analogous and is omitted.

We thus prove that if $G[S] \cong K_3$, then $d_{\overline{G}}(S) \leq 4$.

If there exists a vertex $v \in V(G) - S$ such that $|E_G[v, S]| = 0$, then $\overline{G}[S \cup \{v\}]$ is connected. In view of the arbitrariness of S, we have $sdiam_3(\overline{G}[S]) \leq 3$, as desired. We now assume that

(a) $|E_G[x, S]| \geq 1$ for any vertex $x \in V(G) - S$.

For any $S' = \{v_1, v_2, v_3\} \subseteq V(G)$, if $|S \cap S'| \geq 1$, then $G[S \cup S']$ is connected, and hence $d_G(S') \leq 4$. From the arbitrariness of S', we have $sdiam_3(G) \leq 4$, a contradiction. We now assume $|S \cap S'| = 0$. From (a), $|E_G[v_i, S]| \geq 1$ for $i = 1, 2, 3$. If there exists a vertex $u_i \in S$ such that the subgraph induced by the edges in $E_G[u_i, S']$ is a star $K_{1,3}$, then $d_G(S') \leq 3$. From the arbitrariness of S', we have $sdiam_3(G) \leq 3$, a contradiction. If there exists two vertices $u_i, u_j \in S$ such that the subgraph induced by the edges in $E_G[\{u_i, u_j\}, S']$ equals $P_3 \cup K_2$, then $d_G(S') \leq 4$. In view of the arbitrariness of S', we have $sdiam_3(G) \leq 4$, a contradiction. We now assume that

(b) The subgraph induced by the edges in $E_G[S, S']$ equal $3\,K_2$.

If $G[S']$ is connected, then $d_G(S') = 2$. From the arbitrariness of S', we have $sdiam_3(G) = 2$, a contradiction. So we assume that there exists a 3-subset S' such that $G[S']$ is not connected. We now assume that

(c) $G[S'] \cong K_2 \cup K_1$ or $G[S'] \cong 3\,K_1$.

From (b) and (c), the subgraph induced by the vertices of $S \cup S'$ is either the graph H_1 obtained from a triangle with vertex set $\{u_1, u_2, u_3\}$ by adding three pendent edges u_iv_i, where $1 \leq i \leq 3$, or the graph H_2 obtained from H_1 by adding an edge v_1v_2.

For H_1, the tree in $\overline{G}$ induced by the edges in $\{v_2u_1, v_2u_3, v_1v_2, v_1u_2\}$ is an S-Steiner tree, and hence $d_{\overline{G}}(S) \leq 4$. For H_2, the tree in $\overline{G}$ induced by the edges in $\{v_3u_1, v_3u_3, v_1v_3, v_1u_2\}$ is an S-Steiner tree, and hence $d_{\overline{G}}(S) \leq 4$.

From the above argument, if $G[S] \cong K_3$ or $G[S] \cong P_3$, then $d_{\overline{G}}(S) \leq 4$. From the arbitrariness of S, we have $sdiam_3(\overline{G}) \leq 4$, as desired. ■

Lemma 1.42. [113] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$SW_3(G) + SW_3(\overline{G}) \geq 5\binom{n}{3} \tag{15}$$

and

$$SW_3(G) \cdot SW_3(\overline{G}) \geq 6\binom{n}{3}^2 + (n-2)\binom{n}{3} - (n-2)^2\,. \tag{16}$$

Moreover, the bounds are sharp.

Proof. (1) For any $S \subseteq V(G)$ and $|S| = 3$, $G[S] \cong K_3$ or $G[S] \cong P_3$ or $G[S] \cong K_2 \cup K_1$ or $G[S] \cong 3K_1$. If $G[S] \cong K_3$ or $G[S] \cong P_3$, then $d_G(S) = 2$. If $G[S] \cong K_2 \cup K_1$ or $G[S] \cong 3K_1$, then $d_G(S) \geq 3$. Let $S_1, S_2, \ldots, S_{\binom{n}{3}}$ be all the 3-subsets of $V(G)$. Without loss of generality, let $S_1, S_2, \ldots, S_x$ be all the 3-subsets of $V(G)$ such that $G[S_i] \cong K_3$ or $G[S_i] \cong P_3$, where $1 \leq i \leq x$. Therefore, $d_G(S_i) = 2$ and $d_{\overline{G}}(S_i) \geq 3$ for each i $(1 \leq i \leq x)$. Furthermore, for any S_j $(x+1 \leq j \leq \binom{n}{3})$, $G[S_j] \cong K_2 \cup K_1$ or $G[S_j] \cong 3K_1$. Then $d_G(S_j) \geq 3$ and $d_{\overline{G}}(S_j) = 2$ for each j $(x+1 \leq j \leq \binom{n}{3})$. So

$$SW_3(G) \geq 2x + 3\left[\binom{n}{3} - x\right] = 3\binom{n}{3} - x$$

and

$$SW_3(\overline{G}) \geq 3x + 2\left[\binom{n}{3} - x\right] = 2\binom{n}{3} + x$$

implying inequality (15).

By Corollary 1.2, there exist at least $(n-2)$ subsets of $V(G)$ whose Steiner 3-distances are equal to 2. The same is true for $\overline{G}$. Therefore, $n-2 \leq x \leq \binom{n}{3} - n + 2$, and hence

$$\begin{aligned} SW_3(G) \cdot SW_3(\overline{G}) &\geq \left[3\binom{n}{3} - x\right]\left[2\binom{n}{3} + x\right] \\ &= 6\binom{n}{3}^2 + \binom{n}{3}x - x^2 \geq 6\binom{n}{3}^2 + (n-2)\binom{n}{3} - (n-2)^2 \end{aligned}$$

i.e., inequality (16) holds. ■

The sharpness of the above bounds is illustrated by the following example.

Example 1.1. [113] Let $G \cong P_4$. Then $\overline{G} \cong P_4$. By Lemma 1.37, $SW_3(G) = SW_3(\overline{G}) = 10$, and hence $SW_3(G)+SW_3(\overline{G}) = 20 = 5\binom{n}{3}$ and $SW_3(G)\cdot SW_3(\overline{G}) = 100 = 6\binom{n}{3}^2+(n-2)\binom{n}{3}-(n-2)^2$, which confirms that the lower and upper bounds are sharp.

Let S^* be a tree obtained from a star of order $n-2$ and a path of length 2 by identifying the center of the star and a vertex of degree one in the path. Then $\overline{S^*}$ is a graph obtained from a clique of order $n-1$ by deleting an edge uv and then adding an pendent edge at v.

Observation 1.3. [113]

(1) $SW_3(S^*) = 9\binom{n-3}{2} + 3\binom{n-3}{3} + 8n - 22$;

(2) $SW_3(\overline{S^*}) = 7\binom{n-3}{2} + 2\binom{n-3}{3} + 7n - 18$.

Proof. From the structure of S^* and $\overline{S^*}$, we conclude

$$\begin{aligned} SW_3(S^*) &= 4\binom{n-3}{2} + 2\left[\binom{n-3}{2} + (n-3) + 1\right] + 3\left[\binom{n-3}{2} + \binom{n-3}{3} + 2(n-3)\right] \\ &= 9\binom{n-3}{2} + 3\binom{n-3}{3} + 8n - 22 \end{aligned}$$

and

$$\begin{aligned} SW_3(\overline{S^*}) &= 2\left[2\binom{n-3}{2} + 2(n-3) + \binom{n-3}{3}\right] + 3\left[\binom{n-3}{2} + (n-2)\right] \\ &= 7\binom{n-3}{2} + 2\binom{n-3}{3} + 7n - 18\,. \end{aligned}$$

■

In order to show the sharpness of the above bounds, we consider the following example.

Example 1.2. [113] Let S^* be the same tree as before. From Observation 1.3, we have

$$SW_3(S^*) + SW_3(\overline{S^*}) = 16\binom{n-3}{2} + 5\binom{n-3}{3} + 15n - 40$$

and

$$\begin{aligned} SW_3(S^*) \cdot SW_3(\overline{S^*}) &= 63\binom{n-3}{2}^2 + 6\binom{n-3}{3}^2 + 39\binom{n-3}{2}\binom{n-3}{3} \\ &\quad +(119n-316)\binom{n-3}{2} + (37n-98)\binom{n-3}{3} \\ &\quad +(8n-22)(7n-18)\,. \end{aligned}$$

The following lemmas are preparations for deducing an upper bound on $SW_3(G) + SW_3(\overline{G})$.

Lemma 1.43. [113] *Let $G \in \mathcal{G}(n)$ be a connected graph, and let T be a spanning tree of G. If $sdiam_3(\overline{G}) = 3$, then*

$$SW_3(G) + SW_3(\overline{G}) \leq SW_3(T) + SW_3(\overline{T})\,.$$

Proof. Note that $\overline{G}$ is a spanning subgraph of $\overline{T}$. It suffices to prove that

$$SW_3(\overline{G}) - SW_3(\overline{T}) \leq SW_3(T) - SW_3(G)\,.$$

Since $sdiam_3(\overline{G}) = 3$, it follows that $d_{\overline{G}}(S) = 2$ or $d_{\overline{G}}(S) = 3$ for any $S \subseteq V(G)$ and $|S| = 3$. Since $\overline{G}$ is a spanning subgraph of $\overline{T}$ and $sdiam_3(\overline{G}) = 3$, it follows that $sdiam_3(\overline{T}) \leq 3$, and hence $d_{\overline{T}}(S) = 2$ or $d_{\overline{T}}(S) = 3$ for any $S \subseteq V(T)$ and $|S| = 3$. Then $0 \leq d_{\overline{G}}(S) - d_{\overline{T}}(S) \leq 1$. We claim that $d_{\overline{G}}(S) - d_{\overline{T}}(S) \leq d_T(S) - d_G(S)$ for $S \subseteq V(T)$ and $|S| = 3$. Because $\overline{G}$ is a spanning subgraph of $\overline{T}$, $d_{\overline{G}}(S) \geq d_{\overline{T}}(S)$ for any $S \subseteq V(T)$ and $|S| = 3$. Similarly, since T is a spanning subgraph of G, $d_T(S) \geq d_G(S)$ for any $S \subseteq V(T)$ and $|S| = 3$. If $d_{\overline{G}}(S) - d_{\overline{T}}(S) = 0$, then $d_{\overline{G}}(S) - d_{\overline{T}}(S) = 0 \leq d_T(S) - d_G(S)$, as desired. If $d_{\overline{G}}(S) - d_{\overline{T}}(S) = 1$, then $d_{\overline{G}}(S) = 3$ and $d_{\overline{T}}(S) = 2$, and hence $d_G(S) = 2$ and $d_T(S) \geq 3$. Therefore, $d_T(S) - d_G(S) \geq 1 = d_{\overline{G}}(S) - d_{\overline{T}}(S)$, as desired. The result follows from the arbitrariness of S and the definition of Steiner Wiener index. ■

Lemma 1.44. [113] *Let T be a tree of order n, different from the star S_n. Let S^* be the tree same as in Observation 1.3. If $sdiam_3(\overline{G}) = 3$, then*

$$SW_3(T) + SW_3(\overline{T}) \leq SW_3(P_n) + SW_3(\overline{S^*})\,.$$

Proof. Note first that the complements of all trees, except of the star, are connected. Therefore, $SW_3(\overline{T})$ in Lemma 1.44 is always well defined.

By Lemma 1.36, $SW_3(T) \leq SW_3(P_n)$. It suffices to prove $SW_3(\overline{T}) \leq SW_3(\overline{S^*})$. Since $sdiam_3(\overline{G}) \leq 3$, it follows that $sdiam_3(\overline{T}) \leq 3$. For any $S \subseteq V(T)$ and $|S| = 3$, if $T[S]$ is not connected, then $d_{\overline{T}}(S) = 2$. If $T[S]$ is connected, then $d_{\overline{T}}(S) \geq 3$. So if we want to obtain the maximum value of $SW_3(\overline{T})$ for a tree T, then we need to find as many as possible 3-subsets of $V(T)$ whose induced subgraphs in $\overline{T}$ are disconnected. Since the complement of S_n is not connected, it follows that $\overline{S^*}$ is our desired tree. So $SW_3(\overline{T}) \leq SW_3(\overline{S^*})$, and hence $SW_3(T) + SW_3(\overline{T}) \leq SW_3(P_n) + SW_3(\overline{S^*})$. ■

We are now in the position to complete the proof of Theorem 1.16. This will be achieved by combining Lemmas 1.42 and 1.45.

Let $G \in \mathcal{G}(n)$. If $n = 6, 7$ and $sdiam_3(G) = 5$, then the validity of Theorem 1.16 can be verified by direct checking.

Lemma 1.45. [113] *Let $G \in \mathcal{G}(n)$ be a connected graph. Let $n \geq 8$, or $n \leq 5$, or $n = 6, 7$ and $sdiam_3(G) \neq 5$, or $n = 6, 7$ and $sdiam_3(\overline{G}) \neq 5$. Then the upper bounds in parts (1) and (2) of Theorem 1.16 are obeyed. Moreover, these bounds are sharp.*

Proof. We need to separately examine three cases.

Case 1. $sdiam_3(G) \geq 6$ or $sdiam_3(\overline{G}) \geq 6$.

Without loss of generality, let $sdiam_3(G) \geq 6$. From Corollary 1.1 it is known that $sdiam_3(\overline{G}) = 3$, and hence $SW_3(G) + SW_3(\overline{G}) \leq SW_3(P_n) + SW_3(\overline{S^*})$. By Lemma 1.37, $SW_3(P_n) = 2\binom{n+1}{4}$. Note that $\overline{S^*}$ is a graph obtained from a clique of order $n-1$ by deleting an edge uv and then adding a pendent edge at v. Then $SW_3(\overline{S^*}) = 7\binom{n-3}{2} + 2\binom{n-3}{3} + 7n - 18$, and hence $SW_3(G) + SW_3(\overline{G}) \leq 2\binom{n+1}{4} + 7\binom{n-3}{2} + 2\binom{n-3}{3} + 7n - 18 = 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{1}{2}(7n^2 - 35n + 48)$.

Case 2. $sdiam_3(G) = 5$ or $sdiam_3(\overline{G}) = 5$.

In view of Lemma 1.41, we can assume that $sdiam_3(G) = 5$ and $sdiam_3(\overline{G}) \leq 4$. Let $S_1, S_2, \ldots, S_{\binom{n}{3}}$ be all the 3-subsets of $V(G)$. Without loss of generality, assume that $S_1, S_2, \ldots, S_x$ are the 3-subsets of $V(G)$ for which $G[S_i] \cong K_3$ or $G[S_i] \cong P_3$, where $1 \leq i \leq x$.

For each i $(1 \leq i \leq x)$, $d_G(S_i) = 2$. For any S_j $(x+1 \leq j \leq \binom{n}{3})$, $G[S_j] \cong K_2 \cup K_1$ or $G[S_j] \cong 3K_1$. Since G is connected, it follows that there exists a spanning tree, say T. By Lemmas 1.38 and 1.39, there exist at least $(n-3)$ subsets of $V(T)$ whose Steiner 3-distance is 3, and there exist at least $(n-2)$ subsets of $V(T)$ whose Steiner 3-distance is 2. Therefore, there exist at least $(2n-5)$ subsets of $V(G)$ whose Steiner 3-distance is at most 3. Without loss of generality, let $d_G(S_j) = 3$ for S_j $(x+1 \leq j \leq 2n-5)$. Then $d_G(S_j) \leq 5$ and $d_{\overline{G}}(S_j) = 2$ for each j $(2n-4 \leq j \leq \binom{n}{3})$. For each i $(1 \leq i \leq x)$, $d_G(S_i) = 2$. By Lemma 3.9, there exist at least $(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance is 3. Then there exist at most $x-(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance is 4. If $x \leq 2n-5$, then $SW_3(G) \leq 2x + 3(2n-5-x) + 5\left[\binom{n}{3} - 2n + 5\right]$ and $SW_3(\overline{G}) \leq 3(n-3) + 4(x-n+3) + 2\left[\binom{n}{3} - x\right]$, and hence $SW_3(G) + SW_3(\overline{G}) \leq 7\binom{n}{3} + x - 5n + 13 \leq 7\binom{n}{3} - 3n + 8$. If $x \geq 2n-5$. Then $SW_3(G) \leq 2x + 5\left[\binom{n}{3} - x\right]$ and $SW_3(\overline{G}) \leq 3(n-3) + 4(x-n+3) + 2\left[\binom{n}{3} - x\right]$, and hence $SW_3(G) + SW_3(\overline{G}) \leq 7\binom{n}{3} - x - n + 3 \leq 7\binom{n}{3} - 3n + 8$.

Case 3. $sdiam_3(G) \leq 4$ and $sdiam_3(\overline{G}) \leq 4$.

Let $S_1, S_2, \ldots, S_{\binom{n}{3}}$ be the 3-subsets of $V(G)$. Without loss of generality, let $S_1, S_2, \ldots, S_x$ be the 3-subsets of $V(G)$ for which $G[S_i] \cong K_3$ or $G[S_i] \cong P_3$, where $1 \leq i \leq x$. For each i $(1 \leq i \leq x)$, $d_G(S_i) = 2$. For any S_j $(x+1 \leq j \leq \binom{n}{3})$, $G[S_j] \cong K_2 \cup K_1$ or $G[S_j] \cong 3K_1$. Since G is connected, there exists a spanning tree, say T. By Lemmas 1.38 and 1.39, there exist at least $(n-3)$ subsets of $V(T)$ whose Steiner 3-distance is equal to 3, and there exist at least $(n-2)$ subsets of $V(T)$ whose Steiner 3-distance is 2. Therefore, there exist at least $(2n-5)$ subsets of $V(G)$ whose Steiner 3-distance is at most 3. Without loss of generality, let $d_G(S_j) = 3$ for S_j $(x+1 \leq j \leq 2n-5)$. Then $d_G(S_j) \leq 4$ and $d_{\overline{G}}(S_j) = 2$ for each j $(2n-4 \leq j \leq \binom{n}{3})$. For each i $(1 \leq i \leq x)$, $d_G(S_i) = 2$. By Lemma 1.39, there exist at least $(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance in $\overline{G}$ is 3. Then there exist at most $x-(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance in $\overline{G}$ is 4. If $x \leq 2n-5$, then $SW_3(G) \leq 2x + 3(2n-5-x) + 4\left[\binom{n}{3} - 2n + 5\right]$ and $SW_3(\overline{G}) \leq 3(n-3) + 4(x-n+3) + 2\left[\binom{n}{3} - x\right]$. Thus

$$SW_3(G) + SW_3(\overline{G}) \leq 6\binom{n}{3} + x - 3n + 8 \leq 6\binom{n}{3} - n + 3\,.$$

If $x \geq 2n-5$, then $SW_3(G) \leq 2x + 4\left[\binom{n}{3} - x\right]$ and $SW_3(\overline{G}) \leq 3(n-3) + 4(x-n+3) + 2\left[\binom{n}{3} - x\right]$.

Thus

$$SW_3(G) + SW_3(\overline{G}) \le 6\binom{n}{3} - n + 3\,.$$

For $n \ge 4$, one can check that $2\binom{n+1}{4}+2\binom{n-3}{3}+\frac{1}{2}(7n^2-35n+48) \ge 6\binom{n}{3}-n+3$ and $7\binom{n}{3}-3n+8 \ge 6\binom{n}{3} - n + 3$. So we only need to consider the upper bounds in Cases 1 and 2.

From the above argument, we conclude the following:

(1) For $n \ge 8$,

$$2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{7n^2 - 35n + 48}{2} \ge 7\binom{n}{3} - 3n + 8$$

and

$$SW_3(G) + SW_3(\overline{G}) \le 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{7n^2 - 35n + 48}{2}\,.$$

(2) For $n \le 5$, the upper bound in Case 2 does not exist. Then

$$SW_3(G) + SW_3(\overline{G}) \le 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{7n^2 - 35n + 48}{2}\,.$$

(3) If $n = 6, 7$, $sdiam_3(G) \ne 5$, and $sdiam_3(\overline{G}) \ne 5$, then

$$SW_3(G) + SW_3(\overline{G}) \le 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{7n^2 - 35n + 48}{2}\,.$$

(4) If $n = 6, 7$ and $sdiam_3(G) = 5$, or $n = 6, 7$ and $sdiam_3(\overline{G}) = 5$, then

$$SW_3(G) + SW_3(\overline{G}) \le 7\binom{n}{3} - 3n + 8\,.$$

This completes the proof.

In order to demonstrate the sharpness of the above bounds, we point out the following example.

Example 1.3. [113] Let $G \cong P_4$. Then $\overline{G} \cong P_4$. By Lemma 1.37, $SW_3(G) = SW_3(\overline{G}) = 10$, and hence $SW_3(G) + SW_3(\overline{G}) = 20 = 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{1}{2}\left(7n^2 - 35n + 48\right)$ and $SW_k(G) \cdot SW_k(\overline{G}) = 100 = \left[\binom{n+1}{4} + \binom{n-3}{3} + \frac{1}{4}\left(7n^2 - 35n + 48\right)\right]^2$, which implies that the upper and lower bounds are sharp.

1.9 Harary index

The Harary index of a molecular graph has been introduced in 1993 in this Journal independently by Plavšić, Nikolić, Trinajstić, Mihalić [123] and by Ivanciuc, T. S. Balaban, A. T. Balaban [87] for characterization of G. The *Harary index* $H(G)$ of a graph G is defined by

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}\,.$$

In [154], Zhou, Cai, and Trinajstić obtained the Nordhaus–Gaddum problem for the Harary index.

Theorem 1.17. [154] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected graph. Then*

$$1 + \frac{(n-1)^2}{2} + n\sum_{k=2}^{n-1}\frac{1}{k} \leq H(G) + H(\overline{G}) \leq \frac{3n(n-1)}{4}. \tag{17}$$

with left (right, respectively) equality in (17) if and only if $G = P_n$ or $G = \bar{P}_n$ (both G and G have diameter 2, respectively).

Later, Das, Zhou, and Trinajstić [37] obtained the following bounds for Harary index.

Lemma 1.46. [37] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ be a connected graph with diameter d. Then*

$$H(P_{d+1}) + \frac{n(n-1) + 2(m-d)(d-1)}{2d} - \frac{d+1}{2} \leq H(G) \leq H(P_{d+1}) + \frac{n(n-1)+2m}{4} - \frac{d(d+3)}{4},$$

with left (right, respectively) equality holds if and only if G is a graph of diameter at most 2 or G is a path P_n (G is a graph of diameter at most 2 or G is a path P_n or G is isomorphic to G^*, respectively).

Denote by $G^* = (V, E)$, a graph of diameter d ($3 \leq d \leq 4$ and $|V(G^*)| \geq d+2$) such that any vertex v_i, $v_i \in V(G^*) \setminus V(P_{d+1})$, $\delta(i,j \,|\, G^*) = 1$ or $\delta(i,j \,|\, G^*) = 2$ for any vertex $v_j \in V(G^*)$, $j \neq i$, where P_{d+1} is a path of $d+1$ vertices in G^*. The two graphs depicted in Table 1.3 are of G^* type graph. Then

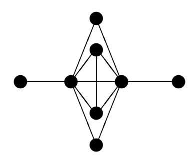	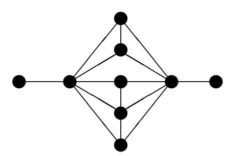
B_1	B_2

Table 1.3 Graphs are of G^* type graph.

Lemma 1.47. [37] *Let P_n be a path of n vertices. Then*

$$H(P_n) \leq \frac{(n-1)(n+2)}{4}.$$

Moreover, equality holds if and only if either $n = 2$ or $n = 3$.

By the above bounds, they gave a lower bound for $H(G) + H(\overline{G})$.

Theorem 1.18. [37] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph. Then*

$$H(G) + H(\overline{G}) \geq H(P_{k+1}) + \frac{n(n-1)}{2}\left(1 + \frac{1}{k}\right) - 3k + \frac{7}{2}, \tag{18}$$

where $k = \max\{d, \bar{d}\}$, d and $\bar{d}$ are diameter of G and $\overline{G}$, respectively. Moreover, the equality holds in (18) if and only if both G and $\overline{G}$ have diameter 2.

Proof. For a connected graph G with $n \geq 2$ vertices, m edges, and diameter d, from Lemma 1.46, we have

$$H(G) \geq H(P_{d+1}) + m + \frac{\overline{m}}{d} - \frac{3}{2}d + \frac{1}{2},$$

where $\overline{m}$ is the number of edges in $\overline{G}$. Using above result, we get

$$\begin{aligned} H(G) + H(\overline{G}) &\geq H(P_{d+1}) + H(P_{\overline{d}+1}) + m + \overline{m} + \frac{\overline{m}}{d} + \frac{m}{\overline{d}} - \frac{3}{2}(d + \overline{d}) + 1 \quad (19) \\ &\geq H(P_{d+1}) + H(P_{\overline{d}+1}) + (m + \overline{m})\left(1 + \frac{1}{k}\right) - 3k + 1 \\ &\quad \text{as } k = \max\{d, \overline{d}\} \quad (20) \\ &\geq H(P_{d+1}) + \frac{n(n-1)}{2}(1 + \frac{1}{k}) - 3k + \frac{7}{2} \\ &\quad \text{as } k = \max\{d, \overline{d}\} \text{ and } d, \overline{d} \geq 2. \quad (21) \end{aligned}$$

Now suppose that (18) holds. Then all inequalities in the above argument must be equalities. Then from (19), we get G is a graph of diameter 2 or G is a path P_n, and $\overline{G}$ is graph of diameter 2 or $\overline{G}$ is a path P_n. From (19), we get $k = d = \overline{d}$. Also from (20), we get either $d = 2$ or $\overline{d} = 2$. Hence both G and $\overline{G}$ have diameter 2.

Conversely, one can easily check that (18) holds for both G and $\overline{G}$ of diameter 2. ■

Remark 1.8. [37] *For graph A_1 in Table 1.2, the lower bound (18) for $H(G) + H(\overline{G})$ is 31.5 better then 29.15, the lower bound given in (17). But for graph G_2, the lower bound (17) is 21.2 better then our lower bound 16.67, given in (18). So the lower bounds are given in (17) and (18), are not comparable.*

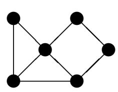	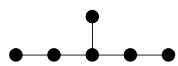
D_1	D_2

Table 1.4 Graphs for Remark 1.2.

They also gave a lower bound for $H(G)+H(\overline{G})$ in terms of the number of vertices n and the diameter d in G.

Theorem 1.19. [37] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph. Then*

$$H(G) + H(\overline{G}) \leq H(P_{d+1}) + \frac{3n(n-1)}{4} - \frac{d(d+3)}{4}. \quad (22)$$

Moreover, the equality holds in (22) if and only if both G and $\overline{G}$ have diameter 2 or G is a path P_n.

Proof. Since G and $\overline{G}$ are connected, it follows that $d \geq 2$ and $\overline{d} \geq 2$. By Lemma 1.46, we get

$$\begin{aligned} H(G) + H(\overline{G}) \leq H(P_{d+1}) &+ \frac{n(n-1) + 2m}{4} - \frac{d(d+3)}{4} \\ + H(P_{\overline{d}+1}) &+ \frac{n(n-1) + 2\overline{m}}{4} - \frac{\overline{d}(\overline{d}+3)}{4}, \quad (23) \end{aligned}$$

where $\overline{m}$ is the number of edges in $\overline{G}$ and $\overline{d}$ is the diameter in $\overline{G}$.

Using Lemma 1.47 in above result, we get

$$H(G) + H(\overline{G}) \leq H(P_{d+1}) + \frac{3n(n-1)}{4} - \frac{d(d+3)}{4} \qquad \text{as } 2\overline{m} = n(n-1) - 2m. \tag{24}$$

Now suppose that equality holds in (22). Then the (23) and (24) hold. From (23), we have G is a graph of diameter at most 2 or G is a path P_n and $\overline{G}$ is a graph of diameter at most 2 or $\overline{G}$ is a path P_n. From (24), we must have

$$H(P_{\overline{d}+1}) = \frac{\overline{d}(\overline{d}+3)}{4}$$

By Lemma 1.47, $\overline{d} = 2$ as $\overline{d} \neq 1$. Hence both G and $\overline{G}$ have diameter 2 or G is a path P_n.

Conversely, one can see easily that (22) holds for both G and $\overline{G}$ have diameter 2 or $G = P_n$. ■

Remark 1.9. [37] *By Lemma 1.46, one can easily that (22) is always better then the upper bound given in (17).*

Remark 1.10. [37] *The lower and upper bounds given by (17) and (22), respectively, are equal when both G and $\overline{G}$ have diameter* 2.

For a triangle- and quadrangle-free graph, they proved the following.

Theorem 1.20. [37] *Let $G \in \mathcal{G}(n, m)$ $(n \geq 2)$ be a triangle- and quadrangle-free graph. Then*

$$H(G) + H(\overline{G}) \leq \frac{1}{6}M_1(G) + \frac{7n(n-1)}{12} + \frac{n(n-1)^2}{12} - \frac{m(n-1)}{3}. \tag{25}$$

Moreover, the equality holds in (25) if and only if both G and $\overline{G}$ have diameter at most 3.

1.10 Szeged index

Let $G = (V, E)$ be a connected graph on n vertices. Let uv be an edge of G. Define two vertex sets in G as

$$\begin{aligned} N_u(uv) &= \{w \in V : d_G(u, w) < d_G(v, w)\} \\ N_v(uv) &= \{w \in V : d_G(v, w) < d_G(u, w)\} \end{aligned}$$

Denote by $n_u(uv)$ and $n_v(uv)$ the cardinalities of $N_u(uv)$ and $N_v(uv)$, respectively. In 1994, Gutman [61] introduced the Szeged index $\mathrm{Sz}(G)$ of a connected graph G as

$$\mathrm{Sz}(G) = \sum_{uv \in E(G)} n_u(uv) n_v(uv).$$

Gutman proposed the Szeged index as an extension of the Wiener index (the sum of all distances) of trees to the connected graphs containing cycles. Indeed, in the class of trees, the Szeged index and the Wiener index are equal.

Das and Gutman [27] first observed:

$$\begin{aligned} 2Sz(\overline{P_n}) &= 2(2+4+\underbrace{6+6+\cdots+6}_{n-4})+2(4+6+\underbrace{9+9+\cdots+9}_{n-5}) \\ &\quad +2(2+4+6+\underbrace{9+9+\cdots+9}_{n-6})+(n-6)(4+4+6+6+\underbrace{9+9+\cdots+9}_{n-7}) \\ &= 2(6n-18)+2(9n-35)+2(9n-42)+(9n-43)(n-6), \end{aligned}$$

that is,

$$Sz(\overline{P_n}) = \frac{1}{2}(9n^2-49n+68).$$

Next, they derived the following lower bound of $\mathrm{Sz}(G)$ for a connected graph G.

Lemma 1.48. [27] *Let G be a connected graph with m edges and diameter d. Then*

$$\mathrm{Sz}(G) \geq m + \frac{1}{6}d(d^2+3d-4) \tag{26}$$

with equality holding if and only if $G \cong K_n$ or $G \cong P_n$.

Nordhaus–Gaddum inequalities for Szeged index were obtained by Das and Gutman [27].

Theorem 1.21. [27] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph on diameter d, and with a connected complement $\overline{G}$. Then*

$$\mathrm{Sz}(G) + \mathrm{Sz}(\overline{G}) \geq \frac{n(n-1)}{2} + \frac{1}{6}(d^3+27d^2-94d+84) \tag{27}$$

with equality holding if and only if $G \cong P_n$.

Proof. Since G has diameter d, it follows that $\overline{P}_{d+1}$ is a subgraph of $\overline{G}$. Thus

$$Sz(\overline{G}) \geq Sz(\overline{P}_{d+1}) + \sum_{e \in E(\overline{G}) \setminus E(\overline{P}_{d+1})} n_1(e\,|\,\overline{G})n_2(e\,|\,\overline{G}) \tag{28}$$

$$\geq \frac{1}{2}(9d^2-31d+28) + \overline{m} - \frac{1}{2}d(d-1) \tag{29}$$

$$= \frac{1}{2}(9d^2-31d+28) + \frac{n(n-1)}{2} - m - \frac{1}{2}d(d-1). \tag{30}$$

From (26) and (30), we get

$$\mathrm{Sz}(G) + \mathrm{Sz}(\overline{G}) \geq \frac{n(n-1)}{2} + \frac{1}{2}(9d^2-31d+28) - \frac{1}{2}d(d-1) + \frac{1}{6}d(d^2+3d-4) \tag{31}$$

and inequality (27) follows.

Suppose now that equality holds in (27). Then equality holds in (28), (29) and (31). Using the same technique as in Lemma 1.48, we conclude that $G \cong P_n$. Conversely, one can easily check that (27) holds for $G \cong P_n$. ∎

It was first observed by Goodman [57] that $t(G) + t(\overline{G})$ is determined by the degree sequence:

Lemma 1.49. [57] *Let $t(G)$ and $t(\overline{G})$ be, respectively, the number of triangles in G and $\overline{G}$. Then*

$$t(G) + t(\overline{G}) = \frac{1}{2}\sum_{i=1}^{n} d_i^2 - (n-1)m + \frac{1}{6}n(n-1)(n-2). \tag{32}$$

Lemma 1.50. [57] *Let $G \in \mathcal{G}(n,m)$ $(n > 2)$ be a connected graph with $t(G)$ triangles. Then*

$$\mathrm{Sz}(G) \leq \frac{1}{4}n^2 m - 3t(G). \tag{33}$$

Moreover, if equality holds in (33), then G is bipartite, n is even and the minimum vertex degree is greater than or equal to 2.

A structure descriptor introduced long time ago [133] is the so-called *first Zagreb index* (M_1) equal to the sum of squares of the degrees of all vertices.

Theorem 1.22. [27] *Let $G \in \mathcal{G}(n,m)$ $(n > 2)$ be a connected graph with $t(G)$ triangles, and with a connected complement $\overline{G}$. Then*

$$\mathrm{Sz}(G) + \mathrm{Sz}(\overline{G}) \leq \frac{1}{8}n(n-1)(n^2-4n+8) - \frac{3}{2}M_1 + 3(n-1)m. \tag{34}$$

Proof. We start by inequality (33). Let $\overline{m}$ be the number of edges of $\overline{G}$. Then

$$\mathrm{Sz}(G) + \mathrm{Sz}(\overline{G}) \leq \frac{1}{4}n^2(m+\overline{m}) - 3\left(t(G) + t(\overline{G})\right). \tag{35}$$

Since $m + \overline{m} = \frac{1}{2}n(n-1)$, inequality (34) is obtained by combining (33) with (35). ■

1.11 Vertex PI index

In view of the considerable success of the Szeged index in chemical graph theory, an additive version of it has been put forward, called the *vertex PI index*:

$$PI(G) = \sum_{uv \in E(G)} [n_u(uv) + n_v(uv)] = \sum_{e \in E(G)} [n_1(e|G) + n_2(e|G)].$$

Das and Gutman [29] first gave a lower bound of $PI(G)$ for a connected graph G.

Lemma 1.51. [29] *Let $G \in \mathcal{G}(n,m)$ be a connected graph on diameter d. Then*

$$PI(G) \geq 2m + d^2 - d. \tag{36}$$

Moreover, the lower bound is reached if and only if $G \cong K_n$ or $G \cong P_n$; the upper bound is reached if and only if G is a bipartite graph or $G \cong K_3$.

Next, they observed that for $n \geq 5$,

$$\begin{aligned} 2PI(\overline{P}_n) &= 2(3+4+\underbrace{5+5+\cdots+5}_{n-4}) + 2(4+5+\underbrace{6+6+\cdots+6}_{n-5}) \\ &+ 2(3+4+5+\underbrace{6+6+\cdots+6}_{n-6}) + (n-6)(4+4+5+5+\underbrace{6+6+\cdots+6}_{n-7}) \\ &= 2(5n-13) + 2(6n-21) + 2(6n-24) + (6n-24)(n-6), \end{aligned}$$

that is,

$$PI(\overline{P}_n) = (n-2)(3n-7).$$

By the above lemma, they proved the Nordhaus–Gaddum inequality for vertex PI index.

Theorem 1.23. [29] *Let $G \in \mathcal{G}(n)$ be a connected graph on diameter d, and with a connected complement $\overline{G}$. Then*

$$PI(G) + PI(\overline{G}) \geq n(n-1) + (d-1)(3d-4) \tag{37}$$

with equality holding if and only if $G \cong P_n$.

Proof. Since G has diameter d, it follows that $\overline{P}_{d+1}$ is a subgraph of $\overline{G}$, and hence

$$PI(\overline{G}) \geq PI(\overline{P}_{d+1}) + \sum_{e \in E(\overline{G}) \setminus E(\overline{P}_{d+1})} [n_1(e \,|\, \overline{G}) + n_2(e \,|\, \overline{G})] \tag{38}$$

$$\geq (d-1)(3d-4) + 2\left[\overline{m} - \frac{1}{2}d(d-1)\right] \tag{39}$$

$$= 2(d-1)(d-2) + n(n-1) - 2m\,. \tag{40}$$

From (36) and (40) we get

$$PI(G) + PI(\overline{G}) \geq 2(d-1)(d-2) + n(n-1) + d^2 - d \tag{41}$$

and inequality (37) follows.

Suppose now that equality holds in (37). Then equality holds in (38), (39), and (41). Using the same way of reasoning as in the proof of Lemma 1.51, we conclude that $G \cong P_n$.

Conversely, one can easily check that (37) holds for $G \cong P_n$. ∎

Lemma 1.52. [29] *Let $G \in \mathcal{G}(n,m)$ be a connected graph, possessing $t(G)$ triangles. Then*

$$PI(G) \leq nm - 3t(G).$$

Moreover, the upper bound is reached if and only if G is a bipartite graph or $G \cong K_3$.

Das and Gutman [26] also obtained an upper bound for $PI(G) + PI(\overline{G})$:

Theorem 1.24. [29] *Let $G \in \mathcal{G}(n,m)$ $(n > 2)$ be a connected graph on diameter d, $t(G)$ triangles, and with a connected complement $\overline{G}$. Then*

$$PI(G) + PI(\overline{G}) \leq (n-1)(3m+n) - \frac{3}{2}M_1(G). \tag{42}$$

Moreover, the equality holds in (42) if and only if $G \cong P_4$.

Proof. Let $\overline{m}$ be the number of edges of $\overline{G}$. By (36), we get

$$PI(G) + PI(\overline{G}) \leq n(m + \overline{m}) - 3[t(G) + t(\overline{G})] \tag{43}$$

$$= \frac{1}{2}n^2(n-1) - \frac{3}{2}\sum_{i=1}^{n} deg(v_i)^2 + 3(n-1)m - \frac{1}{2}n(n-1)(n-2). \tag{44}$$

Since $m + \overline{m} = \frac{n(n-1)}{2}$, inequality (42) is obtained from (44).

Suppose now that equality holds in (42). Then equality holds in (43). From (36) we conclude that both G and $\overline{G}$ are bipartite graphs. So we may assume that $V(G) = A \cup B$ and $A \cap B = \emptyset$. Since $\overline{G}$ is also bipartite, we must have $|A| \leq 2$ and $|B| \leq 2$. Furthermore, since G and $\overline{G}$ both are connected, it must be $G \cong P_4$.

Conversely, one can easily check that (42) holds for $G \cong P_4$. ■

1.12 Co–PI index

Hassani, Khormali, and Iranmanesh [75] introduced a new topological index similar to the vertex version of PI index. This index is called the ***Co-PI index*** of G and defined as:

$$Co - PI_v(G) = \sum_{e=uv \in E(G)} |n_u(e) - n_v(e)|. \tag{45}$$

Here the summation goes over all edges of G. Fath-Tabar, Došlić, and Ashrafi proposed the Szeged matrix and Laplacian Szeged matrix in [49]. Then Su, Xiong, and Xu [131] introduced the Co-PI matrix of a graph. The *adjacent matrix* $(a_{ij})_{n \times n}$ of G is the integer matrix with rows and columns indexed by its vertices, such that the ij-th entry is equal to the number of edges connecting i and j. Let the weight of the edge $e = uv$ be a non-negative integer $|n_u(e) - n_v(e)|$, we can define a weight function: $w : E \to R^+ \cup \{0\}$ on E, which is said to be the ***Co-PI weighting*** of G. The adjacency matrix of G weighted by the Co-PI weighting is said to be its ***Co-PI matrix*** and denoted by $M_{CPI} = (c_{ij})_{n \times n}$. That is,

$$c_{ij} = \begin{cases} |n_{v_i}(e) - n_{v_j}(e)| & \text{if } e = v_i v_j \\ 0 & \text{otherwise.} \end{cases}$$

Its eigenvalues are said to be the ***Co-PI eigenvalues*** of G and denoted by $\lambda_i^*(G)$ for $k = 1, 2, \ldots, |V|$. Easy verification shows that the ***Co-PI index*** of G can be expressed as one half of the sum of all entries of M_{CPI}, i.e.,

$$Co - PI_v(G) = \frac{1}{2}\sum_{i=1}^{n} M_{CPI_i}(G),$$

where M_{CPI_i} is the sum of i-th row of the matrix M_{CPI}.

Kaya and Maden [90] presented Nordhaus–Gaddum type equalities for the largest Co-PI eigenvalue of G. Let G be a connected graph on $n \geq 3$ vertices and m edges. Furthermore, assume that $G \in \mathscr{H}$ has a connected complement $\overline{G}$ with $\overline{m}$ edges. As one can easily prove, the following equality:

$$2(m + \overline{m}) = n(n-1).$$

The following lemma is due to Su, Xiong, and Xu [131].

Lemma 1.53. [131] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 3)$ be connected graph. Then*

$$2m \leq \lambda_1^{*2}(G) + \lambda_2^{*2}(G) + \cdots + \lambda_n^{*2}(G) \leq 2m(n-2)^2.$$

Note that $trace(M_{CPI}) = 0$ and denote by $N = N(G)$ the trace of M_{CPI}^2. Therefore, for $i = 1, 2, \ldots, n$, the eigenvalues $\lambda_i^*(G)$ of M_{CPI} satisfy the relations

$$\sum_{i=1}^{n} \lambda_i^*(G) = 0$$

and

$$\sum_{i=1}^{n} \lambda_i^{*2}(G) = N(G).$$

Let $\mathscr{H}$ be the class of connected graphs whose Co-PI matrices have exactly one positive eigenvalue. In the following, we give upper and lower bounds for $\lambda_1^*(G)$ of graphs in the class $\mathscr{H}$ in terms of the number of vertices and $N(G)$.

Lemma 1.54. [131] *Let $G \in \mathscr{H}$ with $n \geq 2$ vertices. Then*

$$\lambda_1^*(G) \leq \sqrt{\frac{n-1}{n} N(G)}.$$

Lemma 1.55. [131] *Let $G \in \mathscr{H}$ with $n \geq 2$ vertices. Then*

$$\lambda_1^*(G) \geq \sqrt{\frac{N(G)}{2}}.$$

By Lemmas 1.53, 1.54 and 1.55, Kaya and Maden [90] derived the following Nordhaus–Gaddum-type results.

Theorem 1.25. [131] *Let $G \in \mathscr{H}$ with $n \geq 3$ vertices, and let $\overline{G}$ be connected. Then*

$$\lambda_1^*(G) + \lambda_1^*(\overline{G}) \leq \sqrt{\frac{n-1}{n}} \left[\sqrt{2m(n-2)^2} + \sqrt{(n(n-1) - 2m)(n-2)^2} \right].$$

Theorem 1.26. [131] *Let $G \in \mathscr{H}$ with $n \geq 3$ vertices, and let $\overline{G}$ be connected. Then*

$$\lambda_1^*(G) + \lambda_1^*(\overline{G}) \geq \sqrt{m} + \sqrt{\frac{(n(n-1) - 2m)}{2}}.$$

1.13 Second geometric–arithmetic index

The first geometric-arithmetic index GA_1 will be introduced in the next chapter. The *second geometric-arithmetic index*, introduced by [50], is based on the notion of distance. Using the same notation as in the definition of the Szeged index, the formula of GA_2 is

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u(uv) n_v(uv)}}{n_u(uv) + n_v(uv)}.$$

Das, Gutman, and Furtula [32] derived a lower bound of $GA_2(G)$ for a graph G.

Lemma 1.56. [32] *Let $G \in \mathcal{G}(n,m)$ be a connected graph with p pendent vertices. Then*

$$GA_2(G) \geq \frac{2m\sqrt{n-2}}{n-1} - 2p\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right). \tag{46}$$

Equality holds in (46) if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$.

Nordhaus–Gaddum type inequalities for the second geometric-arithmetic index were proved by Das, Gutman, and Furtula [32] in 2010.

Theorem 1.27. [32] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected complement $\overline{G}$. Then*

$$GA_2(G) + GA_2(\overline{G}) \geq \frac{2\sqrt{n-2}}{n-1}\binom{n}{2} - 2(p+\bar{p})\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right), \tag{47}$$

where p and $\bar{p}$ are the number of pendent vertices in G and $\overline{G}$, respectively.

Proof. We have $m + \overline{m} = \binom{n}{2}$ where $\overline{m}$ is the number of edges in $\overline{G}$, Using (46), we get

$$\begin{aligned} GA_2(G) + GA_2(\overline{G}) &\geq \frac{2\sqrt{n-2}}{n-1}(m+\overline{m}) - 2(p+\overline{p})\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right) \\ &= \frac{2\sqrt{n-2}}{n-1}\binom{n}{2} - 2(p+\overline{p})\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right) \end{aligned}$$

Inequality (47) follows now from Lemma 1.56. ■

Let $\mathscr{G}_1$ be the class of graphs $H_1 = (V_1, E_1)$ such that H_1 is connected graph with $n_i = n_j$ for each edge $ij \in E(H_1)$. For example, $K_{1,n-1}, K_n \in \mathscr{G}_1$. Denote by C_n^*, a unicyclic graph of order n and cycle length k, such that each vertex in the cycle is adjacent to one pendent vertex, $n = 2k$. Let $\mathscr{G}_2$ be the class of graphs $H_2 = (V_2, E_2)$, such that H_2 is connected graph with $n_i = n_j$ for each non-pendent edge $ij \in E(H_2)$. For example, $C_n^* \in \mathscr{G}_2$.

Lemma 1.57. [32] *Let $G \in \mathcal{G}(n,m)$ $(n > 2)$ be a connected graph with p pendent vertices. Then*

$$GA_2(G) \leq \frac{2p\sqrt{n-1}}{n} + m - p. \tag{48}$$

Equality in (48) holds if and only if $G \cong K_{1,n-1}$ or $G \in \mathscr{G}_1$ or $G \in \mathscr{G}_2$.

By the above lemma, they derived the following Nordhaus–Gaddum type result for $GA_2(G)$.

Theorem 1.28. [32] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected complement $\overline{G}$. Then*

$$GA_2(G) + GA_2(\overline{G}) \leq \binom{n}{2} - (p+\bar{p})\left(1 - \frac{2\sqrt{n-1}}{n}\right), \tag{49}$$

where p and $\bar{p}$ are the number of pendent vertices in G and $\overline{G}$, respectively.

Proof. By (48), we get

$$\begin{aligned} GA_2(G) + GA_2(\overline{G}) &\leq \frac{2\sqrt{n-1}}{n}(p+\overline{p}) + (m+\overline{m}) - (p+\overline{p}) \\ &= \binom{n}{2} - (p+\overline{p})\left(1 - \frac{2\sqrt{n-1}}{n}\right), \end{aligned}$$

since $m + \overline{m} = \binom{n}{2}$.

The following corollary is immediate.

Corollary 1.3. [32] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected complement $\overline{G}$. Then*

$$GA_2(G) + GA_2(\overline{G}) \leq \binom{n}{2}.$$

1.14 Third geometric–arithmetic index

A further molecular structure descriptor, belonging to the class of GA-indices, is the so-called third geometric-arithmetic index; see [157].

Let $ij \in E(G)$ be an edge of the graph G, connecting the vertices i and j. Let $x \in V(G)$ be any vertex of G. The *distance between x and ij* is denoted by $d(x, ij \mid G)$ and is defined as $\min\{d_G(x,i), d_G(x,j)\}$. For $ij \in E(G)$, let

$$m_i = |\{f \in E(G) : d(i, f \mid G) < d(j, f \mid G)\}|.$$

It is immediate to see that in all cases $m_i \geq 0$ and $m_i + m_j \leq m - 1$.

It should be noted that m_i is not a quantity that is in a unique manner associated with the vertex i of the graph G, but that it depends on the edge ij. Yet, this restriction is not relevant for the definition of GA_3. Then the *third geometric-arithmetic index* is defined as

$$GA_3 = GA_3(G) = \sum_{ij \in E(G)} \frac{\sqrt{m_i m_j}}{\frac{1}{2}[m_i + m_j]}.$$

By $S(2r, s)$ $(r \geq 1,\ s \geq 1)$, we denote the starlike tree with diameter less than or equal to 4, which has a vertex v_1 of degree $r + s$ and which has the property that

$$S(2r, s) \setminus \{v_1\} = \underbrace{P_2 \cup P_2 \cup \ldots \cup P_2}_{r} \cup \underbrace{P_1 \cup P_1 \cup \ldots \cup P_1}_{s}$$

For additional details on $S(2r, s)$, see [32].

In 2010, Das, Gutman and Furtula [31] obtained a lower bound of $GA_3(G)$ for a connected graph G.

Lemma 1.58. [31] *Let $G \in \mathcal{G}(n, m)$ $(n > 2)$ be a connected graph with p pendent vertices. Then*

$$GA_3(G) \geq \frac{2(m-p)\sqrt{m-2}}{m-1}. \tag{50}$$

Equality in (50) holds if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$ or $G \cong S(2r, s)$, $n = 2r + s + 1$.

The following theorem is an immediate consequence of inequality (50).

Theorem 1.29. [31] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected complement $\overline{G}$. Then*

$$GA_3(G) + GA_3(\overline{G}) \geq \frac{2(m-p)\sqrt{m-2}}{m-1} + \frac{2(\overline{m}-\overline{p})\sqrt{\overline{m}-2}}{\overline{m}-1},$$

where $p, \overline{p}$ and $m, \overline{m}$ are the number of pendent vertices and edges in G and $\overline{G}$, respectively.

Let $\mathscr{H}_1$ be the class of graphs $H_1 = (V_1, E_1)$, such that H_1 is connected graph with $m_i = m_j$ for each edge $ij \in E(H_1)$. For example, $K_n, C_n \in \mathscr{H}_1$. Denote by C_n^*, an unicyclic graph of order n and cycle length k, such that each vertex in the cycle is adjacent to one pendent vertex, $n = 2k$. Let $\mathscr{H}_2$ be the class of graphs $H_2 = (V_2, E_2)$, such that H_2 is connected graph with $m_i = m_j$ for each non-pendent edge $ij \in E(H_2)$. For example, $C_n^* \in \mathscr{H}_2$.

Das, Gutman and Furtula [31] stated an upper bound on $GA_3(G)$.

Lemma 1.59. [31] *Let $G \in \mathcal{G}(n, m)$ $(n > 2)$ be a connected graph with p pendent vertices. Then*

$$GA_3(G) \leq m - p. \tag{51}$$

Equality in (51) holds if and only if $G \cong K_{1,n-1}$ or $G \in \mathscr{H}_1$ or $G \in \mathscr{H}_2$.

By the above lemma, they proved the following Nordhaus–Gaddum-type inequality for $GA_3(G)$.

Theorem 1.30. [31] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected complement $\overline{G}$. Then*

$$GA_3(G) + GA_3(\overline{G}) \leq \binom{n}{2} - p - \bar{p}. \tag{52}$$

Proof. By (51),

$$GA_3(G) + GA_3(\overline{G}) \leq (m + \overline{m}) - (p + \overline{p})$$

One arrives at (52) by noting that $m + \overline{m} = \binom{n}{2}$. ■

Directly from Theorem 1.30 follows:

Corollary 1.4. [31] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected complement $\overline{G}$. Then*

$$GA_3(G) + GA_3(\overline{G}) \leq \binom{n}{2}.$$

1.15 Eccentric distance sum

Let $D_G(v)$ be the sum of distances of all vertices in G from v, that is, $D_G(v) = \sum_{u \in V(G)} d_G(v, u)$. The *eccentric distance sum* (EDS) is defined as [60]

$$\xi^d(G) = \sum_{v \in V(G)} ecc_G(v) D_G(v).$$

Hua, Zhang, and Xu [84] gave the Nordhaus–Gaddum type results for EDS of connected graphs in 2012. Suppose that G is a connected triangle-free graph on n vertices such that $\overline{G}$ is connected. Then we clearly have $n \geq 4$. If $n = 4$, then G must be the path P_4, and thus, $\xi^d(G) + \xi^d(\overline{G}) = 52$ by an elementary calculation. So they assumed that $n \geq 5$ in their following theorem.

Theorem 1.31. [84] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected triangle-free graph. If $\overline{G}$ is connected, then*

$$\xi^d(G) + \xi^d(\overline{G}) \geq 6n(n-1),$$

with equality if and only if $G \cong C_5$ or $\overline{G} \cong C_5$.

Proof. It is obvious that $deg_G(v) \leq n-2$ for any $v \in V(G)$, for otherwise, $\overline{G}$ is disconnected, a contradiction. So, $ecc_G(v) \geq 2$. Similarly, we have $ecc_{\overline{G}}(v) \geq 2$ for any $v \in V(G)$, since $G = \overline{\overline{G}}$ is connected. Thus

$$\begin{aligned}
\xi^d(G) + \xi^d(\overline{G}) &\geq 2\left(\sum_{v\in V(G)} D_G(v) + \sum_{v\in V(G)} D_{\overline{G}}(v)\right) \\
&= 2\left[\sum_{v\in V(G)} deg_G(v) + \sum_{v\in V(G)} \sum_{u\in V(G)\setminus N_G[v]} d_G(u,v)\right] \\
&\quad +2\left[\sum_{v\in V(G)} deg_{\overline{G}}(v) + \sum_{v\in V(G)} \sum_{u'\in V(G)\setminus N_{\overline{G}}[v]} d_{\overline{G}}(u',v)\right] \\
&\geq 2n(n-1) + 2\left[\sum_{v\in V(G)} \sum_{u\in V(G)\setminus N_G[v]} 2 + \sum_{v\in V(G)} \sum_{u'\in V(G)\setminus N_{\overline{G}}[v]} 2\right] \\
&= 2n(n-1) + 4\sum_{v\in V(G)} (n - deg_G(v) - 1) + 4\sum_{v\in V(G)} (n - deg_{\overline{G}}(v) - 1) \\
&= 10n(n-1) - 4\sum_{u\in V(G)} (deg_G(v) + deg_{\overline{G}}(v)) = 6n(n-1).
\end{aligned}$$

Assume that $\xi^d(G) + \xi^d(\overline{G}) = 6n(n-1)$. Since both G and $\overline{G}$ are connected, we have $deg_G(v) \leq n-2$ and $deg_{\overline{G}}(v) \leq n-2$ for any vertex v in G. So $V(G) \setminus N_G[v] \neq \emptyset$ and $(G) \setminus N_{\overline{G}}[v] \neq \emptyset$ for any v. Therefore, for each $v \in V(G)$, $u \in V(G) \setminus N_G[v]$, $u' \in V(G) \setminus N_{\overline{G}}[v]$, there exists $ecc_G(v) = 2$ and $d_G(u,v) = 2$, together with $ecc_{\overline{G}}(v) = 2$ and $d_{\overline{G}}(u',v) = 2$.

Suppose that there exists a vertex, say w, in G such that $deg_G(w) = 1$ and let u be its unique neighbor. Note that $ecc_G(u) = 2$. Then there exists a vertex, say x, such that $d_G(u,x) = 2$. But then $ecc_G(w) \geq d_G(w,x) = 3$, a contradiction.

Hence $\delta(G) \geq 2$. If $\Delta(G) = 2$, then G is just a cycle C_n Since $ecc_G(v) = 2$ for any v in G, we thus have $n = 5$, that is, $G \cong C_5$. Assume now that $\Delta(G) \geq 3$. Let v be a vertex in G with $deg_G(v) = \Delta$ and let $N_G(v) = \{v_1, v_2, \cdots, v_\Delta\}$. Since G is a triangle-free, it follows that $G[v_1, v_2, \cdots, v_\Delta]$ is a null graph. Thus, for any vertex u in $V(G) \setminus N_G[v]$, we have $uv_i \in E(G)$ $(i = 1, \cdots, \Delta)$, since $ecc_G(x) = 2$ for any x in G. Let $A = N_G(v) = \{v_1, v_2, \cdots, v_\Delta\}$ and $B = V(G) \setminus A$. If there exist two vertices, say x and y, in $B \setminus \{v\}$ such that $xy \in E(G)$, then G contains triangle v_ixyv_i $(i = 1, \cdots, \Delta)$, a contradiction. Thus, G is the complete bipartite graph $K_{\Delta,n-\Delta}$ with two partite sets being A and B respectively. But then, $\overline{G} = \overline{K_{\Delta,n-\Delta}}$ is disconnected, a contradiction to our assumption. The discussion above shows that $\xi^d(G) + \xi^d(\overline{G}) = 6n(n-1)$ only if $G \cong C_5$.

Conversely, we have $\xi^d(C_5) + \xi^d(\overline{C}_5) = 120 = 6n(n-1)$. This completes the proof. ■

Hua, Zhang, and Xu [84] also obtained an upper bound of $\xi^d(G)$ for a connected graph G.

Lemma 1.60. [84] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph with degree sequence $(d_1, d_2, \ldots, d_n)$. Then*

$$\xi^d(G) \leq (n-1)\sum_{i=1}^{n}(n-d_i)^2,$$

with equality if and only if $d_1 = d_2 = \cdots = d_n = n-1$, that is, $G \cong K_n$.

By Lemma 1.60, they proved the following Nordhaus–Gaddum inequality.

Theorem 1.32. [84] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected graph with degree sequence $(d_1, d_2, \cdots, d_n)$. If $\overline{G}$ is connected, then*

$$\xi^d(G) + \xi^d(\overline{G}) < n(n-1)(n^2+1) + 2(n-1)\sum_{i=1}^{n}[d_i^2 - (n-1)d_i].$$

Proof. By Lemma 1.60, we have

$$\xi^d(G) \leq (n-1)\sum_{i=1}^{n}(n-d_i)^2 \tag{53}$$

and

$$\xi^d(G) \leq (n-1)\sum_{i=1}^{n}[(n-(n-1-d_i)]^2 = (n-1)\sum_{i=1}^{n}(1+d_i)^2.$$

So,

$$\begin{aligned}\xi^d(G) + \xi^d(\overline{G}) &\leq (n-1)\sum_{i=1}^{n}[(n-d_i)^2 + (1+d_i)^2]. \\ &= n(n-1)(n^2+1) + 2(n-1)\sum_{i=1}^{n}[d_i^2 - (n-1)d_i].\end{aligned}$$

Since $\overline{G}$ is a connected, it follows that G cannot be isomorphic to K_n, and thus the equality in the inequality (53) cannot be attained by Lemma 1.60. It follows the present theorem as desired. ■

2. Degree–based parameters

The concept of degree in graph theory is closely related (but not identical) to the concept of valence in chemistry; see [63]. The degree of a vertex of a molecular graph is the number of first neighbors of this vertex. A large number of molecular-graph-based structure descriptors (topological indices) have been conceived, depending on vertex degrees. In [63], Gutman first presented the most familiar distance-based structure descriptors, and then report results on their comparison.

The following Table 2.1 shows the authors contributing the Nordhaus–Gaddum problem for degree-based parameters.

Degree-based Parameters	Authors Contributing N-G Problem
Randić index	Zhang and Wu [144]
Zagreb index	Zhang and Wu [144]
	Su, Xiong, and Xu [130]
Zagreb co-index	Su, Xiong, and Xu [130]
	Hua, Ashrafi, Zhang [82]
Multiplicative Zagreb coindices	Xu, Das, and Tang [140]
Aton-bond connectivity index	Das, Gutman, and Furtula [30]
Augmented Zagreb index	Ali, Raza, and Bhatti [2]
Sum-connectivity index	Zhou and Trinajstić [158]
	Zhou and Trinajstić [159]
General sum-connectivity co-Index	Su and Xu [132]
Geometric-arithmetic index	Das [23]
Edge version of geometric-arithmetic index	Mahmiani, Khormali, and Iranmanesh [110]
Harmonic index	Zhong and Xu [146]

Table 2.1. Degree–based parameters

2.1 Randić index

The *Randić index* $R(G)$, proposed by Randić [125] in 1975, is defined as the sum of the weights $\frac{1}{\sqrt{deg_G(u)deg_G(v)}}$ over all edges uv of G, that is,

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg_G(u)deg_G(v)}},$$

where $deg_G(u)$ denotes the degree of a vertex u of G. The Randić index is one of the most successful vertex-degree-based molecular descriptors (topological indices) in structure property and structure-activity relationship studies [91, 124]. Mathematical properties of this descriptor have also been studied extensively, as summarized in [65, 99]. Fixing $\alpha \in R - \{0\}$, the general Randić index is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} R_\alpha(uv) = \sum_{uv \in E(G)} (deg_G(u)deg_G(v))^\alpha.$$

Hence, $R_{-\frac{1}{2}}(G)$ is the ordinary Randić index of G.

Zhang and Wu [144] obtained the following Nordhaus–Gaddum-type results for the general Randić index.

Theorem 2.1. [144] *Let $G \in \mathcal{G}(n)$ be a graph.*

(1) *If $\alpha > 0$, then*

$$\binom{n}{2}\left(\frac{n-1}{2}\right)^{2\alpha} \leq R_\alpha(G) + R_\alpha(\overline{G}) \leq \binom{n}{2}(n-1)^{2\alpha}.$$

(2) *If* $\alpha < 0$, *then*

$$\binom{n}{2}(n-1)^{2\alpha} \le R_\alpha(G) + R_\alpha(\overline{G}) \le \binom{n}{2}\left(\frac{n-1}{2}\right)^{2\alpha}.$$

Zhang and Wu got the following lemma.

Lemma 2.1. [144] *Define* $f(x) = x^x(a-x)^{a-x}$ *for* $x \in (0,a)$ *and* $f(0) = f(a) = a^a$. *Then* $f(x) \ge (\frac{a}{2})^a$ *for* $x \in [0,a]$.

Proof. By the definition of $f(x)$, both $f'(x)$ and $f''(x)$ are continuous on $[0,a]$, and it is easy to check that $\frac{a}{2}$ is the unique zero of $f'(x)$, and $f''(\frac{a}{2}) > 0$. This means that $f(x) \ge f(\frac{a}{2})$ for any $x \in [0,a]$. ■

We now in a position to give the proof of Theorem 2.1.

Proof of Theorem 2.1: For a graph $G = (V,E)$ of order n, let $e(G) = |E(G)|$ and $N = \binom{n}{2}$. We first consider the upper bound. Since $\alpha > 0$, it follows that

$$\begin{aligned} R_\alpha(G) + R_\alpha(\overline{G}) &= \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha + \sum_{uv\in E(\overline{G})} (d_{\overline{G}}(u)d_{\overline{G}}(v))^\alpha \\ &\le e(G)[(n-1)(n-1)]^\alpha + e(\overline{G})[(n-1)(n-1)]^\alpha \\ &= \binom{n}{2}(n-1)^{2\alpha}. \end{aligned}$$

Now we aim to the lower bound.

$$\begin{aligned} R_\alpha(G) + R_\alpha(\overline{G}) &= \sum_{uv\epsilon E(G)} (d_G(u)d_G(v))^\alpha + \sum_{uv\epsilon E(\overline{G})} (d_{\overline{G}}(u)d_{\overline{G}}(v))^\alpha \\ &\ge N \sqrt[N]{\prod_{uv\in E(G)} (d_G(u)d_G(v))^\alpha \prod_{uv\in E(\overline{G})} (d_{\overline{G}}(u)d_{\overline{G}}(v))^\alpha} \\ &= N \sqrt[N]{\prod_{u\epsilon E(G)} (d_G(u))^{d_G(u)\alpha} \prod_{v\epsilon E(\overline{G})} (d_{\overline{G}}(v))^{d_{\overline{G}}(v)\alpha}} \\ &= N \left[\prod_{u\epsilon E(G)} (d_G(u))^{d_G(u)}(n-1-d_G(u))^{n-1-d_G(u)}\right]^{\frac{\alpha}{N}} \\ &\ge N \left[\prod_{u\epsilon E(G)} \left(\frac{n-1}{2}\right)^{n-1}\right]^{\frac{\alpha}{N}} \\ &= \binom{n}{2}\left[\left(\frac{n-1}{2}\right)^{n(n-1)}\right]^{\frac{2\alpha}{n(n-1)}} = \binom{n}{2}\left(\frac{n-1}{2}\right)^{2\alpha}. \end{aligned}$$

Similarly, we get the bounds for $\alpha < 0$. ■

The bounds are best possible. The complete graph K_n is the unique graph G whose $R_\alpha(G) + R_\alpha(\overline{G})$ attains the upper bound in (1) of Theorem 2.1. For any $n = 4k+1, k \geq 1$, there exists a graph G_n with G_n and $\overline{G}_n$ are $2k$-regular. Then G_n is a graph G whose $R_\alpha(G) + R_\alpha(\overline{G})$ attains the lower bound in (1) of Theorem 2.1. For $\alpha < 0$, K_n and G_n are, in turn, the graphs whose $R_\alpha(G) + R_\alpha(\overline{G})$ attain the lower and upper bound respectively in (2) of Theorem 2.1.

2.2 Zagreb index

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$, defined in [10], are

$$M_1(G) = \sum_{u \in V(G)} (deg_G(u))^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} deg_G(u) deg_G(v),$$

respectively. Note that the second Zagreb index $M_2(G)$ is just the general Randić index $R_1(G)$. Li and Zhao [105] introduced the first general Zagreb index as

$$M_\alpha(G) = \sum_{u \in V(G)} (deg_G(u))^\alpha$$

where $\alpha \in R$ and $\alpha \neq 0$.

2.2.1 Nordhaus–Gaddum type results

Zhang and Wu [144] got the Nordhaus-Goddum-type inequality for the first general Zagreb index for $\alpha \in R$, $\alpha \neq 0$ and $\alpha \neq 1$.

Theorem 2.2. [144] *Let $G \in \mathcal{G}(n)$ be a graph.*

(i) *If $\alpha > 1$, then*

$$2n\left(\frac{n-1}{2}\right)^\alpha \leq M_\alpha(G) + M_\alpha(\overline{G}) \leq n(n-1)^\alpha.$$

(ii) *If $0 < \alpha < 1$, then*

$$n(n-1)^\alpha \leq M_\alpha(G) + M_\alpha(\overline{G}) \leq 2n\left(\frac{n-1}{2}\right)^\alpha.$$

(iii) *If $\alpha < 0$, then*

$$2n\left(\frac{n-1}{2}\right)^\alpha \leq M_\alpha(G) + M_\alpha(\overline{G}) \leq n[1 + (n-2)^\alpha].$$

2.2.2 Generalized Nordhaus–Gaddum type results

Recall that if a real valued function $G(x)$ defined on an interval has a second derivative $G''(x)$, then a necessary and sufficient condition for it to be convex (concave, resp.) on that interval is that $G''(x) \geq 0$ $(G''(x) \leq 0, \text{ resp.})$.

The fundamental discrete Jensen's inequalities show the following lemma.

Lemma 2.2. [73] *Let $\mathbb{C}$ be a convex subset of a real vector space $\mathbb{X}$, let $x_i \in \mathbb{C}$ and $\sigma_i \geq 0$ $(i = 1, 2, \ldots, n)$ with $\sum_{i=1}^{n} \sigma_i = 1$. Then*
(1) $\Phi(\sum_{i=1}^{k} \sigma_i x_i) \leq \sum_{i=1}^{k} \sigma_i \Phi(x_i)$ *if $\Phi(x) : \mathbb{C} \to \mathbb{R}$ is a convex function*
(2) $\Phi(\sum_{i=1}^{k} \sigma_i x_i) \geq \sum_{i=1}^{k} \sigma_i \Phi(x_i)$ *if $\Phi(x) : \mathbb{C} \to \mathbb{R}$ is a concave function.*

Lemma 2.3. [130] *Let G be a graph with two non-adjacent vertices $u, v \in V(G)$. Then $M_\alpha(G+uv) > M_\alpha(G)$ for $\alpha \in (0,1) \cup (1, +\infty)$ and $M_\alpha(G+uv) < M_\alpha(G)$ for $\alpha \in (-\infty, 0)$.*

Let k be an positive integer not less than 2; we define two classes: $\mathcal{P}_k^n = \{\mathcal{D}_k \,|\, \mathcal{D}_k = (G_1, G_1 \cdots, G_k)$ is a k-decomposition of K_n such that each cell G_i is connected and $\delta(G_i) \geq 2\}$, and $\mathcal{Q}_k^n = \{\mathcal{D}_k \,|\, \mathcal{D}_k = (G_1, G_1 \cdots, G_k)$ is a k-decomposition of K_n such that each cell G_i is connected and $\delta(G_i) \geq 1\}$.

Su, Xiong, and Xu [130] obtained the following Nordhaus–Gaddum-type results.

Theorem 2.3. [130] *Let $k \geq 2$ and t be integers, $D_k = (G_1, G_1 \cdots, G_k)$ be a k-decomposition of K_n. Then*

$$(1) \quad n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n(n-1)^\alpha, \text{ if } \alpha > 1,$$

$$(2) \quad n(n-1)^\alpha \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n(n-1)^\alpha k^{1-\alpha}, \text{ if } 0 < \alpha < 1,$$

$$(3) \quad n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq nk, \text{ if } \alpha < 0 \text{ and } \mathcal{D}_k \in \mathcal{Q}_k^n,$$

$$(4) \quad n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n[t + t(n-2)^\alpha], \text{ if } \alpha < 0,$$
$$k = 2t \text{ and } \mathcal{D}_k \in \mathcal{P}_k^n,$$

$$(5) \quad n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k)$$
$$\leq n[t + (t+1)(n-2)^\alpha], \text{ if } \alpha < 0,\ k = 2t+1 \text{ and } \mathcal{D}_k \in \mathcal{P}_k^n,$$

Proof. From the definition of the general Zagreb index, we have

$$\begin{aligned} & M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \\ = & \sum_{u \in V(G_1)} [deg_{G_1}(u)]^\alpha + \sum_{u \in V(G_2)} [deg_{G_2}(u)]^\alpha \cdots + \sum_{u \in V(G_k)} [deg_{G_k}(u)]^\alpha \\ = & \sum_{u \in V(G)} [[deg_{G_1}(u)]^\alpha + [deg_{G_2}(u)]^\alpha + \cdots + [deg_{G_k}(u)]^\alpha] \,. \end{aligned}$$

Let $\rho(x) = x^\alpha$ for $x \geq 0$ and $\alpha \in R \setminus \{0, 1\}$. Easy verification shows that $\rho(x)$ is a convex function if $\alpha \in (-\infty, 0) \cup (1, +\infty)$ and is a concave one otherwise. We distinguish the following three separate cases.

Case 1. $\alpha > 1$.

Noticing $\rho(x)$ is a convex function in the case of $\alpha > 1$, and then we have by Lemma 2.2

$$\begin{aligned} & [deg_{G_1}(u)]^\alpha + [deg_{G_2}(u)]^\alpha + \cdots + [deg_{G_k}(u)]^\alpha \\ \geq\ & k\left[\frac{deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u)}{k}\right]^\alpha = \frac{(n-1)^\alpha}{k^{\alpha-1}}, \end{aligned}$$

which implies that

$$M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \geq \frac{n(n-1)^\alpha}{k^{\alpha-1}}.$$

On the other hand, $deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u) = n - 1$ and

$$\begin{aligned} \frac{\sum_{i=1}^k [deg_{G_i}(u)]^\alpha}{[deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u)]^\alpha} &= \sum_{i=1}^k \left[\frac{deg_{G_i}(u)}{deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u)}\right]^\alpha \\ &\leq \sum_{i=1}^k \left[\frac{deg_{G_i}(u)}{deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u)}\right]^1 \\ &= \frac{n-1}{n-1} = 1 \end{aligned}$$

Then, we have

$$[deg_{G_1}(u)]^\alpha + [deg_{G_2}(u)]^\alpha + \cdots + [deg_{G_k}(u)]^\alpha \leq [deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u)]^\alpha.$$

This gives us the proof of (1)

$$\begin{aligned} M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) &\leq \sum_{u \in V(G)} [deg_{G_1}(u) + deg_{G_2}(u) + \cdots + deg_{G_k}(u)]^\alpha \\ &= n(n-1)^\alpha. \end{aligned}$$

Case 2. $0 < \alpha < 1$.

By analogous reasoning as used in Case 1 we can prove (2), and we omit the proof here, respectively.

Case 3. $\alpha < 0$.

For sake of simplicity, let $x_1 = deg_{G_1}(u), x_2 = deg_{G_2}(u), \cdots, x_k = deg_{G_k}(u)$. Easy verification shows that each cell G_i must be connected when $\alpha < 0$, otherwise there would produce a contradiction to the definition of M_α. Without loss of generality we assume $x_1 \geq x_2 \geq \cdots x_k \geq 1$.

Subcase 3.1. $\mathcal{D}_k \in \mathcal{Q}_k^n$.

Let $\Phi_1(x_1, x_2 \cdots, x_k) = x_1^\alpha + x_2^\alpha + \cdots + x_k^\alpha$. If $x_1 \geq x_2 \geq \cdots x_{k-l} \geq 2 > x_{k-l+1} = \cdots = x_k = 1$, then

$$\begin{aligned} \Phi_1(x_1, x_2 \cdots, x_k) &= x_1^\alpha + x_2^\alpha + \cdots + x_{k-l}^\alpha + x_{k-l+1}^\alpha + x_{k-l+2}^\alpha + \cdots + x_k^\alpha \\ &= x_1^\alpha + x_2^\alpha + \cdots + x_{k-l}^\alpha + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{t\ times} \\ &\quad \text{(since } \rho(x) = x^\alpha \text{ is decreasing for } \alpha < 0) \\ &< \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{k-l\ times} + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{l\ times} = k, \end{aligned}$$

this implies that $M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) < kn$.

If $x_1 = x_2 = \cdots = x_k$, then $\Phi_1(x_1, x_2 \cdots, x_k) = x_1^\alpha + x_2^\alpha + \cdots + x_k^\alpha = k$. Easy verification shows that there exists a k-decomposition $(\frac{n}{2}\ K_2, \frac{n}{2}\ K_2, \cdots, \frac{n}{2}\ K_2)$ of K_n which attains the maximum M_α-value kn when n is even. This completes the upper bound of (3). Note that $\rho(x)$ is a convex function when $\alpha < 0$, then by Lemma 2.2 we obtain the lower bound of (3).

Subcase 3.2. $\mathcal{D}_k \in \mathcal{P}_k^n$.

Let $\Phi_2(x_1, x_2 \cdots, x_k) = \Phi_1(x_1 + 1, \cdots, x_i + 1, x_{i+1} - 1, \cdots, x_{2i+1} - 1, x_{2i+2}, \cdots, x_k)$.

We first need to prove the following claim.

Claim 1. $\Phi_1(x_1, x_2 \cdots, x_k) < \Phi_2(x_1, x_2 \cdots, x_k)$.

Proof of Claim 1. By using Lagrange's mean-value theorem and Lemma 2.3, we conclude that

$$\begin{aligned}
& \Phi_2(x_1, x_2 \cdots, x_k) - \Phi_1(x_1, x_2 \cdots, x_k) \\
= & \big[(x_1+1)^\alpha + \cdots + (x_i+1)^\alpha + (x_{i+1}-1)^\alpha + \cdots + (x_{2i}-1)^\alpha + x_{2i+1}^\alpha + x_{2i+2}^\alpha + \cdots + {x_k}^\alpha)\big] \\
& -[x_1^\alpha + x_2^\alpha + \cdots + x_i^\alpha + x_{i+1}^\alpha + x_{i+2}^\alpha + \cdots + x_{2i}^\alpha + x_{2i+1}^\alpha + x_{2i+2}^\alpha + x_{2i+3}^\alpha + \cdots + x_k^\alpha] \\
= & [(x_1+1)^\alpha - x_1^\alpha] + \cdots + [(x_i+1)^\alpha - x_i^\alpha] + [(x_{i+1}-1)^\alpha - x_{i+1}^\alpha] + \cdots + [(x_{2i}-1)^\alpha - x_{2i}^\alpha] \\
= & \alpha\xi_1^{\alpha-1} + \alpha\xi_2^{\alpha-1} + \cdots + \alpha\xi_i^{\alpha-1} - \alpha\eta_1^{\alpha-1} - \alpha\eta_2^{\alpha-1} - \cdots - \alpha\eta_i^{\alpha-1} \\
= & \alpha[(\xi_1^{\alpha-1} - \eta_1^{\alpha-1}) + (\xi_2^{\alpha-1} - \eta_2^{\alpha-1}) + \cdots + (\xi_i^{\alpha-1} - \eta_i^{\alpha-1})] \\
= & \alpha(\alpha-1)[\zeta_1^{\alpha-2}(\xi_1 - \eta_1) + \zeta_2^{\alpha-2}(\xi_2 - \eta_2) + \cdots + \zeta_i^{\alpha-2}(\xi_i - \eta_i)],
\end{aligned}$$

where $\xi_1 \in (x_1, x_1+1), \xi_2 \in (x_2, x_2+1), \cdots, \xi_i \in (x_i, x_i+1)$; $\eta_1 \in (x_{i+1}-1, x_{i+1}), \eta_2 \in (x_{i+2} - 1, x_{i+2}), \cdots, \eta_i \in (x_{2i}-1, x_{2i})$; $\zeta_1 \in (\xi_1, \eta_1), \zeta_2 \in (\xi_2, \eta_2), \cdots, \zeta_i \in (\xi_i, \eta_i)$. In view of the facts that $x_1 \geq x_2 \geq \cdots \geq x_k$, $x_l < \xi_l < x_l + 1$ and $x_{2l} - 1 < \eta_l < x_{2l}$, we obtain $\xi_l - \eta_l > x_l - x_{2l} \geq x_l - x_l = 0$, this implies $\Phi_1(x_1, x_2 \cdots, x_k) < \Phi_2(x_1, x_2 \cdots, x_k)$ for $\alpha < 0$. ■

From Claim 1 we know that the M_α-value of a graph will increase when replacing the degree consequence $(x_1, x_2, \cdots, x_k)$ by $(x_1 + 1, \cdots, x_i + 1, x_{i+1} + 1, \cdots, x_{2i+1} - 1, x_{2i+2}, \cdots, x_k)$.

To obtain the proof of (4) and (5), it is sufficient to consider the following two claims. Note that the equality $x_1 + x_2 + \cdots + x_k = n - 1$ always holds.

Claim 2. $\Phi_1(x_1, x_2 \cdots, x_k) \leq t(n-2)^\alpha + t$, if $k = 2t$.

Proof of Clam 2. Actually, from Claim 1 we obtain that

$$\begin{aligned}
& \Phi_1(x_1, x_2 \cdots, x_{2t}) \\
= & x_1^\alpha + x_2^\alpha + \cdots + x_t^\alpha + x_{t+1}^\alpha + x_{t+2}^\alpha + \cdots + x_{2t}^\alpha \\
\leq & (x_1+1)^\alpha + (x_2+1)^\alpha + \cdots + (x_t+1)^\alpha + (x_{t+1}-1)^\alpha + (x_{t+1}-1)^\alpha + \cdots + (x_{2t}-1)^\alpha \\
\leq & (x_1+2)^\alpha + (x_2+2)^\alpha + \cdots + (x_t+2)^\alpha + (x_{t+1}-2)^\alpha + (x_{t+1}-2)^\alpha + \cdots + (x_{2t}-2)^\alpha \\
\cdots & \\
\leq & \underbrace{(n-2)^\alpha + (n-2)^\alpha + \cdots + (n-2)^\alpha}_{t \text{ times}} + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{t \text{ times}} \\
= & t(n-2)^\alpha + t.
\end{aligned}$$

This completes the proof of Claim 2. ■

Now we use Claim 2 to prove (4). By taking the sum over all vertices of G for two sides of Claim 2, we obtain the upper bound of (4). Note that $\rho(x)$ is a convex function when $\alpha < 0$, then by Lemma 2.2 we obtain the lower bound of (4).

Claim 3. $\Phi_1(x_1, x_2 \cdots, x_k) \leq t(n-2)^\alpha + t$, if $k = 2t+1$.

Proof of Claim 3. By the same reasoning, one can obtain

$$
\begin{aligned}
\Phi_1(x_1, x_2 \cdots, x_{2t+1}) &= x_1^\alpha + x_2^\alpha + \cdots + x_t^\alpha + x_{t+1}^\alpha + x_{t+2}^\alpha + \cdots + x_{2t}^\alpha + x_{2t+1}^\alpha \\
&\leq (x_1+1)^\alpha + (x_2+1)^\alpha + \cdots + (x_t+1)^\alpha + (x_{t+1}-1)^\alpha + (x_{t+2}-1)^\alpha \\
&\quad + \cdots + (x_{2t}-1)^\alpha + x_{2t+1}^\alpha \\
&\leq (x_1+2)^\alpha + (x_2+2)^\alpha + \cdots + (x_t+2)^\alpha + (x_{t+1}-2)^\alpha + (x_{t+2}-2)^\alpha \\
&\quad + \cdots + (x_{2t}-2)^\alpha + x_{2t+1}^\alpha \\
&\quad \cdots \\
&\leq \underbrace{(n-2)^\alpha + (n-2)^\alpha + \cdots + (n-2)^\alpha}_{t \text{ times}} + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{t \text{ times}} + x_{2t+1}^\alpha \\
&= t(n-2)^\alpha + t \cdot 1^\alpha + (n-2)^\alpha \\
&= (t+1)(n-2)^\alpha + t.
\end{aligned}
$$

This completes the proof of Claim 3. ■

Taking the sum over all vertices of G for two sides of Claim 2, we obtain the upper bound of (5). The lower bound of (5) can be verified by Lemma 2.2 since $\rho(x)$ is a convex function when $\alpha < 0$.

Note that the bounds are best possible. The upper bound of (1) and the lower bound of (2) are the same and are attained uniquely if one of the cells G_i is the complete graph K_n and the others are empty graphs with order n. On the other hand, the lower bound of $(1), (3), (4)$ and (5) and the upper bound of (2) are the same and are attained on the $\frac{n-1}{k}$-regular graphs, since for any $n = \beta k + 1, \beta \geq 1$, there exists a graph G_i and all the $k-1$ graphs $G_1, G_2, \cdots, G_{i-1}, G_{i+1}, \cdots, G_k$ are $\frac{n-1}{k}$-regular and with n orders. The upper bound of (4) attained on the graph H_n is obtained from K_n ba deleting a perfect matching, so this occurs only if n is even.

The following consequence is obvious, just taking $k = 2$ in the following.

Remark 2.1. [130] *Just taking $k = 2$ in the above theorem, we can easily derive the results in Theorem 2.3.*

2.3 Zagreb co–indices

The *first and second Zagreb co-indices* are a pair of recently introduced graph invariants [40], which were originally defined as follows:

$$\overline{M_1}(G) = \sum_{uv \notin V(G)} [deg_G(u) + deg_G(v)] \quad \text{and} \quad \overline{M_2}(G) = \sum_{uv \notin E(G)} [deg_G(u) deg_G(v)].$$

2.3.1 Nordhaus–Gaddum–type results in $\mathcal{G}(n)$

The following relation between Zagreb index and Zagreb co-index is due to Ashrafi, Došlić, and Hamzeh [8].

Lemma 2.4. [8] *Let G be a graph with order n and size m. Then*

$$\overline{M_1}(G) = 2m(n-1) - M_1(G), \ \ \overline{M_2}(G) = M_2(\overline{G}) - (n-1)M_1(\overline{G}) + \overline{m}(n-1)^2.$$

Su, Xiong and Xu [130] obtained the following Nordhaus–Gaddum-type results for Zagreb co-index.

Theorem 2.4. [130] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$0 \leq \overline{M_1}(G) + \overline{M_1}(\overline{G}) \leq 2^{-1}n(n-1)^2.$$

The lower bound attains on K_n, and the upper bound attains on the $\frac{n-1}{2}$-regular graphs.

Proof. By applying Lemma 2.4 to the complement graph $\overline{G}$, one obtains $\overline{M_1}(\overline{G}) = 2\overline{m}(n-1) - M_1(\overline{G})$. Now plugging in the expression for $M_1(\overline{G})$, we have $\overline{M_1}(G) + \overline{M_1}(\overline{G}) = n(n-1)^2 - [M_1(G) + M_1(\overline{G})]$. From Theorem 2.2, we have $2^{-1}n(n-1)^2 \leq M_1(G) + M_1(\overline{G}) \leq n(n-1)^2$. The theorem follows immediately.

Note that the bounds are best possible. By direct calculation, $\overline{M_1}(K_n) + \overline{M_1}(\overline{K_n}) = 0$, the lower bound attains on K_n. The upper bound attains on the $\frac{n-1}{2}$-regular graphs, so $n = 4\beta + 1$ for some integer β. ■

Theorem 2.5. [130] *Let G be a graph with order n. Then*

$$0 \leq \overline{M_2}(G) + \overline{M_2}(\overline{G}) \leq 2^{-1}n(n-1)^3.$$

The lower bound attains on K_n, and the upper bound attains on the $2k$-regular graphs.

Proof. By applying Lemma 2.4 to the complement graph $\overline{G}$, one obtains $\overline{M_2}(\overline{G}) = M_2(G) - (n-1)M_1(G) + m(n-1)^2$, thus $\overline{M_2}(G) + \overline{M_2}(\overline{G}) = [M_2(G) + M_2(\overline{G})] + 2^{-1}n(n-1)^3 - (n-1)[M_1(G) + M_1(\overline{G})]$. From Theorems 2.1 and 2.2, we have $2^{-1}n(n-1)^2 \leq M_1(G) + M_1(\overline{G}) \leq n(n-1)^2$ and $2^{-3}n(n-1)^3 \leq M_2(G) + M_2(\overline{G}) \leq 2^{-1}n(n-1)^3$. Easy verification completes the proof.

Note that the bounds are best possible. By direct calculation, $\overline{M_2}(K_n) + \overline{M_2}(\overline{K_n}) = 0$, the lower bound attains on K_n. The upper bound attains on the $2k$-regular graphs. ■

2.3.2 Nordhaus–Gaddum–type results in $\mathcal{G}(n, m)$

The following results for the first Zagreb index will be used later.

Lemma 2.5. [101] *Let $G \in \mathcal{G}(n, m)$ $(n \geq 2)$ be a graph. Then*

$$M_1(G) \leq m\left(\frac{2m}{n-1} + n - 2\right)$$

with equality if and only if the $G \cong S_n$ or K_n.

Lemma 2.6. [149] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ be a graph. If G is K_{r+1}-free, $2 \leq r \leq n-1$, then*

$$M_1(G) \leq \frac{2r-2}{r} mn$$

with equality if and only if a bipartite graph for $r = 2$, and regular complete r-partite graph for $r \geq 3$.

Let W_n be the graph obtained from the star S_n by adding $\lfloor \frac{n-1}{2} \rfloor$ independent edges. Let $\mathrm{even}(n) = 1$ if n is even, and 0 otherwise.

Lemma 2.7. [153] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ be a connected quadrangle-free graph. Then*

$$M_1(G) \leq n(n-1) + 2m - 2\,\mathrm{even}(n)$$

with equality if and only if $G \cong W_n$.

Lemma 2.8. [153] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a connected triangle- and a quadrangle-free graph. Then*

$$M_1(G) \leq n(n-1)$$

with equality if and only if $G \cong S_n$ or a Moore graph of diameter 2.

Hua, Ashrafi, Zhang [82] obtained the following Nordhaus–Gaddum-type bounds for the first Zagreb co-index.

Theorem 2.6. [82] (i) *If $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ is a graph, then*

$$\overline{M_1}(G) + \overline{M_1}(\overline{G}) \geq 2mn - \frac{4m^2}{n-1}$$

with equality if and only if the $G \cong S_n$ or K_n.

(ii) *If G is a connected K_{r+1}-free graph $2 \leq r \leq n-1$, then*

$$\overline{M_1}(G) + \overline{M_1}(\overline{G}) \geq 4m\left(\frac{n}{r} - 1\right)$$

with equality if and only if G is a bipartite graph for $r = 2$, and regular complete r-partite graph for $r \geq 3$.

(iii) *If G is a connected quadrangle-free graph, then*

$$\overline{M_1}(G) + \overline{M_1}(\overline{G}) \geq 4mn - 2n^2 + 2n - 8m + 4\,\mathrm{even}(n)$$

with equality if and only if $G \cong W_n$.

(iv) *If G is a connected triangle- and a quadrangle-free graph, then*

$$\overline{M_1}(G) + \overline{M_1}(\overline{G}) \geq 2(n-1)(2m-n)$$

with equality if and only if $G \cong S_n$ or a Moore graph of diameter 2.

Proof. It follows from [8] that for any simple graph G, $\overline{M_1}(\overline{G}) = \overline{M_1}(G)$. Hence, $\overline{M_1}(G) + \overline{M_1}(\overline{G}) = 2\overline{M_1}(G)$. From [8], we also have $\overline{M_1}(G) = 2m(n-1) - M_1(G)$ for any simple graph of order n and size m. So,

$$\overline{M_1}(G) + \overline{M_1}(\overline{G}) = 4m(n-1) - 2M_1(G).$$

By Lemmas 2.5, 2.6, 2.7, and 2.8, we have actually completed the proof. ∎

2.4 Multiplicative Zagreb coindices

Narumi and Katayama [116] considered the product of vertex degrees

$$NK(G) = \prod_{v \in V(G)} deg_G(v)$$

but this structure descriptor attracted only a limited attention. However, following a suggestion by Todeschini and Consonni, the multiplicative versions of the Zagreb indices entered the scene. Then $\prod_1(G) = \prod_{v \in V(G)} deg_G(v)^2$, $\prod_2(G) = \prod_{uv \in E(G)} deg_G(u)deg_G(v)$, and $\prod_1^*(G) = \prod_{uv \in E(G)}[deg_G(u) + deg_G(v)]$ are referred to as the "*first multiplicative Zagreb index*", the "*second multiplicative Zagreb index*", and the "*modified first multiplicative Zagreb index*". Evidently, the Narumi-Katayama index and the first multiplicative Zagreb index are simply related as $\prod_1(G) = NK(G)$.

As the multiplicative versions of Zagreb coindices, the *(first and second) multiplicative Zagreb coindices* are defined as

$$\overline{\prod}_1(G) = \prod_{uv \notin E(G)} [deg_G(u) + d_G(v)], \ \overline{\prod}_2(G) = \prod_{uv \notin E(G)} deg_G(u)deg_G(v).$$

The following Table 2.2 shows the relations among Zagreb indices, Zagreb co-indices, multiplicative Zagreb indices, and multiplicative Zagreb co-indices.

	Definitions
First Zagreb index	$M_1(G) = \sum_{v \in V(G)} deg_G(v)^2$
First multiplicative Zagreb index	$\prod_1(G) = \prod_{v \in V(G)} deg_G(v)^2$
First Zagreb co-index	$\overline{M}_1(G) = \sum_{uv \notin V(G)}[deg_G(u) + deg_G(v)]$
First multiplicative Zagreb co-index	$\overline{\prod}_1(G) = \prod_{uv \notin E(G)}[deg_G(u) + d_G(v)]$
Second Zagreb index	$M_2(G) = \sum_{uv \in E(G)} deg_G(u)deg_G(v)$
Second multiplicative Zagreb index	$\prod_2(G) = \prod_{uv \in E(G)} deg_G(u)deg_G(v)$
Second Zagreb co-index	$\overline{M}_2(G) = \sum_{uv \notin E(G)} deg_G(u)deg_G(v)$
Second multiplicative Zagreb co-index	$\overline{\prod}_2(G) = \prod_{uv \notin E(G)} deg_G(u)deg_G(v)$

Table 2.2. Zagreb indices, Zagreb co-indices, multiplicative Zagreb indices, and multiplicative Zagreb co-indices.

Xu, Das, and Tang [140] got the following result.

Lemma 2.9. [140] *For a connected graph G, we have*

$$\overline{\prod}_2(G) = \prod_{u \in V(G)} d_G(v)^{n-1-d_G(v)}.$$

Xu, Das, and Tang [140] obtained the following Nordhaus–Gaddum-type results.

Theorem 2.7. [140] *For a connected graph $G \in \mathcal{G}(n, m)$, we have:*

(1) $0 \leq \overline{\prod}_1(G)\overline{\prod}_1(\overline{G}) \leq \frac{\overline{M}_1(G)^{\binom{n}{2}}}{m^m[\binom{n}{2}-m]^{\binom{n}{2}-m}}$ *with the left equality if and only if G has at least two vertices of degree $n-1$, and the right equality if and only if G is $\frac{2m}{n}$-regular.*

(2) $0 \leq \overline{\prod}_2(G)\overline{\prod}_2(\overline{G}) \leq (\frac{n-1}{2})^{(n-1)n}$ *with the left equality if and only if G has at least one vertex of degree $n-1$, and the right equality if and only if G is a regular self-complementary graph.*

Proof. Let G be a connected graph with vertex set $\{v_1, v_2, \cdots, v_n\}$ such that $d_G(v_i) = d_i$.

(1) For the definition of the first multiplicative Zagreb coindex ($\overline{\prod}_1$), considering Lemma 2.4, we have

$$\begin{aligned}
\overline{\prod}_1(G)\overline{\prod}_1(\overline{G}) &= \prod_{v_iv_j \notin E(G)} (d_i + d_j) \cdot \prod_{v_iv_j \in E(G)} (n-1-d_i+n-1-d_j) \\
&\leq \left(\frac{\sum_{v_iv_j \notin E(G)} (d_i + d_j)}{\binom{n}{2} - m} \right)^{\binom{n}{2}-m} \cdot \left(\frac{\sum_{v_iv_j \in E(G)} [2n-2-(d_i+d_j)]}{m} \right)^m \\
&= \left[\frac{\overline{M}_1(G)}{\binom{n}{2} - m} \right]^{\binom{n}{2}-m} \cdot \left[\frac{2(n-1)m - M_1(G)}{m} \right]^m \\
&= \frac{\overline{M}_1(G)^{\binom{n}{2}}}{m^m[\binom{n}{2} - m]^{\binom{n}{2}-m}}
\end{aligned}$$

with equality holding if and only if $d_1 = d_2 = \cdots = d_n$, i.e., G is $\frac{2m}{n}$-regular, finishing the right part of (1).

For the left part, we can easily obtain $\overline{\prod}_1(G)\overline{\prod}_1(\overline{G}) \geq 0$ with equality holding if and only if G has at least two vertices of degree $n-1$. Thus the proof of (1) is complete.

(2) By Lemma 2.9, we have

$$\begin{aligned}
\overline{\prod}_2(G)\overline{\prod}_2(\overline{G}) &= \prod_{i=1}^{n} d_i^{n-1-d_i}(n-1-d_i)^{d_i} \leq \left(\frac{\sum_{i=1}^{n} d_i^{n-1-d_i}(n-1-d_i)^{d_i}}{n} \right)^n \\
&\leq \left[\frac{\sum_{i=1}^{n} (\frac{2(n-1-d_i)d_i}{n-1})^{n-1}}{n} \right]^n \leq \left[\frac{\sum_{i=1}^{n} \left(\frac{\frac{(n-1)^2}{2}}{n-1} \right)^{n-1}}{n} \right]^n \\
&= \left[\frac{n(\frac{n-1}{2})^{n-1}}{n} \right]^n = \left(\frac{n-1}{2} \right)^{(n-1)n}
\end{aligned}$$

with three equalities holding if and only if $d_1 = d_2 = \cdots = d_n$ and $d_i = n-1-d_i$ for $i = 1, 2, \cdots, n$, which implies that G is a regular self-complementary graph. Thus the proof of the right part is over.

For the left part, clearly, we have

$$\overline{\prod}_2(G)\overline{\prod}_2(\overline{G}) = \prod_{i=1}^{n} d_i^{n-1-d_i}(n-1-d_i)^{d_i} \geq 0.$$

The above equality holds if and only if there is at least one vertex v_i of degree $d_i = n-1$. This completes the proof of this theorem. ∎

If one adds one more condition that $\overline{G}$, i.e., the complement of G, is also connected, it seems to be a bit difficult to find the corresponding extremal graph. So Xu, Das, and Tang [140] proposed the following problem.

Problem 2.1. [140] *Which graph makes $\overline{\prod}_1(G)\overline{\prod}_1(\overline{G})$ achieve its minimal value for $i = 1, 2$ among all connected graphs of order n with their complements being also connected?*

2.5 Atom–bond connectivity index

The *atom-bond connectivity (ABC) index*, introduced by Estrada, Torres, Rodríguez, and Gutman [46], is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{deg_G(u) + deg_G(v) - 2}{deg_G(u)deg_G(v)}}.$$

Das [24] proved that

Lemma 2.10. [24] *Let G be a simple connected graph with m edges and maximal vertex degree Δ. Then*

$$ABC(G) \geq \frac{2^{7/4} m\sqrt{\Delta - 1}}{\Delta^{3/4}(\sqrt{\Delta} + \sqrt{2})} \tag{54}$$

where equality is attained if and only if $G \cong P_n$.

Later, Das, Gutman, and Furtula [30] reported the results for the ABC index.

Theorem 2.8. [30] *Let $G \in \mathcal{G}(n)$ be a connected graph with connected complement $\overline{G}$. Then*

$$ABC(G) + ABC(\overline{G}) \geq \frac{2^{3/4} n(n-1)\sqrt{k-1}}{k^{3/4}(\sqrt{k} + \sqrt{2})}, \tag{55}$$

where $k = \max\{\Delta, n - \delta - 1\}$, and where Δ and δ are the maximal and minimal vertex degrees of G. Moreover, equality in (55) holds if and only if $G \cong P_4$.

Proof. We start by equality in (54). Let m and $\overline{\Delta}$ be the number of edges and maximal vertex degree in $\overline{G}$. Then

$$\begin{aligned} ABC(G) + ABC(\overline{G}) &\geq \frac{2^{\frac{7}{4}} m\sqrt{\Delta - 1}}{\Delta^{\frac{3}{4}}(\sqrt{\Delta} + \sqrt{2})} + \frac{2^{\frac{7}{4}} \overline{m}\sqrt{\overline{\Delta} - 1}}{\overline{\Delta}^{\frac{3}{4}}(\sqrt{\overline{\Delta}} + \sqrt{2})} \\ &= \frac{2^{\frac{3}{4}} 2m\sqrt{\Delta - 1}}{\Delta^{\frac{3}{4}}(\sqrt{\Delta} + \sqrt{2})} + \frac{2^{\frac{3}{4}}(n(n-1) - 2m)\sqrt{n - \delta - 2}}{(n - \delta - 1)^{\frac{3}{4}}(\sqrt{n - \delta - 1} + \sqrt{2})}. \end{aligned} \tag{56}$$

Consider the function

$$f = \frac{\sqrt{x - 1}}{x^{\frac{3}{4}}(\sqrt{x} + \sqrt{2})}$$

for which one can easily show that it monotonically decreases in the interval $[2, \infty)$. Thus

$$\frac{\sqrt{\Delta - 1}}{\Delta^{\frac{3}{4}}(\sqrt{\Delta} + \sqrt{2})} \geq \frac{\sqrt{k - 1}}{k^{\frac{3}{4}}(\sqrt{k} + \sqrt{2})} \leq \frac{\sqrt{n - \delta - 2}}{(n - \delta - 1)^{\frac{3}{4}}(\sqrt{n - \delta - 1} + \sqrt{2})}, \tag{57}$$

since $k \geq \Delta$ and $k \geq n - \delta - 1$. Since $2\overline{m} = n(n-1) - 2m$, combing the above results with (56), we arrive at (55).

It remains to examine the equality case. It is easy to check that equality in (55) holds if $G \cong P_4$. Suppose now that the equality in (55). Then all inequalities in (57) must be equalities, and we get $k = \Delta = n - 1 - \delta$. Equality in (56) implies $G \cong P_n$ and $\overline{G} \cong P_n$. Hence $G \cong P_4$. By this proof of Theorem 2.8 has been completed. ∎

Das [23] proved that

Lemma 2.11. [23] *For a connected graph G with m edges and maximum degree Δ,*

$$ABC(G) \leq p\sqrt{1-\frac{1}{\Delta}} + \frac{m-p}{\delta_1}\sqrt{2(\delta_1-1)}, \tag{58}$$

where p and δ_1 are the number of pendent vertices and minimal non-pendent vertex degrees in G.

By this upper bound, they derived the following result.

Theorem 2.9. [30] *Let $G \in \mathcal{G}(n)$ be a connected graph with connected complement $\overline{G}$. Then*

$$ABC(G) + ABC(\overline{G}) \leq (p+\bar{p})\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right) + \binom{n}{2}\sqrt{\frac{2}{k}-\frac{2}{k^2}}, \tag{59}$$

where $p, \bar{p}$ and $\delta_1, \bar{\delta}_1$ are the number of pendent vertices and minimal non-pendent vertex degrees in G and $\overline{G}$, respectively, and $k = \min\{\delta_1, \bar{\delta}_1\}$. Equality holds in (59) if and only if $G \cong P_4$ or G is an r-regular graph of order $2r+1$.

Proof. We have $\Delta \leq n-2$, as G and $\overline{G}$ are connected, and hence

$$1-\frac{1}{\Delta} \leq \frac{n-3}{n-2} \text{ and } \frac{2}{\delta_1} - \frac{2}{\delta_1^2} \geq \frac{2(n-3)}{(n-2)^2}.$$

Bearing in mind (58), we get

$$\begin{aligned} ABC(G) &\leq p\sqrt{\frac{n-3}{n-2}} - p\sqrt{\frac{2(n-3)}{(n-2)^2}} + m\sqrt{\frac{2}{\delta_1}-\frac{2}{\delta_1^2}} \\ &= p\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right) + m\sqrt{\frac{2}{\delta_1}-\frac{2}{\delta_1^2}}. \end{aligned} \tag{60}$$

from which there holds

$$\begin{aligned} ABC(G) + ABC(\overline{G}) &\leq (p+\overline{p})\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right) + m\sqrt{\frac{2}{\delta_1}-\frac{2}{\delta_1^2}} + \overline{m}\sqrt{\frac{2}{\overline{\delta}_1}-\frac{2}{\overline{\delta}_1^2}} \quad (61) \\ &\leq (p+\overline{p})\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right) + (m+\overline{m})\sqrt{\frac{2}{k}-\frac{2}{k^2}}. \quad (62) \end{aligned}$$

as $k \leq \delta_1, \overline{\delta}_1$. Since $m + \overline{m} = \binom{n}{2}$, from (62), we get the required result (59).

We now examine the equality case. Suppose that equality holds in (59). Then all inequalities in the above argument must be equalities. From equality in (60) we get $\Delta = \delta_1 = n-2, p \neq 0$, that is, $G \cong P_4$ or G is isomorphic to a regular graph. Equality in (61) implies that (i) $G \cong P_4$ or G is isomorphic to a regular graph and (ii) $\overline{G} \cong P_4$ or $\overline{G}$ is isomorphic to a regular graph. From equality in (62), we get $\delta_1 = \overline{\delta}_1$.

Using the above results, and recalling that $\overline{P}_4 \cong P_4$ we conclude that $G \cong P_4$ or G is isomorphic to an r-regular graph with $n = 2r+1$.

Conversely, one can easily see that equality in (59) holds for the path P_4 and for an r-regular graph of order $2r+1$. ■

2.6 Augmented Zagreb index

Inspired by the work done on the ABC index, Furtula, Graovac, and Vukičević [54] proposed the following modified version of the ABC index and named it as *augmented Zagreb index* (AZI):

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{deg_G(u)deg_G(v)}{deg_G(u) + deg_G(v) - 2} \right)^3.$$

To proceed, we need some lemmas.

Lemma 2.12. [85] *Let G be a connected graph with $m \geq 2$ edges and maximum degree Δ. Then*

$$AZI(G) \leq \frac{m\Delta^6}{8(\Delta - 1)^3} \tag{63}$$

with equality holding if and only if G is a path or a Δ-regular graph.

A graph G is said to be (r_1, r_2)-*regular* (or simply *biregular*) if $\Delta \neq \delta$ and $deg_G(u) = r_1$ or r_2, for every vertex u of G. Let Φ_1 denote the collection of those connected graphs whose pendent edges are incident with the maximum degree vertices and all other edges have at least one end-vertex of degree 2. Let Φ_2 be the collection of connected graphs having no pendent vertices but all the edges have at least one end-vertex of degree 2.

Lemma 2.13. [136] *Let G be a connected graph of order $n \geq 3$ with m edges, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$AZI(G) \geq p \left(\frac{\Delta}{\Delta - 1} \right)^3 + (m - p) \left(\frac{\delta_1^2}{2\delta_1 - 2} \right)^3 \tag{64}$$

with equality if and only if G is isomorphic to a $(1, \Delta)$-biregular graph or G is isomorphic to a regular graph or $G \in \Phi_1$ or $G \in \Phi_2$.

Ali, Raza, and Bhatti [2] obtained the following Nordhaus–Gaddum-type results.

Theorem 2.10. [2] *Let $G \in \mathcal{G}(n)$ $(n \geq 3)$ be a connected graph such that its complement $\overline{G}$ is connected. Let Δ, δ_1, p and $\overline{\Delta}, \overline{\delta_1}, \overline{p}$ denote the maximum degree, minimum non-pendent vertex degree, the number of pendent vertices in G and $\overline{G}$ respectively. If $\alpha = \min\{\delta_1, \overline{\delta_1}\}$ and $\beta = \max\{\Delta, \overline{\Delta}\}$, then*

$$\begin{aligned} (p + \overline{p}) \left(\frac{n-2}{n-3} \right)^3 \left(1 - \left(\frac{n-2}{2} \right)^3 \right) + \binom{n}{2} \left(\frac{\alpha^2}{2\alpha - 2} \right)^3 &\leq AZI(G) + AZI\left(\overline{G}\right) \\ &\leq \binom{n}{2} \left(\frac{\beta^2}{2\beta - 2} \right)^3 \end{aligned} \tag{65}$$

with equalities if and only if $G \cong P_4$ or G is isomorphic to r-regular graph with $2r + 1$ vertices.

Proof. Suppose that m and $\overline{m}$ are the number of edges in G and $\overline{G}$ respectively. Firstly, we will prove the lower bound. Since both G and $\overline{G}$ are connected, it follows that $\delta_1 \leq \Delta \leq n-2$. Note that both the functions $f(x) = -\frac{x^2}{2x-2}$ and $g(x) = \frac{x}{x-1}$ are decreasing in the interval $[2, \infty)$. Then

$$-\frac{\delta_1^2}{2\delta_1 - 2} \geq -\frac{(n-2)^2}{2(n-3)} \text{ and } \frac{\Delta}{\Delta - 1} \geq \frac{n-2}{n-3}.$$

Hence from (64), we have

$$\begin{aligned} AZI(G) &\geq p\left(\frac{n-2}{n-3}\right)^3 + m\left(\frac{\delta_1^2}{2\delta_1 - 2}\right)^3 - p\left(\frac{(n-2)^2}{2(n-3)}\right)^3 \\ &= m\left(\frac{\delta_1^2}{2\delta_1 - 2}\right)^3 + p\left(\frac{n-2}{n-3}\right)^3\left(1 - \left(\frac{n-2}{2}\right)^3\right), \end{aligned} \tag{66}$$

this implies

$$\begin{aligned} AZI(G) + AZI\left(\overline{G}\right) &\geq m\left(\frac{\delta_1^2}{2\delta_1 - 2}\right)^3 + \overline{m}\left(\frac{\overline{\delta_1}^2}{2\overline{\delta_1} - 2}\right)^3 \\ &\quad + (p + \overline{p})\left(\frac{n-2}{n-3}\right)^3\left(1 - \left(\frac{n-2}{2}\right)^3\right). \end{aligned} \tag{67}$$

Since the function $-f$ is increasing in the interval $[2, \infty)$ and $\delta_1, \overline{\delta_1} \geq \alpha \geq 2$, from (67) it follows that

$$\begin{aligned} AZI(G) + AZI\left(\overline{G}\right) &\geq m\left(\frac{\alpha^2}{2\alpha - 2}\right)^3 + \overline{m}\left(\frac{\alpha^2}{2\alpha - 2}\right)^3 \\ &\quad + (p + \overline{p})\left(\frac{n-2}{n-3}\right)^3\left(1 - \left(\frac{n-2}{2}\right)^3\right). \end{aligned} \tag{68}$$

After using the fact $m + \overline{m} = \binom{n}{2}$ in (68), one obtains the desired lower bound.

Now, we prove the upper bound. From (63), it follows that

$$AZI(G) + AZI\left(\overline{G}\right) \leq \frac{m\Delta^6}{8(\Delta - 1)^3} + \frac{\overline{m}\overline{\Delta}^6}{8(\overline{\Delta} - 1)^3} \tag{69}$$

Since the function $h(x) = \frac{x^6}{8(x-1)^3}$ is increasing in the interval $[2, \infty)$ and $\Delta, \overline{\Delta} \geq 2$, from (69) we have

$$AZI(G) + AZI\left(\overline{G}\right) \leq \frac{m\beta^6}{8(\beta - 1)^3} + \frac{\overline{m}\beta^6}{8(\beta - 1)^3} = \binom{n}{2}\left(\frac{\beta^2}{2\beta - 2}\right)^3. \tag{70}$$

Now, let us discuss the equality cases. If $G \cong P_4$ then $\overline{G} \cong P_4$ and if G is isomorphic to r-regular graph with $2r+1$ vertices then $\overline{G}$ is also isomorphic to r-regular graph. Hence in either case, both lower and upper bounds are attained. Conversely, first let us suppose that left equality in (65) hold. Then all the Inequalities (66), (67), (68) must be equalities.

$a)$. Equality in (68) implies that $\delta_1 = \overline{\delta_1}$.

$b)$. Equality in (67) implies

- G is isomorphic to regular graph or $G \cong P_4$, and
- $\overline{G}$ is isomorphic to regular graph or $\overline{G} \cong P_4$.

c). Equality in (66) implies that either $\delta_1 = \Delta = n-2$ and $p \neq 0$, or G is isomorphic to a regular graph.

Using the fact $P_4 \cong \overline{P}_4$ and combining all the results derived in a), b), c), we obtain the desired conclusion. Finally, suppose that right equality in (65) holds, then both the Inequalities (69) and (70) must be equalities. Equality in (70) implies that $\Delta = \overline{\Delta} = \beta$. Equality in (69) implies that

• $G \cong P_4$ or G is isomorphic to regular graph and

• $\overline{G} \cong P_4$ or $\overline{G}$ is isomorphic to regular graph.

Therefore, either $G \cong P_4$ or G is isomorphic to r-regular graph with $2r+1$ vertices. ■

2.7 Sum–connectivity index

Zhou and Trinajstić [158] proposed a new invariant to measure the molecular connectivity in chemistry. It is the *sum-connectivity index* $\mathrm{SC}(G)$ of a graph G defined by

$$\mathrm{SC}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg_G(u) + deg_G(v)}}.$$

The first Nordhaus–Gaddum inequality for sum-connectivity index appeared in the same paper [158].

Theorem 2.11. [158] *If $G \in \mathcal{G}(n)$ is a graph, then*

$$\mathrm{SC}(G) + \mathrm{SC}(\overline{G}) \geq \frac{n\sqrt{n-1}}{2\sqrt{2}}$$

with equality if and only if G or $\overline{G}$ is the complete graph K_n.

In the next year, the same authors, in another paper [159], extended the sum-connectivity index SC(G) to the *general sum-connectivity index* $\mathrm{SC}_\alpha(G)$, which is defined as

$$\mathrm{SC}_\alpha(G) = \sum_{uv \in E(G)} (deg_G(u) + deg_G(v))^\alpha,$$

where α is a real number.

Lemma 2.14. [159] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a graph. If $0 < \alpha < 1$, then*

$$\mathrm{SC}_\alpha(G) \geq M_1(G)^\alpha$$

with equality if and only if $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$, and if $\alpha < 0$, then

$$\mathrm{SC}_\alpha(G) \leq 2^{-1+\alpha} n(n-1)$$

with equality if and only if $G = K_2$.

Zhou and Trinajstić [159] proved the following Nordhaus–Gaddum-type results for general sum-connectivity index.

Theorem 2.12. [159] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a graph.*

(1) *If $\alpha > 0$, then*

$$\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) \leq 2^{\alpha-1} n(n-1)^{\alpha+1}$$

with equality if and only if G or $\overline{G}$ is the complete graph K_n,

$$\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) \geq 2^{-1} n(n-1)^{\alpha+1}$$

for $\alpha \geq 1$; with equality if and only if G is a regular graph of degree $\frac{n-1}{2}$, and

$$\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) > 2^{-\alpha} n^\alpha (n-1)^{2\alpha}$$

for $0 < \alpha < 1$.

(2) *If $\alpha < 0$, then*

$$2^{\alpha-1} n(n-1)^{\alpha+1} \leq \mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) < 2^\alpha n(n-1)$$

with left equality if and only if G or $\overline{G}$ is the complete graph K_n.

Proof. Let m and $\overline{m}$ be respectively the number of edges of G and $\overline{G}$. Then $m + \overline{m} = \frac{n(n-1)}{2}$. If $\alpha > 0$, then

$$\begin{aligned} \mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) &= \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)]^\alpha + \sum_{uv \in E(\overline{G})} [deg_{\overline{G}}(u) + deg_{\overline{G}}(v)]^\alpha \\ &\leq m(2n-2)^\alpha + \overline{m}(2n-2)^\alpha \\ &= (m + \overline{m})(2n-2)^\alpha \\ &= 2^{-1+\alpha} n(n-1)^{1+\alpha} \end{aligned}$$

with equality if and only if either $deg_G(u) = deg_G(v) = n-1$ for every edge $uv \in E(G)$ or $E(G) = \emptyset$, i.e., $G = K_n$ or $G = \overline{K}_n$. Similarly, if $\alpha < 0$, then $\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) \geq 2^{-1+\alpha} n(n-1)^{1+\alpha}$ with equality if and only if $G = K_n$ or $G = \overline{K_n}$.

It is easily seen that:

$$\begin{aligned} \mathrm{SC}_1(G) + \mathrm{SC}_1(\overline{G}) &= \sum_{u \in V(G)} [deg_G(u)^2 + deg_{\overline{G}}(u)^2] \\ &\geq \sum_{u \in V(G)} \frac{[deg_G(u) + deg_{\overline{G}}(u)]^2}{2} = \frac{n(n-1)^2}{2} \end{aligned}$$

with equality if and only if $deg_G(u) = deg_{\overline{G}}(u)$ for all $u \in V(G)$, i.e., G is a regular graph of degree $\frac{n-1}{2}$. If $\alpha > 1$, then x^α is strictly convex and thus:

$$\begin{aligned}
& \mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) \\
\geq\ & (m+\overline{m}) \left[\frac{\sum_{uv\in E(G)}(deg_G(u) + deg_G(v)) + \sum_{uv\in E(\overline{G})}(deg_{\overline{G}}(u) + deg_{\overline{G}}(v))}{m+\overline{m}} \right]^\alpha \\
=\ & (m+\overline{m})^{1-\alpha}[\mathrm{SC}_1(G) + \mathrm{SC}_1(\overline{G})]^\alpha \\
\geq\ & (m+\overline{m})^{1-\alpha} \left[\frac{n(n-1)^2}{2} \right]^\alpha \\
=\ & 2^{-1}n(n-1)^{1+\alpha}
\end{aligned}$$

with equality if and only if G is a regular graph of degree $\frac{n-1}{2}$. If $0 < \alpha < 1$, then

$$\begin{aligned}
\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) &\geq \left[\sum_{uv\in E(G)} (deg_G(u) + deg_G(v)) + \sum_{uv\in E(\overline{G})} (deg_{\overline{G}}(u) + deg_{\overline{G}}(v)) \right]^\alpha \\
&= [\mathrm{SC}_1(G) + \mathrm{SC}_1(\overline{G})]^\alpha \\
&\geq \left[\frac{n(n-1)^2}{2} \right]^\alpha \\
&\geq 2^{-\alpha}n^\alpha(n-1)^{2\alpha}
\end{aligned}$$

and thus $\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) > 2^{-\alpha}n^\alpha(n-1)^{2\alpha}$. This is because a graph G with $|E(G) \cup E(\overline{G})| \leq 1$ is not possible to be a regular graph of degree $\frac{n-1}{2}$ for $n \geq 2$.

If $\alpha < 0$, then it follows from Lemma 2.14 that

$$\mathrm{SC}_\alpha(G) + \mathrm{SC}_\alpha(\overline{G}) < 2^{-1+\alpha}n(n-1) + 2^{-1+\alpha}n(n-1) = 2^\alpha n(n-1).$$

The proof is now completed. ■

2.8 General sum–connectivity co–index

The first Zagreb index can be viewed as the contribution of pairs of adjacent vertices to additively weighted versions of Wiener numbers and polynomials; see [94]. Curiously enough, it turns out that analogous contribution of non-adjacent pairs of vertices must be taken into account when calculating the weighted Wiener polynomials of certain composite graphs [40]. Such quantity is said to be the first Zagreb co-index since the sums involved run over the edges of graph $\overline{G}$. The *first Zagreb co-index* of a graph G is more formally defined as

$$\overline{M}_1(G) = \sum_{uv\notin E(G)} [deg_G(u) + deg_G(v)]$$

Zhou and his co-workers [159] proposed a graph invariant, called the *general sum-connectivity index*

$$\mathrm{SC}_\alpha(G) = \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)]^\alpha.$$

Su and Xu [132] focused their attention to contributions from the pairs of non-adjacent vertices of graph G and introduced a new invariant, the *general sum-connectivity co-index*, which is defined as:

$$\overline{\mathrm{SC}}_\alpha(G) = \sum_{uv \notin E(G)} [deg_G(u) + deg_G(v)]^\alpha.$$

In [132], Su and Xu obtained the following.

Lemma 2.15. [132] *Let $G \in \mathcal{G}(n)$ be a simple graph. Then*

$$0 \leq \overline{M}_1(G) + \overline{M}_1(\overline{G}) \leq 2^{-1} n(n-1)^2.$$

The lower bound attains on $G = K_n$, and the upper bound attains uniquely on $\frac{n-1}{2}$-regular graphs.

Lemma 2.16. [132] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a simple graph. Each of the following holds:*

(1) *If $0 < \alpha < 1$, then $\overline{\mathrm{SC}}_\alpha(G) \geq \overline{M}_1(G)^\alpha$. The lower bound attains either on $G = \overline{K_2} \cup K_{n-2}$ or $G = K_n$.*

(2) *If $\alpha < 0$, then $\overline{\mathrm{SC}}_\alpha(G) \leq 2^{\alpha-1} n(n-2)$. The upper bound attains uniquely on $\frac{n}{2}$ K_2.*

Theorem 2.13. [132] *Let G be a simple graph with order n. The following hold:*

(1) *If $\alpha > 1$, then*

$$0 \leq \overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G}) \leq 2^{1-\alpha} n(n-1)^{1+\alpha}.$$

The lower bound attains either on $G = K_n$ or $G = \overline{K_n}$, and the upper bound attains uniquely on $\frac{n-1}{2}$-regular graphs.

(2) *If $\alpha < 0$, then*

$$0 \leq \overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G}) \leq 2^\alpha n(n-2).$$

The lower bound attains uniquely on $\frac{n}{2} K_2$, and the upper bound attains either on $G = K_n$ or $G = \overline{K_n}$.

Proof. (1) If $\alpha > 1$, then $\Phi(x) = x^\alpha$ is a strictly convex function. From Lemma 2.15, we have

$$\begin{aligned}
& \overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G}) \\
= & \sum_{uv \notin E(G)} [deg_G(u) + deg_G(v)]^\alpha + \sum_{uv \notin E(\overline{G})} [deg_{\overline{G}}(u) + deg_{\overline{G}}(v)]^\alpha \\
\geq & (\overline{m} + m) \left[\frac{\sum_{uv \notin E(G)} [deg_G(u) + deg_G(v)] + \sum_{uv \notin E(\overline{G})} [deg_{\overline{G}}(u) + deg_{\overline{G}}(v)]}{m + \overline{m}} \right]^\alpha \\
= & (\overline{m} + m)^{1-\alpha} [\overline{M}_1(G) + \overline{M}_1(\overline{G})]^\alpha \geq 0
\end{aligned}$$

with equality if and only if either $deg_G(u) + deg_G(v) = n - 1$ for each edge uv or there is no edge in graph G. This implies that $G = K_n$ or $G = \overline{K_n}$. On the other hand,

$$\begin{aligned}
\overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G}) &= \sum_{uv \notin E(G)} [deg_G(u) + deg_G(v)]^\alpha + \sum_{uv \notin E(\overline{G})} [deg_{\overline{G}}(u) + deg_{\overline{G}}(v)]^\alpha \\
&\leq \overline{m} \left[\frac{n-1}{2} + \frac{n-1}{2}\right]^\alpha + m \left[\frac{n-1}{2} + \frac{n-1}{2}\right]^\alpha \\
&= (\overline{m} + m)(n-1)^\alpha \\
&= 2^{-1} n (n-1)^{\alpha+1}.
\end{aligned}$$

Note that the upper bound is best possible. In fact, for any $n = 4k + 1$, $k \geq 1$, there exists a graph G_n with G_n and $\overline{G_n}$ are $\frac{n-1}{2}$-regular. Then G_n is a graph whose $\overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G})$ attains the upper bound.

(2) If $\alpha < 0$, then it follows from Lemma 2.16 that

$$\overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G}) \leq 2^{\alpha-1} n(n-2) + 2^{\alpha-1} n(n-2) = 2^\alpha n(n-2).$$

The upper bound attains uniquely on $\frac{n}{2}K_2$. By analogous arguments as (1), we obtain that $\overline{\mathrm{SC}}_\alpha(G) + \overline{\mathrm{SC}}_\alpha(\overline{G}) \geq 0$ for $\alpha < 0$, and the lower bound attains uniquely on $G = K_n$ or $G = \overline{K_n}$. This completes the proof. ■

2.9 Geometric–arithmetic index

In [134], Vukičević and Furtula defined a new topological index "geometric-arithmetic index" of a graph G, denoted by $GA(G)$ and is defined by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{deg_G(u) deg_G(v)}}{deg_G(u) + deg_G(v)}$$

Let $G = (V(G), E(G))$. If $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree s, then G is a (r, s)-*semiregular graph*. When $r = s$, G is called a *regular graph*.

Das [23] first got the following upper bound of $GA(G)$ for a connected graph G.

Lemma 2.17. [23] *Let G be a simple connected graph of m edges with maximum vertex degree Δ and minimum vertex degree δ. Then*

$$GA(G) \geq \frac{2m\sqrt{\Delta\delta}}{\Delta + \delta}, \tag{71}$$

with equality holding in (71) if and only if G is isomorphic to a regular graph or G is isomorphic to a bipartite semiregular graph.

By the above lower bound, Das next derived the following Nordhaus–Gaddum-type result for the geometric-arithmetic index in 2010.

Theorem 2.14. [23] *Let $G \in \mathcal{G}(n)$, and $G, \overline{G}$ are both connected. Then*

$$GA(G) + GA(\overline{G}) \geq \frac{2k}{k^2+1}\binom{n}{2}, \tag{72}$$

where $k = \max\left\{\sqrt{\frac{\Delta}{\delta}}, \sqrt{\frac{n-1-\delta}{n-1-\Delta}}\right\}$; Δ, δ are the maximum vertex degree and minimum vertex degree in G, respectively. Moreover, the equality holds in (72) if and only if G is isomorphic to a regular graph.

Proof. We have $\overline{m} = \binom{n}{2} - m$, $\overline{\Delta} = n-1-\delta$ and $\overline{\delta} = n-1-\Delta$, where $\overline{m}$, $\overline{\Delta}$ and $\overline{\delta}$ are the number of edges, maximum vertex degree and minimum vertex degree in $\overline{G}$, respectively. Using (71), we get

$$GA(G) + GA(\overline{G}) \geq \frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{(n(n-1)-2m)\sqrt{(n-1-\delta)(n-1-\Delta)}}{2(n-1)-\Delta-\delta}. \tag{73}$$

Since

$$k \geq \sqrt{\frac{\Delta}{\delta}} \geq 1 \text{ and } 1 - \frac{\sqrt{\delta}}{k\sqrt{\Delta}} \geq 0,$$

we have

$$\left(k - \sqrt{\frac{\Delta}{\delta}}\right)\left(1 - \frac{\sqrt{\delta}}{k\sqrt{\Delta}}\right) \geq 0$$

i.e.

$$\frac{\sqrt{\Delta\delta}}{\Delta+\delta} \geq \frac{k}{k^2+1}. \tag{74}$$

Again, since $k \geq \sqrt{(n-1-\delta)/(n-1-\Delta)}$, it follows that

$$\frac{\sqrt{(n-1-\delta)(n-1-\Delta)}}{2(n-1)-\Delta-\delta} \geq \frac{k}{k^2+1}. \tag{75}$$

Using (74) and (75) in (73), we get the required result (72).

By Lemma 2.17, the equality holds in (73) if and only if G is a regular graph, as G and $\overline{G}$ are connected. Moreover, all inequalities in the above argument must be equalities for regular graph. Thus the equality holds in (72) if and only if G is isomorphic to a regular graph. ■

Das [23] also got the following lower bound of $GA(G)$ for a connected graph G.

Lemma 2.18. [23] *Let G be a simple connected graph of m edges with minimum nonpendent vertex degree δ_1. Then*

$$GA(G) \leq \frac{2p\sqrt{\delta_1}}{\delta_1+1} + m - p \tag{76}$$

where p is the number of pendent vertices in G. Moreover, the equality holds in (76) if and only if G is isomorphic to a regular graph or G is isomorphic to a $(\delta_1, 1)$-semiregular graph.

By the above upper bound, Das [23] derived the following result.

Theorem 2.15. [23] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected $\overline{G}$. Then*

$$GA(G) + GA(\overline{G}) \leq \binom{n}{2} - p\frac{(\sqrt{\delta_1} - 1)^2}{\delta_1 + 1} - \bar{p}\frac{(\sqrt{\bar{\delta}_1} - 1)^2}{\bar{\delta}_1 + 1}, \tag{77}$$

where $p, \bar{p}$ and $\delta_1, \bar{\delta}_1$ are the number of pendent vertices and minimum non-pendent vertex degrees in G and $\overline{G}$, respectively. Moreover, the equality holds in (77) if and only if G is isomorphic to a regular graph.

Proof. By (76), we get

$$GA(G) + GA(\overline{G}) \leq m - p + \frac{2p\sqrt{\delta_1}}{\delta_1 + 1} + \overline{m} - \overline{p} + \frac{2\overline{p}\sqrt{\bar{\delta}_1}}{\bar{\delta}_1 + 1}.$$

Since $m + \overline{m} = \binom{n}{2}$, we get the required result (77). By Lemma 2.18, the equality holds in (77) if and only if G is isomorphic to a regular graph. ∎

The following corollary is immediate from Theorem 2.14.

Corollary 2.1. [23] *Let G be a connected graph on n vertices with a connected $\overline{G}$. Then*

$$GA(G) + GA(\overline{G}) \leq \binom{n}{2} \tag{78}$$

with equality holding in (78) if and only if G is isomorphic to a regular graph.

In [134], the following lower and upper bounds for $GA(G)$ was established:

Lemma 2.19. [134] *Let $G \in \mathcal{G}(n)$ be a connected graph. Then*

$$\frac{2(n-1)^{3/2}}{n} \leq GA(G) \leq \binom{n}{2}. \tag{79}$$

Lower bound is achieved if and only if $G \cong K_{1,n-1}$ and upper bound is achieved if and only if $G \cong K_n$.

Remark 2.2. [23] *The upper bound of $GA(G)$ in (79) is $\binom{n}{2}$, but this is our upper bound for $GA(G) + GA(\overline{G})$.*

Remark 2.3. [23] *The lower and upper bounds given by (72) and (77), respectively, are equal when G is a regular graph.*

2.10 Edge version of geometric–arithmetic index

Mahmiani, Khormali, and Iranmanesh [110] introduced the edge version of geometric-arithmetic index based on the end-vertex degrees of edges in a line graph of G as follows

$$EGA(G) = \sum_{ef \in E(L(G))} \frac{2\sqrt{deg_G(e) deg_G(f)}}{deg_G(e) + deg_G(f)},$$

where $deg_G(e)$ denotes the degree of the edge e in G.

For the edge version of geometric-arithmetic index, they first obtained the following upper and lower bounds.

Lemma 2.20. [110] *Let $G \in \mathcal{G}(n,m)$ be a connected graph. Therefore, we have*

$$EGA(G) \leq \sum_{u \in V(G)} deg_G(u)^2 - 2m.$$

Lemma 2.21. [110] *Let $G \in \mathcal{G}(n,m)$ be a simple graph. Then*

$$n - 4 + \frac{4\sqrt{2}}{3} \leq EGA(G) \leq \frac{n(n-1)^2}{2}.$$

By the above two lemmas, they derived the following Nordhaus–Gaddum-type results.

Theorem 2.16. [110] *Let $G \in \mathcal{G}(n)$. Then*

$$\frac{3(n^2-n-4)+8\sqrt{2}}{6} \leq EGA(G) + EGA(\overline{G}) \leq \frac{(n-2)(n-1)n(n+1)}{8}.$$

Proof. From Lemma 2.21, we have $EGA(G) \geq m-2+\frac{4\sqrt{2}}{3}$. Therefore, by replacing $\binom{n}{2}$ instead of m in last equation, the lower bound is concluded. From Lemma 2.20, we have $EGA(G) \leq |E(L(G))| \leq \binom{m}{2}$. Then by replacing $\binom{n}{2}$ instead of m in last equation, the upper bound is concluded. ■

2.11 Harmonic index

The *harmonic index* $HA(G)$ is a vertex-degree-based topological index. This index first appeared in [47], and was defined as

$$HA(G) = \sum_{uv \in E(G)} \frac{2}{deg_G(u) + deg_G(v)}.$$

Zhong and Xu [146] gave the following upper and lower bounds of $HA(G)$ in terms of Randić index.

Lemma 2.22. [146] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$\frac{2\sqrt{n-1}}{n} R(G) \leq HA(G) \leq R(G).$$

The lower bound is attained if and only if $G \cong S_n$, and the upper bound is attained if and only if all connected components of G are regular.

By the above lemma, Zhong and Xu [146] derived the following Nordhaus–Gaddum-type result for harmonic index.

Theorem 2.17. [146] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$\frac{n}{2} \leq HA(G) + HA(\overline{G}) \leq n. \tag{80}$$

The lower bound is attained if and only if $G \cong K_n$ or $\overline{G} \cong K_n$, and the upper bound is attained if and only if G is a k-regular graph with $1 \leq k \leq n-2$.

Proof. Let m and $\overline{m}$ be the number of edges order n with connected in G and $\overline{G}$. respectively. Then

$$
\begin{aligned}
& HA(G) + HA(\overline{G}) \\
= & \sum_{uv \in E(G)} \frac{2}{deg_G(v) + deg_G(u)} + \sum_{uv \in E(\overline{G})} \frac{2}{(n-1-deg_G(v)) + (n-1-deg_G(u))} \\
\geq & \sum_{uv \in E(G)} \frac{2}{2n-2} + \sum_{uv \in E(\overline{G})} \frac{2}{2n-2} = \frac{2}{2n-2}(m+\overline{m}) = \frac{2}{2n-2} \cdot \frac{n(n-1)}{2} = \frac{n}{2}
\end{aligned}
$$

with equality if and only if either $deg_G(u) = deg_G(v) = n-1$ for every edge uv of G or $E(G) = \emptyset$, i.e., $G \cong K_n$ or $\overline{G} \cong K_n$. So the lower bound of (80) holds.

We now prove the upper bound of (80). By Lemma 2.22, we have

$$HA(G) + HA(\overline{G}) \leq R(G) + R(\overline{G}) \leq \frac{n}{2} + \frac{n}{2} = n$$

with equalities if and only if both G and $\overline{G}$ contain no isolated vertices (i.e., $1 \leq \delta(G) \leq \Delta(G) \leq n-2$) and all connected components of G and $\overline{G}$ are regular. We claim that G must be a regular graph. For otherwise, there exist two vertices u, v in G such that $deg_G(u) \neq deg_G(v)$. Then u and v are contained in two different connected components of G, and hence $uv \in E(\overline{G})$. But this forces u and v lie in the same component of $\overline{G}$, a contradiction. So Theorem 2.17 holds. ■

3. Eigenvalue–based parameters

In this section, we consider eigenvalue-based parameters, which are defined using eigenvalues of one or more of the matrices associated to a graph. We first introduce four basic matrices and their eigenvalues.

Eigenvalues of the adjacent matrix: Let $G = (V, E)$ be a graph on n vertices. The *adjacency matrix* $A = (a_{i,j})$ is defined by $a_{i,j} = 1$ if vertices v_i and v_j of the graph G are adjacent and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of the adjacency matrix of G.

Eigenvalues of the Laplacian matrix: The *Laplacian matrix* of a graph is defined by $L = Diag - A$ where $Diag$ is the diagonal matrix with degrees of the vertices on the main diagonal. We denote its eigenvalues by $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$.

Eigenvalues of the signless Laplacian matrix: The *signless Laplacian matrix* is defined by $Q = Diag + A$. Denote by $q_1 \geq q_2 \geq \ldots \geq q_n$ its eigenvalues.

Eigenvalues of the distance matrix: Let G be a simple connected graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The distance $d_{i,j}$ between v_i and v_j of G is the length of the shortest path between those two vertices. The *distance matrix* D is the $n \times n$ matrix (D_{ij}) such that $D_{ij} = d_{i,j}$. Since D is a symmetric matrix, its eigenvalues are real. Denote by $p_1 \geq p_2 \geq \ldots \geq p_n$ its eigenvalues.

The following Table 3.1 shows the authors contributing the Nordhaus–Gaddum problem for eigenvalue-based parameters.

Eigenvalue Parameters	Authors Contributing N-G Problem
Spectral radius	Nosal [122]
	Amin and Hakimi [3]
	Nikiforov [118]
	Li [102]
	Shi [128]
	Hong and Shu [77]
	Nikiforov [120]
Energy	Zhou and Gutman [156]
	Das and Gutman [28]
Laplacian spectral radius	Shi [128]
	Liu, Lu, and Tian [107]
Laplacian energy	Zhou and Gutman [156]
	Zhou [147]
Laplacian-energy-like invariant	Gutman, Zhou, and Furtula [72]
Laplacian Estrada Index	Chen and Hou [16]
Laplacian Estrada-like invariant	Güngoör [59]
Kirchhoff index	Zhou and Trinajstić [162]
	Yang, Zhang, and Klein [142]
	Das, Yang and Xu [36]
Signless Laplacian spectral radius	Gutman, Kiani, Mirzakhah, and Zhou [67]
Incidence energy	Gutman, Kiani, Mirzakhah, and Zhou [67]
Distance spectral radius	Zhou and Trianjstić [161]
Reciprocal distance spectral radius	Zhou and Trinajstić [160]
	Zhou, Cai, and Trianjstić [154]
	Das [25]

Table 3.1. Eigenvalue–based parameters

3.1 Eigenvalues of the adjacent matrix

The determinant of a square matrix A is denoted by $|A|$ or by $\det A$. The characteristic polynomial $|\lambda I - A|$ of the adjacency matrix A of G is called the *characteristic polynomial* of G and denoted by $P_G(\lambda)$. The eigenvalues of A (i.e. the zeros of $|\lambda I - A|$) and the spectrum of A (which consists of the eigenvalues) are also called the *eigenvalues* and the *spectrum* of G, respectively. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G, then the whole spectrum is denoted by $Sp(G) = \{\lambda_1, \lambda_2, \cdots, \lambda_n\}$. In this section, we let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Then $\lambda_1(G)$ is called the *spectral radius* of G.

Let G be a simple graph on n vertices. The eigenvalues of G are the eigenvalues of its adjacency matrix $A(G)$; see [19]. These eigenvalues, arranged in a non-increasing order, will be denoted as $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$. Then the *energy* of the graph G is defined as

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

3.1.1 Spectral radius

Nosal [122] showed that for every graph G of order n,

$$n - 1 \leq \lambda_1(G) + \lambda_1(\overline{G}) \leq \sqrt{2}(n-1). \tag{81}$$

Amin and Hakimi [3] obtained the following result for spectral radius.

Theorem 3.1. [3] *Let $G \in \mathcal{G}(n)$ be a simple graph. Then*

$$n - 1 \leq \lambda_1(G) + \lambda_1(\overline{G}) \leq \frac{1+\sqrt{3}}{2}(n-1).$$

The lower bound is attained if and only if the graph is regular.

The lower bound has been improved in 2007 by Nikiforov [118].

Theorem 3.2. [118] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$\lambda_1(G) + \lambda_1(\overline{G}) \geq (n-1) + \sqrt{2}\,\frac{s^2(G)}{n^3},$$

where $s(G) = \sum_{u \in V(G)} |deg_G(u) - \frac{2m}{n}|$.

Before giving the proof of Theorem 3.2, they first stated a more general problem.
Problem 1. [118] For every $1 \leq k \leq n$ find

$$f_k(n) = \max_{|V(G)|=n} |\lambda_k(G)| + \left|\lambda_k(\overline{G})\right|.$$

It is difficult to determine $f_k(n)$ precisely for every n and k, so at this stage it seems more practical to estimate it asymptotically. In [118], they showed that

$$\frac{4}{3}n - 2 \leq f_1(n) < (\sqrt{2} - c)n$$

for some $c > 10^{-7}$ independent of n.

We recall two auxiliary results whose proofs can be found in [119]. Given a graph $G = G(n, m)$, recall that

$$s(G) = \sum_{u \in V(G)} \left| deg_G(u) - \frac{2m}{n} \right|.$$

Proposition 3.1. [118] *For every graph $G = G(n,m)$,*

$$\frac{s^2(G)}{2n^2\sqrt{2m}} \leq \lambda_1(G) - \frac{2m}{n} \leq \sqrt{s(G)}, \tag{82}$$

and

$$\lambda_n(G) + \lambda_n(\overline{G}) \leq -1 - \frac{s^2(G)}{2n^3}. \tag{83}$$

Decreasing the constant $\sqrt{2}$ in (81) happened to be a surprisingly challenging task for the author. The little progress that has been made is given in the following theorem.

Theorem 3.3. [118] *There exists $c \geq 10^{-7}$ such that*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq (\sqrt{2} - c)n.$$

for every graph G of order n.

Proof. Assume the opposite, let $\varepsilon = 10^{-7}$ and let there exist a graph G of order n such that

$$\lambda_1(G) + \lambda_1(\overline{G}) > (\sqrt{2} - \varepsilon)n.$$

Writing $A(G)$ for the adjacency matrix of G, we have

$$\sum_{i=1}^{n} \lambda_i^2(G) = \operatorname{tr}(A^2(G)) = 2e(G),$$

implying that

$$\lambda_1^2(G) + \lambda_n^2(G) + \lambda_1^2(\overline{G}) + \lambda_n^2(\overline{G}) \leq 2e(G) + 2e(\overline{G}) < n^2.$$

From

$$\lambda_1^2(G) + \lambda_1^2(\overline{G}) \geq \frac{1}{2}(\lambda_1(G) + \lambda_1(\overline{G}))^2 > \left(1 - \frac{\varepsilon}{\sqrt{2}}\right)^2 n^2 > (1 - \sqrt{2}\varepsilon)n^2$$

we find that

$$|\lambda_n(G)| + \left|\lambda_n(\overline{G})\right| \leq \sqrt{2(\lambda_n^2(G) + \lambda_n^2(\overline{G}))} < \sqrt{2\sqrt{2}\varepsilon}n, \tag{84}$$

and so, $\lambda_n(G) + \lambda_n(\overline{G}) > -2^{3/4}\varepsilon^{1/2}n$. Hence, by (83), we have $s^2(G) \leq 2^{7/4}\varepsilon^{1/2}n^4$. On the other hand, by (82) and in view of $s(G) = s(\overline{G})$, we see that

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq n - 1 + 2\sqrt{s(G)} < n + 2\sqrt{s(G)} \leq n + 2^{23/16}\varepsilon^{1/8}n,$$

and, by (84), it follows that

$$(\sqrt{2} - \varepsilon)n < n + 2^{23/16}\varepsilon^{1/8}n.$$

Dividing by n, we obtain $(\sqrt{2} - 1) < \varepsilon + 2^{23/16}\varepsilon^{1/8}$, a contradiction for $\varepsilon = 10^{-7}$. ■

It is certain that the upper bound given by Theorem 3.3 is far from the best one. We shall give below a lower bound on $f_1(n)$ which seems to be tight.

Given $1 \leq r < n$, let G be a the join of K_r and $\overline{K}_{n-r}$. Then G satisfies (see, e.g. [78])

$$\begin{aligned}\lambda_1(G) + \lambda_1(\overline{G}) &= \frac{r-1}{2} + \sqrt{nr - \frac{3r^2 + 2r - 1}{4}} + n - r - 1 \\ &= n - \frac{r+3}{2} + \sqrt{nr - \frac{3r^2 + 2r - 1}{4}}.\end{aligned}$$

The right-hand side of this equality is increasing in r for $0 \leq r \leq (n-1)/3$ and we find that

$$f_1(n) > \frac{4n}{3} - 2.$$

This give some evidence for the following conjecture.

Conjecture 3.1. [118]

$$f_1(n) = \frac{4n}{3} + O(1).$$

We conclude this section with an improvement of the lower bound in (81). Using the first of (82) obtain

$$\begin{aligned}\lambda_1(G) + \lambda_1(\overline{G}) &\geq n - 1 + \frac{s^2(G)}{2n^2}\left(\frac{1}{\sqrt{2e(G)}} + \frac{1}{\sqrt{2e(\overline{G})}}\right) \\ &\geq n - 1 + \sqrt{2}\,\frac{s^2(G)}{n^3}.\end{aligned}$$

The currently best upper bound was given by Csikvári [18] in 2009. The following conjecture has been formulated after some experiments with AutoGraphiX, a computer conjecture making system.

Conjecture 3.2. [6] *For any graph $G \in \mathcal{G}(n)$,*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \frac{4}{3}n - \frac{5}{3} - \begin{cases} f_1(n) & \text{if } n \mod (3) = 1, \\ 0 & \text{if } n \mod (3) = 2, \\ f_2(n) & \text{if } n \mod (3) = 0, \end{cases}$$

where $f_1(n) = \frac{3n-2-\sqrt{9n^2-12n+12}}{6}$ *and* $f_2(n) = \frac{3n-1-\sqrt{9n^2-6n+9}}{6}$.

This bound is sharp and attained if and only if G or $\overline{G}$ is a complete split graph with independent set on $\lfloor \frac{n}{3} \rfloor$ vertices (or $\lceil \frac{n}{3} \rceil$ if $n \mod (3) = 2$).

Upper bounds on the sum $\lambda_1(G) + \lambda_1(\overline{G})$ using the order and the minimum and maximum degrees of G were proved first by Li [102] in 1996 and then by Shi [128] in 2007.

Theorem 3.4. [102] *Let $G \in \mathcal{G}(n)$ be a graph with minimum and maximum degrees δ and Δ, respectively. Then*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \sqrt{2n(n-1) - 4\delta(n-1-\Delta) + 1} - 1.$$

Lemma 3.1. [128] *Let $G \in \mathcal{G}(n,m)$ be a graph with no isolated vertex. Let $\Delta = \Delta(G)$ and $\delta = \delta(G)$. Then*

$$(2m - \Delta n + \Delta\delta + \Delta - \delta)^{1/2} \leq \lambda_1(G) \leq (2m - \delta n + \Delta\delta - \Delta + \delta)^{1/2}.$$

Moreover, if G is connected then the first equality holds if and only if G is regular and the second holds if and only if G is a regular graph or a star.

Shi [128] gave some sharp upper bounds on the spectral radius of the Nordhaus–Gaddum type for a connected graph G and its connected complement $\overline{G}$.

Theorem 3.5. [128] *Let $G \in \mathcal{G}(n)$ be a graph with minimum and maximum degrees δ and Δ, respectively, such that $0 < \delta(G) \leq \Delta(G) < n-1$. Then*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \sqrt{2[(n-1)^2 - 2\delta n + 2\Delta\delta - \Delta + 3\delta]}.$$

Moreover, if both G and $\overline{G}$ are connected, then the equality holds if and only if G is $\frac{n-1}{2}$-regular.

Proof. Let $f(m,\Delta,\delta) = (2m - \delta n + \Delta\delta - \Delta + \delta)^{1/2}$. Note that $\Delta(\overline{G}) = n-1-\delta$, $\delta(\overline{G}) = n-1-\Delta$ and $m(\overline{G}) = \binom{n}{2} - m$. Lemma 3.1 gives that

$$\lambda_1(G) \leq f(m,\Delta,\delta) \text{ and } \lambda_1(\overline{G}) \leq f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right).$$

Now let $g(m) = f(m,\Delta,\delta) = f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)$. Then

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq g(m)$$

Since

$$\frac{dg}{dm} = 1/f(m,\Delta,\delta) - 1/f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right),$$

it is easy to check that $\frac{dg}{dm} \geq 0$ if and only if $f(m,\Delta,\delta) \leq f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)$ i.e. $m \leq [(n-1)^2 + \Delta + \delta]/4$. Thus

$$\begin{aligned}\lambda_1(G) + \lambda_1(\overline{G}) &\leq g([(n-1)^2 + \Delta + \delta]/4) \\ &= 2f([(n-1)^2 + \Delta + \delta]/4, \Delta, \delta) \\ &= \sqrt{2[(n-1)^2 - 2\delta n + 2\Delta\delta - \Delta + 3\delta]}.\end{aligned}$$

If the sum of spectral radii attains the upper bound, then the spectral radii of G and $\overline{G}$ both attain their upper bounds and $m = [(n-1)^2 + \Delta + \delta]/4$. Now if both G and $\overline{G}$ are connected, then Lemma 3.1 implies that $\Delta = \delta$. Thus

$$2\delta n = (n-1)^2 + 2\delta$$

This implies that $\delta = (n-1)/2$ and hence G is $(n-1)/2$-regular. Conversely, if G is a $(n-1)/2$-regular, then $\lambda_1(G) + \lambda_1(\overline{G}) = n-1$. ■

Lemma 3.2. [128] *Let $G \in \mathcal{G}(n,m)$ be a graph. Let $\Delta = \Delta(G)$ and $\delta = \delta(G)$. If $\Delta < 2n-1-[(2n-1)^2-8m-1]^{1/2}$, then*

$$\lambda_1(G) \le \frac{1}{2}\left(\Delta - 1 - \sqrt{(\Delta+1)^2 + 4(2m - \Delta n)}\right) \tag{85}$$

or

$$\frac{1}{2}\left(\Delta - 1 + \sqrt{(\Delta+1)^2 + 4(2m - \Delta n)}\right) \le \lambda_1(G) \le \frac{1}{2}\left(\delta - 1 + \sqrt{(\delta+1)^2 + 4(2m - \delta n)}\right). \tag{86}$$

Moreover, if G is connected, then the upper bound in (85) is strict, the first equality in (86) holds if and only if G is regular, and the second in (86) holds if and only if G is either a regular graph or a bidegreed graph with all vertices of degree δ or $n-1$.

By the above upper bound, Shi [128] derived the following Nordhaus–Gaddum-type result.

Theorem 3.6. [128] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$\lambda_1(G) + \lambda_1(\overline{G}) \le \left\{n - \Delta + \delta - 3 + \sqrt{2[(n-\Delta)^2 + 4n(\Delta - \delta) + (\delta+1)^2]}\right\}/2.$$

Moreover, if both G and $\overline{G}$ are connected, then the equality holds if and only if G is $(n-1)/2$-regular.

Proof. Let $f(m, \Delta, \delta) = [(\delta+1)^2 + 4(2m - \delta n)]^{1/2}$. Note that $\Delta(\overline{G}) = n - 1 - \delta$, $\delta(\overline{G}) = n - 1 - \Delta$ and $m(\overline{G}) = \binom{n}{2} - m$. Lemma 3.2 gives that

$$\lambda_1(G) \le [\delta - 1 + f(m, \Delta, \delta)]/2$$

and

$$\lambda_1(\overline{G}) \le \left[n - \Delta - 2 + f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)\right]/2.$$

Now let $g(m) = f(m, \Delta, \delta) + f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)$. Then

$$\lambda_1(G) + \lambda_1(\overline{G}) \le [n - \Delta + \delta - 3 + g(m)]/2$$

Since

$$\frac{dg}{dm} = 4/f(m, \Delta, \delta) - 4/f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right),$$

it is easy to check that $\frac{dg}{dm} \ge 0$ if and only if $f(m, \Delta, \delta) \le f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)$ i.e. $m \le [(n-\Delta)^2 + 4n(\Delta+\delta) - (\delta+1)^2]/16$. Thus

$$\begin{aligned}
\lambda_1(G) + \lambda_1(\overline{G}) &\le \{n - \Delta + \delta - 3 + g([(n-\Delta)^2 + 4n(\Delta+\delta) - (\delta+1)^2]/16)\}/2 \\
&= \{n - \Delta + \delta - 3 + 2f([(n-\Delta)^2 + 4n(\Delta+\delta) - (\delta+1)^2]/16, \Delta, \delta)\}/2 \\
&= \{n - \Delta + \delta - 3 + \sqrt{2[(n-\Delta)^2 + 4n(\Delta-\delta) + (\delta+1)^2]}\}/2.
\end{aligned}$$

If the sum of spectral radii attains the upper bound, then the spectral radii of G and $\overline{G}$ both attain their upper bounds and $m = [(n-\Delta)^2 + 4n(\Delta+\delta) - (\delta+1)^2]/16$. Now if both G and $\overline{G}$ are connected, then Lemma 3.2 implies that $\Delta = \delta$. Thus

$$8\delta n = (n-\delta)^2 + 8\delta n - (\delta+1)^2.$$

This implies that $\delta = (n-1)/2$ and hence G is $(n-1)/2$-regular. Conversely, if G is $(n-1)/2$-regular, then $\lambda_1(G) + \lambda_1(\overline{G}) = n-1$. ■

Remark 3.1. [128] *It is easy to see that our upper bounds are incomparable to the bounds of Nosal and Li. However, if $\Delta = o(n)$ or $\delta = n - o(n)$, then Theorem 3.6 implies that $\lambda_1(G) + \lambda_1(G^c) = O((\sqrt{2}+1)n/2)$ which is better than the bounds $O(\sqrt{2}n)$ of Nosal and Li and of Theorem 3.5.*

The following inequality, which is of Nordhaus–Gaddum type, was proved by Hong and Shu [77] in 2000.

Theorem 3.7. [77] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$\lambda_1(G) + \lambda_1(\overline{G}) \le \sqrt{\left(2 - \frac{1}{\chi(G)} - \frac{1}{\chi(\overline{G})}\right) n(n-1)},$$

where χ denotes the chromatic number. Equality holds if and only if G or $\overline{G}$ is a complete graph K_n.

A *complete k-partite graph* is a graph whose vertex set can be partitioned into k non-empty subsets $V_1, V_2, \ldots, V_k$ in such a way that any vertex in V_i is adjacent to every vertex in V_j, $j \ne i$, and no two vertices of V_i are adjacent $(1 \le i \le n)$. If the vertex number of V_i is n_i, the graph is denote by $K(n_1, n_2, \ldots, n_k)$. If $n_i = t$ for all i, the graph $K(t, t, \ldots, t)$ is called an *equi-complete k-partite graph*.

Lemma 3.3. [43,76] *Let G be a simple graph with m edges and chromatic number k. Then*

$$\lambda_1(G) \le \sqrt{\frac{2(k-1)m}{k}}$$

with equality if and only if G is an equi-complete k-partite graph or an empty graph.

Proof of Theorem 3.7: From Lemma 3.3, we have

$$\lambda_1(G) \le \sqrt{\frac{2(k-1)m}{k}} = \sqrt{2m\left(1 - \frac{1}{k}\right)}$$

and

$$\lambda_1(\overline{G}) \le \sqrt{\frac{2(\overline{k}-1)\overline{m}}{\overline{k}}} = \sqrt{2\overline{m}\left(1 - \frac{1}{\overline{k}}\right)},$$

where $\overline{m}$ is the edge number of the complement $\overline{G}$. So $2\overline{m} = n(n-1) - 2m$. Let us suppose that $s = 1 - 1/k$, $\overline{s} = 1 - 1/\overline{k}$ and

$$f(m) = \lambda_1(G) + \lambda_1(\overline{G}) = \sqrt{2ms} + \sqrt{(n(n-1) - 2m)\overline{s}}.$$

It is easy to show that

$$f(m) \le f\left(\frac{s}{2(s+\overline{s})} n(n-1)\right) = \sqrt{(s+\overline{s})n(n-1)}.$$

Therefore, we have

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \sqrt{\left(2 - \frac{1}{k} - \frac{1}{\overline{k}}\right) n(n-1)}.$$

Equality holds if and only if each of G and $\overline{G}$ are empty graph or equi-complete k-partite graph. Moreover, $m = s/(2(s+\overline{s}))n(n-1)$. Thus, G must be a complete graph or an empty graph. The proof is completed. ■

A similar inequality was given in 2002 by Nikiforov [120] using the clique number ω instead of the chromatic number χ.

Theorem 3.8. [120] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \sqrt{\left(2 - \frac{1}{\omega(G)} - \frac{1}{\omega(\overline{G})}\right) n(n-1)},$$

where ω denotes the clique number.

3.1.2 Energy

Zhou and Gutman [156] obtained the first Nordhaus–Gaddum-type result for graph energy.

Theorem 3.9. [156] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$E(G) + E(\overline{G}) \geq 2(n-1) \tag{87}$$

with equality if and only if G is the complete graph K_n or its complement, the empty graph (the n-vertex graph without edges).

Proof. We first observe that $E(G) \geq 2\lambda_1$ with equality if and only if G has at most one positive eigenvalue, i.e., if G is the empty graph or a complete multipartite graph [19]. Therefore,

$$E(G) + E(\overline{G}) \geq 2(\lambda_1 + \overline{\lambda_1}) \geq 2(n-1).$$

If equality holds in (87), then both G and $\overline{G}$ are empty or complete multipartite graphs, and so G must be the complete graph or the empty graph. Conversely, knowing the spectrum of K_n and $\overline{K_n}$, see [19], it is easily shown that (87) is an equality if $G \cong K_n$ or $G \cong \overline{K_n}$. ■

In [98] it was shown that for an (n, m)-graph G,

$$E(G) \leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}. \tag{88}$$

From this upper bound it could be deduced that [96]

$$E(G) \leq \frac{n}{2}(\sqrt{n} + 1)$$

which immediately implies

$$E(G) + E(\overline{G}) \leq n(\sqrt{n} + 1).$$

In what follows Zhou and Gutman [156] improved the latter upper bound.

Theorem 3.10. [156] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$E(G) + E(\overline{G}) < \sqrt{2}n + (n-1)\sqrt{n-1}. \tag{89}$$

Proof. Let m and $\overline{m}$ denote, respectively, the number of edges of G and $\overline{G}$. By (88) and (81), we have

$$\begin{aligned}
E(G) + E(\overline{G}) &\leq \lambda_1 + \overline{\lambda_1} + \sqrt{(n-1)(2m-\lambda_1^2)} + \sqrt{(n-1)\left(2\overline{m} - \overline{\lambda_1}^2\right)} \\
&\leq \lambda_1 + \overline{\lambda_1} + \sqrt{2(n-1)\left[2m + 2\overline{m} - (\lambda_1^2 + \overline{\lambda_1}^2)\right]} \\
&\leq \lambda_1 + \overline{\lambda_1} + \sqrt{2(n-1)\left[n(n-1) - \frac{1}{2}(\lambda_1 + \overline{\lambda_1})^2\right]} \\
&< \sqrt{2}n + \sqrt{2(n-1)\left[n(n-1) - \frac{1}{2}(n-1)^2\right]} \\
&= \sqrt{2}n + (n-1)\sqrt{n-1}.
\end{aligned}$$

This completes the proof. ∎

Remark 3.2. [156] *Let $G \in \mathcal{G}(n)$ be a regular graph of degree r. Then (88) becomes $E(G) \leq r + \sqrt{(n-1)r(n-r)}$ and we have*

$$\begin{aligned}
E(G) + E(\overline{G}) &\leq n - 1 + \sqrt{n-1}\left[\sqrt{r(n-r)} + \sqrt{(r+1)(n-r-1)}\right] \\
&\leq (n-1)(\sqrt{n+1} + 1).
\end{aligned}$$

which for $n \geq 6$ is better than (89).

Remark 3.3. [156] *A strongly regular graph G with parameters (n, r, ρ, σ) is an r-regular graph on n vertices, in which each pair of adjacent vertices has ρ common neighbors and each pair of non-adjacent vertices has σ common neighbors. If $\sigma \geq 1$ and G is non-complete, then the eigenvalues of G are [19] r, s, and t , with multiplicities 1, m_s, and m_t, where s and t are the solutions of the equation $x^2 + (\sigma - \rho)x + (\sigma - r) = 0$, and m_s and m_t are determined by $m_s + m_t = n - 1$ and $r + m_s s + m_t t = 0$. If G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$ (for some conveniently chosen value of n), then*

$$E(G) + E(\overline{G}) = \frac{n}{2}(\sqrt{n}+1) + \frac{n}{2}(\sqrt{n}+1) - \sqrt{n} - 2 = (n-1)(\sqrt{n}+1) - 1.$$

If we consider a Paley graph H, which is a strongly regular graph with parameters $(n, (n-1)/2, (n-5)/4, (n-1)/4)$, then

$$E(H) + E(\overline{H}) = (n-1)(\sqrt{n}+1).$$

The results stated in Remark 3.3 show that the bound in (89) is asymptotically tight.

Remark 3.4. [156] *Using Theorem 3.8, from the proof of Theorem 3.10, we have*

$$E_1(G)+E_1(\overline{G})\le\sqrt{\left(2-\frac{1}{\omega(G)}-\frac{1}{\omega(\overline{G})}\right)n(n-1)}+(n-1)\sqrt{n-1},$$

where ω *denotes the clique number of* G.

Das, Mojallal, and Gutman [34] have given the following lower bound, valid for non-singular graphs:

Lemma 3.4. [34] *Let* $G\in\mathcal{G}(n,m)$ *be a connected non-singular graph. Then*

$$E(G)\ge\frac{2m}{n}+n-1+\ln\left(\frac{n|\det A|}{2m}\right),\tag{90}$$

where $\det A$ $(\neq 0)$ *is the determinant of the adjacent matrix.*

Das and Gutman [28] derived the following upper bound for graph energy.

Lemma 3.5. [28] *Let* $G\in\mathcal{G}(n,m)$ *be a connected non-singular graph. Then*

$$E(G)\le 2m-\frac{2m}{n}\left(\frac{2m}{n}-1\right)-\ln\left(\frac{n|\det A|}{2m}\right),\tag{91}$$

where $\det A$ $(\neq 0)$ *is the determinant of the adjacent matrix. Equality holds if and only if* $G\cong K_n$.

Motivated by the seminal work of Noradhaus and Gaddum, Das and Gutman [28] reported here analogous results for graph energy.

Theorem 3.11. [28] *Let* G *and* $\overline{G}$ *be both connected non-singular graphs. If* $G\in\mathcal{G}(n,m)$, *then*

$$\begin{aligned}3(n-1)+\ln\left(\frac{n^2|\det(A\overline{A})|}{2m(n(n-1)-2m)}\right)&\le E(G)+E(\overline{G})\\ &\le 2(n-1)+\frac{4m(n(n-1)-2m)}{n^2}-\ln\left(\frac{n^2|\det(A\overline{A})|}{2m(n(n-1)-2m)}\right),\end{aligned}\tag{92}$$

where $\det A$ $(\neq 0)$ *and* $\det\overline{A}$ $(\neq 0)$ *are the determinants of the adjacency matrices of* G *and* $\overline{G}$, *respectively.*

Proof. By (90),

$$E(G)+E(\overline{G})\ge\frac{2m+2\overline{m}}{n}+2(n-1)+\ln\left(\frac{n|\det A|}{2m}\right)+\ln\left(\frac{n|\det\overline{A}|}{2\overline{m}}\right)$$

where m and $\overline{A}$ are the numbers of edges and the adjacency matrix of $\overline{G}$. Since $2m+2\overline{m}=n(n-1)$ and $\det A\overline{A}=\det A\det\overline{A}$, the lower bound in (92) follows.

By (91), we have

$$E(G)+E(\overline{G})\le 2m+2\overline{m}+\frac{2m+2\overline{m}}{n}-\frac{4m^2+4\overline{m}^2}{n^2}-\ln\left(\frac{n|\det A|}{2m}\right)-\ln\left(\frac{n|\det\overline{A}|}{2\overline{m}}\right).$$

This straightforwardly leads to the upper bound in (92). ∎

The following inequality is due to Dragomir.

Lemma 3.6. [41] *Let $a_1, a_2, \dots, a_n$ and $b_1, b_2, \dots, b_n$ be non-negative real numbers. If $p > 1$, then*

$$\left(\sum_{i=1}^{n}(a_i+b_i)^p\right)^{1/p} \leq \left(\sum_{i=1}^{n} a_i^p\right)^{1/p} + \left(\sum_{i=1}^{n} b_i^p\right)^{1/p}.$$

Moreover, the above equality holds if and only if the rows $\{a_i\}$ and $\{b_i\}$ are proportional.

Theorem 3.12. [28] *Let $G \in \mathcal{G}(n,m)$ be a graph. Then*

$$E(G)+E(\overline{G}) \leq n+\Delta-\delta-1 + \left[(n-1)\left(n-1+\frac{4m(n(n-1)-2m)}{n^2}+\frac{2}{n^2}\sqrt{2m(2m+n)(n^2-2m)(n^2-2m-n)}\right)\right]^{\frac{1}{2}}, \tag{93}$$

where Δ and δ are the maximum degree and minimum degree of G, respectively.

Proof. By Lemma 3.6, we have

$$\left(\sum_{i=2}^{n}(|\lambda_i|+|\overline{\lambda}_i|)^2\right)^{\frac{1}{2}} \leq \left(\sum_{i=2}^{n}\lambda_i^2\right)^{\frac{1}{2}} + \left(\sum_{i=2}^{n}\overline{\lambda}_i^2\right)^{\frac{1}{2}}$$

where λ_i and $\overline{\lambda_i}$ are eigenvalues of G and $\overline{G}$, respectively. Since

$$\sum_{i=1}^{n}\lambda_i^2 = 2m \text{ and } \sum_{i=1}^{n}\overline{\lambda}_1^2 = 2\overline{m},$$

we get

$$\begin{aligned}
\left(\sum_{i=2}^{n}|\lambda_i|+|\overline{\lambda}_i|\right)^2 &\leq \sum_{i=2}^{n}\lambda_i^2+\sum_{i=2}^{n}\overline{\lambda}_i^2+2\sqrt{\sum_{i=2}^{n}\lambda_i^2\sum_{i=2}^{n}\overline{\lambda}_i^2} \\
&= 2m-\lambda_1^2+2\overline{m}-\overline{\lambda}_1^2+2\sqrt{(2m-\lambda_1^2)(2\overline{m}-\overline{\lambda}_1^2)} \\
&\leq n(n-1)-\frac{4m^2+4\overline{m}^2}{n^2}+2\sqrt{\frac{4m\overline{m}}{n^4}(n^2-2m)(2m+n)} \\
&= n-1+\frac{4m(n(n-1)-2m)}{n^2} \\
&\quad +\frac{2}{n^2}\sqrt{2m(n^2-2m-n)(n^2-2m)(2m+n)}.
\end{aligned} \tag{94}$$

Since $\lambda_1 \leq \Delta$, using the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}
E(G)+E(\overline{G}) &= |\lambda_1|+|\overline{\lambda}_1|+\sum_{i=2}^{n}(|\lambda_i|+|\overline{\lambda}_i|) \\
&\leq \Delta+n-\delta-1+\sqrt{(n-1)\sum_{i=2}^{n}(|\lambda_i|+|\overline{\lambda}_i|)^2}
\end{aligned}$$

Together with (94) this yields (93). ■

3.2 Eigenvalues of the Laplacian matrix

Recall that *Laplacian matrix* of a graph is defined as $L = Diag - A$ where $Diag$ is the diagonal matrix with degrees of the vertices on the main diagonal. In this section, we denote its eigenvalues by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$, except in Section 3.2.6.

The *Laplacian energy* of a graph G, denoted by $LE(G)$, has been defined as [71]

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

Liu and Liu [106] proposed another Laplacian-spectrum based "energy", and called it *Laplacian-energy-like invariant*, LEL, which is defined as

$$LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i}.$$

In analogy to the Estrada index, the *Laplacian Estrada index* of a graph G was introduced in [48] as

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

Güngör [59] proposed another Laplacian spectrum based on "Estrada index", and called it *Laplacian Estrada-like invariant*, denoted by LEEL. In fact it is defined as

$$LEEL(G) = \sum_{i=1}^{n} e^{\sqrt{\mu_i}} \,. \tag{95}$$

In 1993, Klein and Randić [95] introduced a new distance function named resistance distance, based on the theory of electrical networks. They viewed G as an electrical network N by replacing each edge of G with a unit resistor. The *resistance distance* between the vertices u and v of the graph G, denoted by $R(u, v) = R(u, v \,|\, G)$, is then defined to be the effective resistance between the nodes u and v in N. Similar to the long recognized shortest–path distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical properties, but also with a substantial potential for chemical applications [93, 95, 138, 139].

The *Kirchhoff index* (or resistance index) is defined in analogy to the Wiener index as:

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} R(u, v).$$

Then a long time known result for the Kirchhoff index [69] is

$$Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}. \tag{96}$$

Let G be a simple, undirected, connected molecular graph and the vertices of it will be labelled by $v_1, v_2, \cdots, v_n$. The shortest path distance between two vertices v_i and v_j is denoted by d_{ij}, whereas the resistance distance between v_i and v_j is denoted by r_{ij}. It is well known that $r_{ij} \leq d_{ij}$ with equality iff v_i and v_j are connected by only one path. Palacios and Renom gave the following lower bound on the resistance distance:

$$r_{ij} \geq \begin{cases} \frac{deg_G(v_i)+deg_G(v_j)-2}{deg_G(v_i)deg_G(v_j)-1} & \text{if } v_iv_j \in E(G), \\ \frac{1}{deg_G(v_i)} + \frac{1}{deg_G(v_j)} & \text{if } v_iv_j \notin E(G), \end{cases} \tag{97}$$

3.2.1 Laplacian spectral radius

The well known bound $\mu_1 \leq 2\Delta$ easily implies the simplest upper bound on the sum of Laplacian spectral radii of a graph G and its complement $\overline{G}$:

$$\mu_1(G) + \mu_1(\overline{G}) \leq 2(n-1) + 2(\Delta - \delta).$$

Shi [128] derived the following upper bound of $\mu_1(G)$ for a connected irregular graph G in terms of the order and maximum degree.

Lemma 3.7. [128] *Let $G \in \mathcal{G}(n)$ be a connected irregular graph with maximum degree Δ. Then*

$$\mu_1(G) < 2\Delta - \frac{2}{2n^2 - n}.$$

If both G and $\overline{G}$ are connected and irregular then Lemma 3.7 implies a slightly better upper bound as follows:

$$\mu_1(G) + \mu_1(\overline{G}) \leq 2\left\lfloor n - 1 - \frac{2}{2n^2 - n} \right\rfloor + 2(\Delta - \delta).$$

Liu, Lu, and Tian [107] proved that

$$\mu_1(G) + \mu_1(\overline{G}) \leq n - 2 + \sqrt{(\Delta + \delta + 1 - n)^2 + n^2 + 4(\Delta - \delta)(n-1)}.$$

The following bounds are given by Shi [128] in 2007, which will be used later.

Lemma 3.8. [128] *Let $G \in \mathcal{G}(n,m)$ be a graph with no isolated vertex. Let $\Delta = \Delta(G)$ and $\delta = \delta(G)$. Then*

$$\mu_1(G) \leq [2\Delta^2 + 4m - 2\delta(n-1) + 2\Delta(\delta - 1)]^{1/2}.$$

Moreover, if G is connected then the equality holds if and only if G is a regular bipartite graph. In particular, if G is bipartite then

$$\mu_1(G) \geq [2\delta^2 + 4m - 2\Delta(n-1) + 2\delta(\Delta - 1)]^{1/2}.$$

Moreover, if G is connected then the equality holds if and only if G is regular.

By the above lemma, they obtained the following Nordhaus–Gaddum-type result for Laplacian spectral radius.

Theorem 3.13. [128] *Let $G \in \mathcal{G}(n)$ be a graph with $0 < \delta(G) \leq \Delta(G) < n-1$. Then*

$$\mu_1(G) + \mu_1(\overline{G}) \leq 2\sqrt{2(n-1)^2 - 3\delta(n-1) + (\Delta+\delta)^2 - \Delta + \delta}.$$

Moreover, if both G and $\overline{G}$ are connected then the upper bound is strict.

Proof. Let $f(m, \Delta, \delta) = [2\Delta^2 + 4m - 2\delta(n-1) + 2\Delta(\delta-1)]^{1/2}$. Note that $\Delta(\overline{G}) = n-1-\delta$, $\delta(\overline{G}) = n-1-\Delta$ and $m(\overline{G}) = \binom{n}{2} - m$. Lemma 3.8 gives that

$$\mu_1(G) \leq f(m, \Delta, \delta) \text{ and } \mu(\overline{G}) \leq f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right).$$

Now let $g(m) = f(m, \Delta, \delta) + f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)$. Then

$$\mu_1(G) + \mu_1(\overline{G}) \leq g(m).$$

Since

$$\frac{dg}{dm} = 2/f(m, \Delta, \delta) - 2/f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right),$$

it is easy to check that $\frac{dg}{dm} \geq 0$ if and only if $f(m, \Delta, \delta) \leq f\left(\binom{n}{2} - m, n-1-\delta, n-1-\Delta\right)$ i.e. $m \leq [2(n-1)^2 - \delta(n-2) - \Delta^2 + \delta^2 + \Delta]/4$. Thus

$$\begin{aligned}
\mu_1(G) + \mu_1(\overline{G}) &\leq g([2(n-1)^2 - \delta(n-2) - \Delta^2 + \delta^2 + \Delta]/4) \\
&= 2f([2(n-1)^2 - \delta(n-2) - \Delta^2 + \delta^2 + \Delta]/4, \Delta, \delta) \\
&= 2\sqrt{2(n-1)^2 - 3\delta(n-1) + (\Delta+\delta)^2 - \Delta + \delta}
\end{aligned}$$

If both G and $\overline{G}$ are connected, then either G or $\overline{G}$ fails to be a bipartite regular graph. Lemma 3.8 implies that the Laplacian spectral radius of either G or $\overline{G}$ fails to attain its upper bound and so does the sum. ■

3.2.2 Laplacian energy

Zhou and Gutman [156] got the following result for Laplacian eigenvalues.

Lemma 3.9. [156] *If G is not the complete graph, and has at least one edge, then $\mu_1 - \mu_{n-1} > 1$.*

Proof. Since G has at least one edge, it follows that $\mu_1 \geq \Delta + 1$, where Δ is the maximum vertex degree of G. If G is connected, then equality holds if and only if $\Delta = n-1$. Suppose that G is connected. Then $\mu_1 - \mu_{n-1} \geq \Delta - 2m/n + 1 \geq 1$. If $\mu_1 - \mu_{n-1} = 1$, then $2m/n = \Delta = n-1$ and then it would be $G \cong K_n$, a contradiction. If G is not connected, then $\mu_1 - \mu_{n-1} = \mu_1 \geq \Delta + 1 > 1$. ■

Let $d(G)$ be the *average degree* of G, i.e., $d(G) = \frac{1}{n}\sum_{u \in V(G)} deg_G(u) = \frac{2m}{n}$, where n and m are respectively the numbers of vertices and edges of G. The *discrepancy* of the graph G with n vertices is defined as

$$disc(G) = \frac{1}{n}\sum_{u \in V(G)} |deg_G(u) - d(G)|.$$

By the above lemma, they [156] derived the Nordhaus–Gaddum-type results for Laplacian energy.

Theorem 3.14. [156] *Let $G \in \mathcal{G}(n)$ be a graph. Then*

$$2n-2 \le LE(G) + LE(\overline{G}) < n\sqrt{n^2-1}.$$

The lower bound attains if and only if G is isomorphic to K_n or $\overline{K_n}$.

Proof. We only give the proof of the lower bound. If G is isomorphic to K_n or $\overline{K_n}$, then it is easy to show that $LE(G) + LE(\overline{G}) = 2n-2$. Suppose that $n \ge 3$ and that G is different from K_n and $\overline{K_n}$. Then

$$\begin{aligned} LE(G) + LE(\overline{G}) &= \mu_1 - \mu_{n-1} + \frac{2m}{n} + \sum_{i=2}^{n-2} \left| \mu_i - \frac{2m}{n} \right| \\ &\quad + \mu_1 - \mu_{n-1} + \frac{2\overline{m}}{n} + \sum_{i=2}^{n-2} \left| n - \mu_i - \frac{2\overline{m}}{n} \right| \\ &\ge 2(\mu_1 - \mu_{n-1}) + n - 1 + \sum_{i=2}^{n-2} 1 \\ &= 2(\mu_1 - \mu_{n-1}) + 2n - 4. \end{aligned}$$

By Lemma 3.9, we have $LE(G) + LE(\overline{G}) > 2n-2$. ■

Zhou [147] improved the upper bound in Theorem 3.14, and obtained the following result.

Proposition 3.2. [147] *Let $G \in \mathcal{G}(n)$ $(n \ge 3)$ be a graph. Then*

$$LE(G) + LE(\overline{G}) < n - 1 + (n-1)\sqrt{n+1} + 2a(2n - 1 - \sqrt{4na+1})$$

$$LE(G) + LE(\overline{G}) < n - 1 + (n-1)\sqrt{n+1} + \frac{4[(2n-1)(n+1)(n-2) + 2(n^2-n+1)^{3/2}]}{27n}.$$

Proof. Let m be the number of edges of G. Note that $\sum_{i=1}^{n} \lambda_i^2 = 2m$ and by the Cauchy-Schwarz inequality,

$$E(G) \le \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}$$

with equality if and only if $|\lambda_2| = \cdots = |\lambda_n|$, where λ_1 is the largest eigenvalue of G. Let $\overline{\lambda_1}$ be the largest eigenvalue of $\overline{G}$. Then

$$\begin{aligned} E(G) + E(\overline{G}) &\le \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)} + \overline{\lambda_1} + \sqrt{(n-1)[n(n-1) - 2m - \overline{\lambda_1}^2]} \\ &\le \lambda_1 + \overline{\lambda_1} + \sqrt{2(n-1)\left[n(n-1) - (\lambda_1^2 + \overline{\lambda_1}^2)\right]} \\ &\le \lambda_1 + \overline{\lambda_1} + \sqrt{2(n-1)\left[n(n-1) - \frac{1}{2}(\lambda_1 + \overline{\lambda_1})^2\right]}. \end{aligned}$$

Note that the function

$$f(x) = x + \sqrt{2(n-1)\left[n(n-1) - \frac{x^2}{2}\right]}$$

is monotonously decreasing for $x \geq \sqrt{2(n-1)}$ and that by Weyl's theorem [79], $\lambda_1 + \overline{\lambda_1}$ is no less than the largest eigenvalue $n-1$ of the matrix $A(G) + A(\overline{G}) = A(K_n)$, implying that $\lambda_1 + \overline{\lambda_1} \geq n-1 \geq \sqrt{2(n-1)}$. Thus,

$$E(G) + E(\overline{G}) \leq f(n-1) = n-1+(n-1)\sqrt{n+1},$$

and if equality is attained then G is regular, $\lambda_1 = \overline{\lambda_1} = \frac{n-1}{2}$, and thus

$$\sqrt{\frac{1}{n-1}(2m-\lambda_1^2)} = \frac{\sqrt{n+1}}{2}$$

is an eigenvalue of G with multiplicity $\frac{n-1}{2}(1-\frac{1}{\sqrt{n+1}})$, which can not be an integer for $n \geq 3$. Then the above bound for $E(G) + E(\overline{G})$ can not be attained. Now the result follows from the bound for $n \cdot disc(G)$. ■

Let $G = K_q \cup \overline{K_{n-q}}$. Then $d(G) = \frac{q(q-1)}{n}$. The Laplacian spectrum of G consists of q ($q-1$ times) and 0 ($n-q+1$ times). It follows that

$$LE(G) = \frac{nq - q(q-1)}{n}(q-1) + \frac{q(q-1)}{n}(n-q+1) = \frac{2q(q-1)(n-q+1)}{n}.$$

Let $q = \frac{2n}{3}$. Then

$$LE(G) = \frac{4(2n-3)(n+3)}{27}.$$

Note that $d(\overline{G}) = \frac{n(n-1)-q(q-1)}{n}$ and the Laplacian spectrum of $\overline{G}$ consists of n ($n-q$ times), $n-q$ ($q-1$ times) and 0 (1 times). Therefore, we have

$$\begin{aligned} LE(\overline{G}) &= \frac{n+q(q-1)}{n}(n-q) + \frac{nq-n-q(q-1)}{n}(q-1) + \frac{n^2-n-q(q-1)}{n} \\ &= \frac{2(n-q)[n+q(q-1)]}{n} \\ &= \frac{2n(4n+3)}{27}. \end{aligned}$$

This example and the previous two propositions imply.

In [147], Zhou proved that:

Proposition 3.3. [147] *Let G be a graph. Then*

$$LE(G) \leq E(G) + \sum_{u \in V(G)} |deg_G(u) - d(G)|.$$

Proposition 3.4. [147] *Let $\mathcal{G}_n$ be the class of graphs with n vertices. Let*

$$LE(n) = \max\{LE(G) : G \in \mathcal{G}_n\}$$

$$NGLE(n) = \max\{LE(G) + LE(\overline{G}) : G \in \mathcal{G}_n\}$$

Then

$$\lim_{n\to\infty} \frac{LE(n)}{n^2} = \frac{8}{27}$$

$$\lim_{n\to\infty} \frac{NGLE(n)}{n^2} = \frac{16}{27}.$$

Recall that the first Zagreb index of the graph G is $M_1(G) = \sum_{u\in V(G)} deg_G(u)^2$. Let G be a graph with n vertices and m edges. By the Cauchy-Schwarz inequality,

$$\sum_{u\in V(G)} |deg_G(u) - d(G)| \leq \sqrt{n \sum_{u\in V(G)} [|deg_G(u) - d(G)|]^2} = \sqrt{nM_1(G) - 4m^2}$$

with equality if and only if $|deg_G(u) - d(G)|$ is a constant for each $u \in V(G)$. We note that $\frac{1}{n}\sum_{u\in V(G)}[|deg_G(u) - d(G)|]^2$ was called the *variance* of G. From Proposition 3.3, we have

$$LE(G) \leq E(G) + \sqrt{nM_1(G) - 4m^2}.$$

Remark 3.5. [147] *We may give somewhat finer upper bounds for the Laplacian energy by applying Proposition 3.3. We give an example. Let G be a graph with $n \geq 2$ vertices, m edges and the first Zagreb index M_1. Then [150]*

$$E(G) \leq \sqrt{\frac{M_1}{n}} + \sqrt{(n-1)\left(2m - \frac{M_1}{n}\right)}$$

with equality if and only if G is K_n, $\overline{K_n}$, mK_2 (m copies of vertex-disjoint K_2), or a non-complete connected strongly regular graph with two non-trivral eigenvalus both with absolute value $\sqrt{\frac{2m-(2m/n)^2}{n-1}}$. Thus,

$$LE(G) \leq \sqrt{\frac{M_1}{n}} + \sqrt{(n-1)\left(2m - \frac{M_1}{n}\right)} + \sqrt{nM_1(G) - 4m^2}$$

with equality if and only if G is K_n, $\overline{K_n}$, mK_2, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-(2m/n)^2}{n-1}}$; and

$$LE(G) \leq \sqrt{\frac{M_1}{n}} + \sqrt{(n-1)\left(2m - \frac{M_1}{n}\right)} + a\left(2n - 1 - \sqrt{4na+1}\right).$$

with equality if and only if $G = K_n$ or $G = \overline{K_n}$.

Remark 3.6. [147] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 3,\ m > 0)$ be a graph. If G is K_{r+1}-free with $2 \leq r \leq n-1$, then [151]*

$$M_1(G) \leq \frac{2r-2}{r} nm$$

with equality for $r = 2$ if and only if G is a complete bipartite graph, and thus

$$LE(G) \leq E(G) + \sqrt{\frac{2r-2}{r} n^2 m - 4m^2}.$$

In particular, if G is bipartite $(r = 2)$, then [97]

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

and thus

$$\begin{aligned} LE(G) &\leq E(G) + \sqrt{n^2 m - 4m^2} \\ &< \frac{n(\sqrt{n} + \sqrt{2})}{\sqrt{8}} + \frac{n^2}{4}. \end{aligned}$$

The second inequality is strict because the bounds for $E(G)$ can not be attained for the complete bipartite graph, which is equal to $2\sqrt{s(n-s)} \le n$ for some $1 \le s \le \lfloor \frac{n}{2} \rfloor$. Note that for rational number α with $0 < \alpha \le \frac{1}{2}$, $LE(K_{an,(1-\alpha)n}) = 2\alpha n + 2\alpha(1-\alpha)(1-2\alpha)n^2$. Let $LE_{bip}(n)$ be the maximum Laplacian energy of n-vertex bipartite graphs. Then $2\alpha(1-\alpha)(1-2\alpha) < \lim_{n\to\infty} \frac{LE_{bip}(n)}{n^2} \le 0.25$. For real x with $0 < x \le \frac{1}{2}$, $x(1-x)(1-2x)$ is maximum if and only if $x = \frac{3-\sqrt{3}}{6}$. Let $\alpha = 0.211 < \frac{3-\sqrt{3}}{6}$. Then $0.19 < \lim_{n\to\infty} \frac{LE_{bip}(n)}{n^2} \le 0.25$. If G is a tree, then $Zg(G) \le n(n-1)$, and thus

$$LE(G) \le E(G) + \sqrt{n-1}(n-2).$$

3.2.3 Laplacian–energy–like invariant

Grone and Merris [58] got the following result.

Lemma 3.10. [58] *Let G be a graph with at least one edge and maximum vertex degree Δ. Then*

$$\mu_1 \ge 1 + \Delta$$

with equality for connected graphs if and only if $\Delta = n-1$.

Gutman, Zhou, and Furtula [72] obtained the following Nordhaus–Gaddum-type result for Laplacian-energy-like invariant.

Theorem 3.15. [72] *Let $G \in \mathcal{G}(n)$ $(n \ge 2)$ be a graph. Then*

$$\sqrt{n}(n-1) \le LEL(G) + LEL(\overline{G}) < \sqrt{2(n+1)} + \sqrt{2(n-2)(n^2-2n-1)}$$

with left equality if and only if $G \cong K_n$ and $G \cong \overline{K}_n$.

Proof. Let m and $\overline{m}$ be respectively the number of edges of G and $\overline{G}$. Let $\overline{\mu}_1, \overline{\mu}_2, \ldots, \overline{\mu}_n$ be the Laplacian eigenvalues of $\overline{G}$ arranged in an non-increasing order. Then $\overline{\mu}_i = n - \mu_{n-i}$ for $i = 1, 2, \ldots, n-1$. It follows that

$$LEL(G) + LEL(\overline{G}) = \sum_{i=1}^{n-1}(\sqrt{\mu_i} + \sqrt{n-\mu_i}) \ge \sum_{i=1}^{n-1} \sqrt{n} = (n-1)\sqrt{n}$$

with equality if and only if either $\mu_1 = \cdots = \mu_{n-1} = n$ and then $G \cong K_n$, or (by Lemma 3.10) $\mu_1 = \cdots = \mu_{n-1} = 0$ and then $G \cong \overline{K}_n$.

On the other hand, by the Cauchy-Schwarz inequality,

$$\begin{aligned} LEL(G) + LEL(\overline{G}) &\le \sqrt{\mu_1} + \sqrt{\overline{\mu}_1} + \sqrt{(n-2)(2m-\mu_1)} + \sqrt{(n-2)(2\overline{m}-\overline{\mu}_1)} \\ &\le \sqrt{2(\mu_1+\overline{\mu}_1)} + \sqrt{2(n-2)[n(n-1)-(\mu_1+\overline{\mu}_1)]}. \end{aligned}$$

Consider the function $g(x) = \sqrt{2x} + \sqrt{2(n-2)[n(n-1)-x]}$. It is decreasing for $x \ge n$.

If one of G or $\overline{G}$ is empty, then $\mu_1 + \overline{\mu}_1 = n$. Otherwise, since one of G and $\overline{G}$ is connected, we have by Lemma 3.10 that $\mu_1 + \overline{\mu}_1 \ge 1 + \Delta + 1 + (n-1-\delta) = n + 1 + \Delta - \delta > n+1$, where Δ and δ are respectively the maximum and minimum vertex degree of G. Thus,

$$LEL(G) + LEL(\overline{G}) < g(n+1) = \sqrt{2(n+1)} + \sqrt{2(n-2)(n^2-2n-1)},$$

as desired. ■

Note that

$$LEL(K_{n/2,n/2}) = \sqrt{n} + \frac{\sqrt{2}}{2}(n-1)\sqrt{n} \text{ and } LEL(\overline{K_{n/2,n/2}}) = \frac{\sqrt{2}}{2}(n-2)\sqrt{n}.$$

Then

$$LEL(K_{n/2,n/2}) + LEL(\overline{K_{n/2,n/2}}) = \sqrt{n} + \sqrt{2}\left(n - \frac{3}{2}\right)\sqrt{n}.$$

This example shows that the upper bound in the previous proposition is asymptotically best possible. More precisely: Let max$LEL_{NG(n)}$ be the maximum value of $LEL(G) + LEL(\overline{G})$ over all graphs with n vertices. Then

$$\lim_{n\to\infty} \frac{\max LEL_{NG(n)}}{n^{3/2}} = \sqrt{2}.$$

3.2.4 Laplacian Estrada Index

Chen and Hou [16] first obtained a lower bound of $LEE(G)$ for a connected graph G.

Lemma 3.11. [16] *Let $G \in \mathcal{G}(n)$ $(n > 3)$ be a connected graph with a connected complement G. Let $\Delta(G) = \Delta$ and $\delta(G) = \delta$. Then*

$$LEE(G) \geq 1 + e^{\Delta+1} + e^{\delta} + (n-3)e^{\frac{2m-\Delta-\delta-1}{n-3}},$$

with equality holding if and only if $G \cong 2K_1 \vee K_{n-2}$, or $G \cong K_{1,n-1}$, or $G \cong (K_1 \cup K_{n-2}) \vee K_1$.

Next, they derived the following Nordhaus–Gaddum-type result.

Proposition 3.5. [16] *Let $G \in \mathcal{G}(n)$ $(n > 3)$ be a connected graph with a connected complement $\overline{G}$. Let $\Delta(G) = \Delta$ and $\delta(G) = \delta$. Then*

$$LEE(G) + LEE(\overline{G}) > e^{\Delta+1} + e^{n-1-\Delta} + e^{\delta} + e^{n-\delta} + 2(n-3)e^{\frac{n}{2}} + 2.$$

Proof. For convenience, we let

$$f(m,\Delta,\delta) = 1 + e^{\Delta+1} + e^{\delta} + (n-3)e^{\frac{2m-\Delta-\delta-1}{n-3}}.$$

Observing that $|E(\overline{G})| = \frac{n(n-1)}{2} - m$, $\Delta(\overline{G}) = n-1-\delta$, and $\delta(\overline{G}) = n-1-\Delta$. From Lemma 3.11, we have

$$\begin{aligned} LEE(G) + LEE(\overline{G}) &> f(m,\Delta,\delta) + f\left(\frac{n(n-1)}{2} - m, n-1-\delta, n-1-\Delta\right) \\ &= 2 + e^{\Delta+1} + e^{\delta} + e^{n-\delta} + e^{n-1-\Delta} \\ &\quad +(n-3)\left(e^{\frac{2m-\Delta-\delta-1}{n-3}} + e^{\frac{(n-1)(n-2)-2m+\Delta+\delta-1}{n-3}}\right) \\ &\geq e^{\Delta+1} + e^{n-1-\Delta} + e^{\delta} + e^{n-\delta} + 2(n-3)e^{\frac{n}{2}} + 2, \end{aligned}$$

where the first inequality holds strictly since $\overline{G}$ is required to be connected, while the second inequality follows from the fact that $e^a + e^b \geq 2e^{\frac{a+b}{2}}$ holds for $a, b \geq 0$, which is a direct consequence of the arithmetic-geometric inequality. The proof is completed. ■

Remark 3.7. [16] *Zhou [152] showed that,*

$$LEE(G) + LEE(\overline{G}) > (n-1)e^{\frac{n}{2}} + 2. \tag{98}$$

Observing that $e^x + e^{n-x} \geq 2e^{\frac{n}{2}}$ holds for $0 \leq x \leq n$, one can see easily that the bound in Proposition 3.5 is always better than the bound (98).

3.2.5 Laplacian Estrada–like invariant

Güngoör [59] got the upper and lower bounds for Laplacian Estrada-like invariant.

Lemma 3.12. [59] *Let $G \in \mathcal{G}(n,m)$ be a graph. Then*

$$\sqrt{n[(n-1)e^{2LEL(G)/n} + 1] + 2LEL(G) + 4m} \leq LEEL(G) \leq n - 1 + e^{\sqrt{2m}}.$$

By these bounds, they derived the following Nordhaus–Gaddum-type results.

Theorem 3.16. [59] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ be a connected graph with a connected component $\overline{G}$. Then*

$$n\sqrt{2e^{\sqrt{n}}} \leq LEEL(G) + LEEL(\overline{G}) \leq 2(n-1) + e^{\sqrt{2m}} + e^{\sqrt{n(n-1)-2m}}.$$

Proof. Let $\overline{\mu_1}, \overline{\mu_2}, \cdots, \overline{\mu_n}$ be the Laplacian eigenvalues of $\overline{G}$ arranged in a nonincreasing order. Then, for $i = 1, 2, \cdots, n-1$, $\overline{\mu_i} = n - \mu_{n-i}$. By considering (95), a direct calculation gives that

$$LEEL(G) + LEEL(\overline{G}) = \sum_{i=1}^{n} (e^{\sqrt{\mu_i}} + e^{\sqrt{n-\mu_i}}) \geq \sum_{i=1}^{n} \sqrt{2e^{\sqrt{n}}} = n\sqrt{2e^{\sqrt{n}}}.$$

By Lemma 3.12, we did obtain an upper bound $n - 1 + e^{\sqrt{2m}}$ for $LEEL(G)$. Now recalling that $\overline{m} = (n(n-1) - 2m)/2$, again a direct calculation shows that

$$LEEL(G) + LEEL(\overline{G}) \leq 2(n-1) + e^{\sqrt{2m}} + e^{\sqrt{n(n-1)-2m}}.$$

Hence the result is attained. ■

3.2.6 Kirchhoff index

A *strongly regular graph* with parameters (n,k,a,c), denoted by $srg(n,k,a,c)$, is a k-regular graph on n vertices such that for every pair of adjacent vertices there are a vertices adjacent to both, and for every pair of non-adjacent vertices there are c vertices adjacent to both. We exclude $k = 0$ and $k = n-1$ from being strongly regular. In this section, we let $\mu_{n-1} \geq \mu_{n-2} \geq \cdots \geq \mu_1 \geq \mu_0 = 0$ be the eigenvalues of G.

It is well known [56] that a $\mathrm{srg}(n,k,a,c)$ has eigenvalues

$$k, \text{ and } \theta_{\pm} = \frac{a - c \pm \sqrt{\Delta}}{2}$$

with corresponding multiplicities

$$1, \text{ and } m_{\mp} = \frac{1}{2}\left(n-1 \mp \frac{(n-1)(c-a)-2k}{\sqrt{\Delta}}\right),$$

where $\Delta = (a-c)^2 + 4(k-c) > 0$.

A *conference graph* is a strongly regular graph with multiplicities $m_+ = m_-$.

In [162], Zhou and Trinajstić obtained a Nordhaus–Gaddum-type result for the Kirchhoff index.

Theorem 3.17. [162] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected (molecular) graph with a connected complement $\overline{G}$. Then*

$$4n - 2 \leq Kf(G) + Kf(\overline{G}) < \frac{n^3 + 3n^2 + 2n - 6}{6}. \tag{99}$$

Later, Yang, Zhang, and Klein [142] improved their results by showing that

Theorem 3.18. [142] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected (molecular) graph with a connected complement $\overline{G}$. Then*

$$4n \leq Kf(G) + Kf(\overline{G}) < \frac{n^3 + 17n - 18}{6}, \tag{100}$$

and equality holds (at the lower bound) if and only if G is a conference graph.

Zhou [148] proved the following result.

Lemma 3.13. [148] *Let $G \in \mathcal{G}(n)$ be a connected graph. Then $\lambda_1 = \lambda_2 = \ldots = \lambda_{n-1}$ if and only if $G \cong K_n$.*

Lemma 3.14. [56] *A connected regular graph with exactly three distinct eigenvalues is strongly regular.*

Lemma 3.15. [142] *Let G ba a connected* $\mathrm{srg}(n, \frac{n-1}{2}, a, c)$. *Then*

$$a + c = \frac{n-3}{2}.$$

We are now in a position to give the proof of Theorem 3.18.

Proof of Theorem 3.18: We first prove the lower bound. Let $d_1 \leq d_2 \leq \cdots \leq d_n$ and $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the vertex degrees and the Laplacian eigenvalues of G, respectively. Then it is well known that [19]

$$S(\overline{G}) = (0, n - \lambda_{n-1}, n - \lambda_{n-2}, \cdots, n - \lambda_1).$$

From (96), we have

$$\begin{aligned} Kf(G) + Kf(\overline{G}) &= n\sum_{i=1}^{n-1}\frac{1}{\lambda_i} + n\sum_{i=1}^{n-1}\frac{1}{n-\lambda_i} \\ &= n\sum_{i=1}^{n-1}\left(\frac{1}{\lambda_i} + \frac{1}{n-\lambda_i}\right) \\ &= n^2\sum_{i=1}^{n-1}\frac{1}{\lambda_i(n-\lambda_i)}, \end{aligned}$$

and by the Cauchy-Schwarz inequality, we have

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i(n-\lambda_i)} \geq \frac{(n-1)^2}{\sum_{i=1}^{n-1} \lambda_i(n-\lambda_i)}. \tag{101}$$

Since

$$\operatorname{tr}(L(G)) = \sum_{i=1}^{n} d_i = \sum_{i=0}^{n-1} \lambda_i$$

and

$$\operatorname{tr}(L(G)^2) = \sum_{i=1}^{n} (d_i^2 + d_i) = \sum_{i=0}^{n-1} \lambda_i^2,$$

it follows that

$$\begin{aligned} \sum_{i=1}^{n-1} \lambda_i(n-\lambda_i) &= n\sum_{i=1}^{n-1} \lambda_i - \sum_{i=1}^{n-1} \lambda_i^2 = n\sum_{i=1}^{n} d_i - \sum_{i=1}^{n} (d_i^2 + d_i) \\ &= \sum_{i=1}^{n} d_i(n-1-d_i) \leq \sum_{i=1}^{n} \left(\frac{n-1}{2}\right)^2 \\ &= \frac{n(n-1)^2}{4}, \end{aligned} \tag{102}$$

and thus

$$Kf(G) + Kf(\overline{G}) = n^2 \sum_{i=1}^{n-1} \frac{1}{\lambda_i(n-\lambda_i)} \geq n^2 \frac{(n-1)^2}{\frac{n(n-1)^2}{4}} = 4n. \tag{103}$$

To show the sharpness of the lower bound, we can see that equality holds in (103) if and only if equalities in both (101) and (102) hold. Equality can only hold in (101) if for all $1 \leq i \neq j \leq n-1$,

$$\lambda_i(n-\lambda_i) = \lambda_j(n-\lambda_j),$$

or equivalently

$$(\lambda_i - \lambda_j)(n - \lambda_i - \lambda_j) = 0,$$

which indicates that either $\lambda_i = \lambda_j$ or $\lambda_i + \lambda_j = n$; and equality can only hold in (102) if G is $(n-1)/2$-regular. From our hypothesis G is not complete, so by Lemma 3.13 we know $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$ is impossible, and equality can only hold in (101) if G has exactly two distinct non-zero Laplacian eigenvalues λ_1 and $n - \lambda_1$; in other words, G has exactly three distinct Laplacian eigenvalues $0, \lambda_1$ and $n - \lambda_1$. Since G is $(n-1)/2$-regular, it follows that G also has exactly three distinct adjacency-matrix eigenvalues

$$\frac{n-1}{2}, \frac{n-1}{2} - \lambda_1 \text{ and } \lambda_1 - \frac{n+1}{2}. \tag{104}$$

By Lemma 3.14, G is strongly regular and thus we may suppose that G is a $\operatorname{srg}(n, \frac{n-1}{2}, a, c)$. Then by the spectral property of a strongly regular graph we get that the three distinct eigenvalues of G are

$$\frac{n-1}{2}, \text{ and } \theta_{\pm} = \frac{a - c \pm \sqrt{\Delta}}{2}, \tag{105}$$

where $\Delta = (a-c)^2 + 4((n-1)/2 - c)$. Comparing (104) with (105), we know

$$\theta_+ + \theta_- = \frac{a-c+\sqrt{\Delta}}{2} + \frac{a-c-\sqrt{\Delta}}{2} = a - c = \frac{n-1}{2} - \lambda_1 + \lambda_1 - \frac{n+1}{2} = -1,$$

that is

$$c - a = 1. \tag{106}$$

On the other hand, by Lemma 3.15,

$$a + c = \frac{n-3}{2}. \tag{107}$$

Combining (106) and (107), one finds $a = \frac{n-5}{4}$ and $c = \frac{n-1}{4}$. Hence G is a $\mathrm{srg}(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4})$ and it follows that G is a conference graph. Hence

$$Kf(G) + Kf(\overline{G}) \geq 4n$$

with equality if and only if G is a conference graph.

To prove the upper bound, we use the famous Foster's formula [53], which states that the sum of resistance distance between all pairs of adjacent vertices in a connected n-vertex graph is $n-1$, whence $\sum_{i<j,\ d_{ij}(G)=1} r_{ij}(G) + \sum_{i<j,\ d_{ij}(\overline{G})=1} r_{ij}(\overline{G}) = 2(n-1)$. Clearly, $\sum_{i<j,\ d_{ij}(G)=1} d_{ij}(G) + \sum_{i<j,\ d_{ij}(\overline{G})=1} d_{ij}(\overline{G}) = \frac{n(n-1)}{2}$ and recall that [144] $W(G) + W(\overline{G}) \leq \frac{n^3+3n^2+2n-6}{6}$ with equality if and only if $G = P_n$ or $G = \overline{P_n}$. Then it follows that

$$Kf(G) + Kf(\overline{G}) \leq W(G) + W(\overline{G}) - \left(\frac{n(n-1)}{2} - 2(n-1)\right) \leq \frac{n^3 + 17n - 18}{6}. \tag{108}$$

For equality in (108) to hold requires not only $G = P_n$ or $G = \overline{P_n}$, but also the resistance distance between every pair of nonadjacent vertices in both G and $\overline{G}$ be equal to the distance between them. But this is impossible since the resistance distance between every pair of nonadjacent vertices in $\overline{P_n}$ is less than the shortest-path distance between them because they are connected by more than one path. So

$$Kf(G) + Kf(\bar{G}) < \frac{n^3 + 17n - 18}{6},$$

and the proof is completed. ∎

Though the upper bound is not sharp, they showed that it is nearly the best possible with an example. Take the n-vertex path P_n for an example. It is well known that

$$Kf(P_n) = W(P_n) = \frac{n^3 - n}{6},$$

so it suffices to compute $Kf(\overline{P_n})$. Since [5]

$$S(P_n) = \left(0, 4\sin^2\frac{\pi}{2n}, 4\sin^2\frac{2\pi}{2n}, \cdots, 4\sin^2\frac{(n-1)\pi}{2n}\right),$$

it follows that

$$S(\overline{P_n}) = \left(0, n - 4\sin^2\frac{\pi}{2n}, n - 4\sin^2\frac{2\pi}{2n}, \cdots, n - 4\sin^2\frac{(n-1)\pi}{2n}\right).$$

Then by (96), we have

$$Kf(\overline{P_n}) = n\sum_{k=1}^{n-1}\frac{1}{n - 4\sin^2\frac{k\pi}{2n}}$$

Thus

$$Kf(P_n) + Kf(\overline{P_n}) = \frac{n^3-n}{6} + n\sum_{k=1}^{n-1}\frac{1}{n - 4\sin^2\frac{k\pi}{2n}} > \frac{n^3-n}{6} + n - 1 = \frac{n^3+5n-6}{6}.$$

Comparing $Kf(P_n) + Kf(\overline{P_n})$ with the upper bound in Theorem 3.18, we can conclude that the upper bound is nearly the best possible.

The above example illustrates that the upper bound is the best possible. Yang, Zhang, and Klein proposed the following conjecture.

Conjecture 3.3. [142] *Let $G \in \mathcal{G}(n)$ be a connected graph with a connected $\overline{G}$. Then*

$$Kf(G) + Kf(\overline{G}) \leq \frac{n^3-n}{6} + n\sum_{k=1}^{n-1}\frac{1}{n - 4\sin^2\frac{k\pi}{2n}}$$

with equality holding if and only if $G = P_n$ or $G = \overline{P_n}$.

The *diameter* of a graph G, denote by $d(G)$, is the maximum shortest-path distance between any two vertices in G. In their paper, Yang, Zhang, and Klein [142] gave bounds for the product of $Kf(G)$ and $Kf(\bar{G})$ in terms of the vertex number n and the maximum diameter of G and $\overline{G}$.

Theorem 3.19. [142] *Suppose that $d = \max\{d(G), d(\overline{G})\}$. Then*

$$4(n-1)^2 < Kf(G) \times Kf(\overline{G}) < \begin{cases} \frac{1}{16}(9n^4 + 6n^3 - 23n^2 - 8n + 16), & \text{if } d = 3 \\ \frac{d}{8}n^4 + \frac{1}{2}n^3 - \frac{d^2+2d-2}{4d}n^2 - \frac{d+2}{2d}n + \frac{d^2+4d+4}{8d}, & \text{otherwise.} \end{cases}$$

Proof. We only prove the upper bound, since the lower bound has been improved. Without loss of generality, suppose that $d = d(G)$. If $d = 3$, then $d(\overline{G}) \leq 3$ and

$$\begin{aligned} Kf(G) \times Kf(\overline{G}) &= \left[\sum_{i<j} r_{ij}(G)\right]\left[\sum_{i<j} r_{ij}(\overline{G})\right] \\ &= \left[\sum_{i<j,\ d_{ij}(G)=1} r_{ij}(G) + \sum_{i<j,\ 2\leq d_{ij}(G)\leq 3} r_{ij}(G)\right] \\ &\quad \times \left[\sum_{i<j,\ d_{ij}(\overline{G})=1} r_{ij}(\overline{G}) + \sum_{i<j,\ 2\leq d_{ij}(\overline{G})\leq 3} r_{ij}(\overline{G})\right]. \end{aligned}$$

But then nothing that by Foster's theorem $\sum_{ij\in E} r_{ij} = n-1$,and further for $2 \le d_{ij} \le 3$ that the corresponding $r_{ij} \le d_{ij} \le 3$, we have

$$\begin{aligned} Kf(G)\times Kf(\overline{G}) &< \left[n-1+3\left(\frac{n(n-1)}{2}-m\right)\right][n-1+3m] \\ &= (n-1)^2+3(n-1)\frac{n(n-1)}{2}+9\left(\frac{n(n-1)}{2}-m\right)m \\ &\le (n-1)^2+3(n-1)\frac{n(n-1)}{2}+9\left(\frac{n(n-1)}{4}\right)^2 \\ &= \frac{1}{16}(9n^4+6n^3-23n^2-8n+16). \end{aligned}$$

Else, $d=2$ or $d>3$. If $d(G)>3$, then $d(\overline{G})<3$, and hence it holds for both $d=2$ and $d>3$ that $d(\bar{G}=2)$. Thus if $d=2$ or $d>3$, then

$$\begin{aligned} Kf(G)\times Kf(\overline{G}) &= \left[\sum_{i<j} r_{ij}(G)\right]\left[\sum_{i<j} r_{ij}(\overline{G})\right] \\ &= \left[\sum_{\substack{i<j\\ d_{ij}(G)=1}} r_{ij}(G)+\sum_{\substack{i<j\\ 2\le d_{ij}(G)\le d}} r_{ij}(G)\right] \\ &\quad\times\left[\sum_{\substack{i<j\\ d_{ij}(\overline{G})=1}} r_{ij}(\overline{G})+\sum_{\substack{i<j\\ d_{ij}(\overline{G})=2}} r_{ij}(\overline{G})\right] \\ &< \left[n-1+d\left(\frac{n(n-1)}{2}-m\right)\right][n-1+2m] \\ &= -2dm^2+(n-1)(dn-d+2)m+\frac{n(n-1)^2d}{2}+(n-1)^2 \\ &= -2d\left[m-\frac{(n-1)(dn-d+2)}{4d}\right]^2+\frac{d}{8}n^4+\frac{1}{2}n^3 \\ &\quad -\frac{d^2+2d-2}{4d}n^2-\frac{d+2}{2d}n+\frac{d^2+4d+4}{8d} \\ &\le \frac{d}{8}n^4+\frac{1}{2}n^3-\frac{d^2+2d-2}{4d}n^2-\frac{d+2}{2d}n+\frac{d^2+4d+4}{8d}. \end{aligned}$$

■

If we choose G to be a conference graph on n vertices, then as indicated in the proof of Theorem 3.18,

$$Kf(G)=Kf(\bar{G})=2n$$

Thus

$$Kf(G) \times Kf(\bar{G}) = 2n \times 2n = 4n^2,$$

which enables us to conclude that the lower bound obtained in Theorem 3.19 is nearly the best possible. However, as far as the upper bound is concerned, it can be seen from the proof process that it is somewhat rough, so we have every reason to believe that it will be improved in the future.

Das, Yang and Xu [36] gave a new lower bound for $Kf(G) \times Kf(\overline{G})$ in terms of n. For this we need the following result:

Lemma 3.16. [53] *Let $G \in \mathcal{G}(n)$ be a connected graph. Then the sum of resistance distances between all pairs of adjacent vertices is equal to $n-1$, i.e.,*

$$\sum_{v_i v_j \in E(G)} r_{ij} = n - 1. \tag{109}$$

By the above lemma, they derived the new lower bound of $Kf(G) \times Kf(\overline{G})$.

Theorem 3.20. [36] *Let $G \in \mathcal{G}(n)$ be a connected graph with connected complement $\overline{G}$. Then*

$$Kf(G) \times Kf(\overline{G}) \geq (2n-1)^2.$$

Proof. By the arithmetic-harmonic mean inequality, we have

$$\begin{aligned}
&\sum_{i=1}^{n} \frac{d_i}{n-d_i-1} \sum_{i=1}^{n} \frac{n-d_i-1}{d_i} \\
&= \left[-n + (n-1)\sum_{i=1}^{n} \frac{1}{n-d_i-1}\right]\left[-n + (n-1)\sum_{i=1}^{n} \frac{1}{d_i}\right] \\
&\geq \left[-n + (n-1)\frac{n^2}{n(n-1)-2m}\right]\left[-n + (n-1)\frac{n^2}{2m}\right] \\
&= \frac{2mn}{n(n-1)-2m} \frac{n^2(n-1)-2mn}{2m} = n^2.
\end{aligned} \tag{110}$$

One can easily see that

$$\frac{d_i}{n-d_i-1} + \frac{n-d_i-1}{d_i} \geq 2. \tag{111}$$

Using (109), we get

$$
\begin{aligned}
Kf(G)\times Kf(\overline{G}) &= \sum_{i<j} r_{ij} \sum_{i<j} \overline{r_{ij}} \\
&= \left(n-1+\sum_{d_{ij}\geq 2} r_{ij}\right)\left(n-1+\sum_{\overline{d_{ij}}\geq 2} \overline{r_{ij}}\right) \\
&= (n-1)^2+(n-1)\left(\sum_{d_{ij}\geq 2} r_{ij}+\sum_{\overline{d_{ij}}\geq 2} \overline{r_{ij}}\right)+\sum_{d_{ij}\geq 2} r_{ij}\sum_{\overline{d_{ij}}\geq 2} \overline{r_{ij}} \\
&\geq (n-1)^2+(n-1)\left[\sum_{d_{ij}\geq 2}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)+\sum_{\overline{d_{ij}}\geq 2}\left(\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}\right)\right] \\
&\quad +\sum_{d_{ij}\geq 2}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)\sum_{\overline{d_{ij}}\geq 2}\left(\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}\right) \text{ by (97)} \\
&= (n-1)^2+(n-1)\sum_{i=1}^{n}\left(\frac{d_i}{n-d_i-1}+\frac{n-d_i-1}{d_i}\right)+\sum_{i=1}^{n}\frac{d_i}{n-d_i-1}\sum_{i=1}^{n}\frac{n-d_i-1}{d_i} \\
&\geq (n-1)^2+2n(n-1)+n^2=(2n-1)^2,
\end{aligned}
$$

by (110) and (111). This completes the proof. ■

Remark 3.8. [36] *Since* $(2n-1)^2 > 4(n-1)^2$, *the result is better than the previous result in Theorem 3.19.*

3.3 Eigenvalues of the signless Laplacian matrix

Recall that the signless Laplacian matrix is defined by $Q = Diag + A$ where $Diag$ is the diagonal matrix with degrees of the vertices on the main diagonal. We denote its eigenvalues by $q_1 \geq q_2 \geq \cdots \geq q_n$. It is well known that $q_1 \leq 2\Delta$, which easily implies that

$$q_1(G) + q_1(\overline{G}) \leq 2(n-1) + 2(\Delta - \delta)$$

with equality if and only if the graph is regular.

The concept of graph energy was extended to any matrix by Nikiforov [117] in the following manner. The singular values of a real (not necessarily square) matrix M are the square roots of the eigenvalues of the (square) matrix MM^t, where M^t denotes the transpose of M. The *energy* $E(M)$ of the matrix M is then defined [117] as the sum of its singular values. Obviously, $E(G) = E(A(G))$.

Let $I(G)$ be the (vertex-edge) incidence matrix of the graph G. For a graph G with vertex set $\{v_1, v_2, \ldots, v_n\}$ and edge set $\{e_1, e_2, \ldots, e_m\}$, the (i, j)-entry of $I(G)$ is 1 if v_i is incident with e_j and 0 otherwise. (In what follows, the unit matrix of order p will be denoted by I_p, and it should not be confused with the incidence matrix.)

Motivated by Nikiforov's idea, Jooyandeh, Kiani, and Mirzakhah [89] introduced the concept of *incidence energy* $IE(G)$ of a graph G, defining it as the sum of the singular values of the incidence matrix $I(G)$. Some basic properties of this quantity were established in [66, 89].

If the singular values of $I(G)$ are $\sigma_1, \sigma_2, \ldots, \sigma_n$, then, by definition [89],

$$IE(G) = \sum_{i=1}^{n} \sigma_i.$$

A well known fact is the identity [114, 115]:

$$I(G)I(G)^t = D(G) + A(G), i.e., I(G)I(G)^t = Q(G).$$

Its immediate consequence is that $\sigma_i = \sqrt{q_i}$ and therefore,

$$IE(G) = \sum_{i=1}^{n} \sqrt{q_i}.$$

3.3.1 Signless Laplacian spectral radius

The well known inequality $2\lambda_1 \leq q_1$ and Theorem 3.1 directly leads to the following result of Gutman, Kiani, Mirzakhah, and Zhou obtained in 2009.

Theorem 3.21. [67] *Let $G \in \mathcal{G}(n)$ be a simple graph. Then*

$$q_1(G) + q_1(\overline{G}) \geq 2n - 2$$

with equality if and only if the graph is regular.

Concerning the upper bounds, Aouchiche and Hansen [7] obtained the following conjecture using the AutoGraphix system.

Conjecture 3.4. [7] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a simple graph. Then*

$$q_1(G) + q_1(\overline{G}) \leq 3n - 4,$$

$$q_1(G) \cdot q_1(\overline{G}) \leq 2n(n - 2).$$

The equalities hold if and only if the graph is the star.

3.3.2 Incidence energy

Gutman, Kiani, Mirzakhah, and Zhou [67] obtained a lower bound for the incidence energy.

Lemma 3.17. [67] *Let $G \in \mathcal{G}(n, m)$ be a graph. Then*

$$IE(G) \geq \frac{2m}{\sqrt{n}}$$

with equality if and only if $G \cong \overline{K_n}$ or $G \cong K_2$.

By the above result, they [67] derived Nordhaus–Gaddum-type results for the incidence energy.

Theorem 3.22. [67] *Let $G \in \mathcal{G}(n)$ $(n \geq 2)$ be a graph. Then*

$$\sqrt{n}(n-1) \leq IE(G) + IE(\overline{G}) < 2\sqrt{n-1} + (n-1)\sqrt{2n-4},$$

with left equality if and only if $n = 2$.

Proof. Let m and $\overline{m}$ be, respectively, the number of edges of G and $\overline{G}$. By Lemma 3.17, we have

$$IE(G) + IE(\overline{G}) \geq \frac{2m + 2\overline{m}}{\sqrt{n}} = \sqrt{n}(n-1), \tag{112}$$

with equality if and only if $m, \overline{m} = 0, 1, i.e, n = 2$ for $n \geq 2$.

Let $\overline{q}_1$ be the largest signless Laplacian eigenvalue of $\overline{G}$. By the Cauchy-Schwarz inequality,

$$\begin{aligned} IE(G) + IE(\overline{G}) &\leq \sqrt{q_1} + \sqrt{\overline{q_1}} + \sqrt{(n-1)(2m - q_1)} + \sqrt{(n-1)(2\overline{m} - \overline{q_1})} \\ &\leq \sqrt{2(q_1 + \overline{q_1})} + \sqrt{2(n-1)[n(n-1) - (q_1 + \overline{q_1})]} \end{aligned}$$

and if equalities are attained, then $q_1 = \overline{q_1}$ and $q_2 = \cdots = q_n$. Consider the function $g(x) = \sqrt{2x} + \sqrt{2(n-1)[n(n-1) - x]}$. It is decreasing for $x \geq n-1$. Note that

$$q_1 + \overline{q_1} \geq \frac{4m}{n} + \frac{4\overline{m}}{n} = 2(n-1),$$

with equality if and only if G is regular. Now

$$IE(G) + IE(\overline{G}) \leq g(2(n-1)) = 2\sqrt{n-1} + (n-1)\sqrt{2(n-2)}$$

and the equality can not be attained, otherwise, $\lambda_2(G) = \cdots = \lambda_n(G) = -\frac{1}{2}$, which is impossible, because by the interlacing theorem, $\lambda_n(G) = 0$ or $\lambda_n(G) \leq -1$. ■

They [67] also gave two examples. For the complete graph K_n,

$$IE(K_n) + IE(\overline{K_n}) = IE(K_n) = \sqrt{2n-2} + (n-1)\sqrt{n-2}$$

For the complete bipartite graph $K_{n/2,n/2}$, with n even,

$$IE(K_{n/2,n/2}) = \sqrt{n} + \frac{\sqrt{2}}{2}(n-1)\sqrt{n}$$

and

$$IE(\overline{K_{n/2,n/2}}) = 2\sqrt{n-2} + \frac{\sqrt{2}}{2}(n-2)\sqrt{n-4}$$

Thus,

$$IE(K_{n/2,n/2}) + IE(\overline{K_{n/2,n/2}}) = \sqrt{n} + \frac{\sqrt{2}}{2}(n-1)\sqrt{n} + 2\sqrt{n-2} + \frac{\sqrt{2}}{2}(n-2)\sqrt{n-4}.$$

These examples and the Theorem 3.22 imply:

Theorem 3.23. [67] *Let* $\min IE_{NG}(n)$ *and* $\max IE_{NG}(n)$ *be respectively the minimum and maximum values of* $IE(G) + IE(\overline{G})$ *over all graphs with* n *vertices. Then*

$$\lim_{n\to\infty} \frac{\min IE_{NG}(n)}{n^{3/2}} = 1 \text{ and } \lim_{n\to\infty} \frac{\max IE_{NG}(n)}{n^{3/2}} = \sqrt{2}.$$

By using structural parameters other than the number of vertices, the upper bound in Theorem 3.22 was improved as follows. Let

$$\kappa = \frac{2}{\sqrt{n}} \left[\sqrt{M_1(G)} + \sqrt{n(n-1)^2 - 4m(n-1) + M_1(G)} \right].$$

Theorem 3.24. [67] *Under the same conditions as in Theorem 3.22*

$$IE(G) + IE(\overline{G}) < \sqrt{2\kappa} + \sqrt{2(n-1)[n(n-1) - \kappa]}\,. \qquad (113)$$

Proof. Repeat the reasoning in the proof of Theorem 3.22 until (112). From the proof of Lemma 3.17 we get

$$\begin{aligned} q_1 + \overline{q_1} &\geq \alpha(G) + \alpha(\overline{G}) \\ &= \frac{2}{\sqrt{n}} \left[\sqrt{\sum_{i=1}^{n} d_i(G)^2} + \sqrt{\sum_{i=1}^{n} d_i(\overline{G})^2} \right] \\ &= \frac{2}{\sqrt{n}} \left[\sqrt{\sum_{i=1}^{n} d_i(G)^2} + \sqrt{\sum_{i=1}^{n} (n-1-d_i(G))^2} \right] \\ &= \frac{2}{\sqrt{n}} \left[\sqrt{M_1(G)} + \sqrt{n(n-1)^2 - 4m(n-1) + M_1(G)} \right]. \end{aligned}$$

with equality if and only if G is regular. As explained in the proof of Theorem 3.22 we now have $IE(G) + IE(\overline{G}) \leq g(\kappa)$ which immediately implies (113). ■

3.4 Eigenvalues of the distance matrix

Recall that the *distance matrix* D is the $n \times n$ matrix (D_{ij}) such that $D_{ij} = d_{ij}$. Such D is a symmetric matrix, its eigenvalues are real. We denote the largest eigenvalue of (D_{ij}) by Λ_1.

The *reciprocal distance matrix* RD of G, also called the *Harary matrix*, is an $n \times n$ matrix (RD_{ij}), defined by

$$RD_{ij} = \begin{cases} \frac{1}{d_{ij}} & \text{if } i \neq j, \\ 0 & \text{if } i = j. \end{cases}$$

3.4.1 Distance spectral radius

Let $\mathcal{A}$ be the class of connected graphs for which the distance matrix of each graph has exactly one positive eigenvalue.

In 2007, Zhou and Trianjstić [161] obtained the following upper and lower bounds for distance spectral radius.

Lemma 3.18. [161] *Let* $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ *be a connected graph. Then*

$$\Lambda_1(G) \geq 2(n-1) - \frac{2m}{n}$$

with equality if and only if $G = K_n$ *or* G *is a regular graph of diameter two.*

Lemma 3.19. [161] *Let* $G \in \mathcal{G}(n)$ $(n \geq 2)$ *be a connected graph. Let* $D_i = \sum_{j=1}^{n} D_{ij}$ *for* $i = 1, \ldots, n$. *Then*

$$\Lambda_1(G) \leq \max_{1 \leq i \leq n} \sum_{j=1}^{n} D_{ij} \sqrt{\frac{D_j}{D_i}}$$

with equality if and only if $D_1 = \ldots = D_n$.

By the above bounds, they [161] gave the following Nordhaus–Gaddum-type result for Λ_1.

Theorem 3.25. [161] *Let* $G \in \mathcal{G}(n)$ $(n \geq 4)$ *be connected graph with a connected* $\overline{G}$. *Then*

$$3(n-1) \leq \Lambda_1(G) + \Lambda_1(\overline{G}) < \frac{n(n+3)}{2} - 3 \tag{114}$$

with left equality if and only if G *and* $\overline{G}$ *are both regular graphs of diameter two. Moreover, if* $G \in \mathcal{A}$ *or* $\overline{G} \in \mathcal{A}$, *then*

$$\Lambda_1(G) + \Lambda_1(\overline{G}) < \sqrt{\frac{(n+1)n(n-1)^2}{6}} + 2n - 3. \tag{115}$$

Proof. Let m and $\overline{m}$ be respectively the number of edges of G and $\overline{G}$. Then $2(m + \overline{m}) = n(n-1)$. By Lemma 3.18,

$$\Lambda_1(G) + \Lambda_1(\overline{G}) \geq 4(n-1) - \frac{2(m+\overline{m})}{n} = 3(n-1)$$

with equality if and only if G and $\overline{G}$ are both regular graphs of diameter two.

Let $f(n) = \frac{n(n+3)}{2} - 3$. By Lemma 3.19, the maximum sum of the distance matrix of G is an upper bound for $\Lambda_1(G)$, and it is attained if and only if the row sums are all equal. We have $\Lambda_1(G) < \frac{1}{2}n(n-1)$, moreover, if G has diameter two then $\Lambda_1(G) < 1 + 2(n-2) = 2n-3$. Thus, if one of G and $\overline{G}$ has diameter two, then $\Lambda_1(G) + \Lambda_1(\overline{G}) < \frac{n(n-1)}{2} + 2n - 3 = f(n)$.

Suppose that both G and $\overline{G}$ has diameter three. For $n = 4$, we have $G = \overline{G} = P_4$, and so $\Lambda_1(G) + \Lambda_1(\overline{G}) < 10.3246 < 11 = f(4)$. Suppose that $n \geq 5$. Then we have either

$$\Lambda_1(G) + \Lambda_1(\overline{G}) < [1 + 2 + 3(n-3)] + [1 + 2(n-3) + 3] = 5n - 8$$

or $\Lambda_1(G) + \Lambda_1(\overline{G}) < 2 \cdot [1 + 2 + 3(n-3) - 1] = 6n - 14$. Thus for $n = 5$, $\Lambda_1(G) + \Lambda_1(\overline{G}) < 17 = f(5)$, and for $n \geq 6$, $\Lambda_1(G) + \Lambda_1(\overline{G}) < 6n - 14 < f(n)$. Now the right inequality in (114) follows.

Suppose that $G \in \mathcal{A}$ or $\overline{G} \in \mathcal{A}$. Recall that $\Lambda_1(G) < \sqrt{\frac{(n+1)n(n-1)^2}{6}}$ if $G \in \mathcal{A}$. Thus if one of G and $\overline{G}$ has diameter two, then (115) holds. Suppose that both G and $\overline{G}$ has diameter three. From the argument above, it is easy to see that (115) follows for $n \neq 5$. If $n = 5$, then one of G or $\overline{G}$ is G_1, G_2 or G_3, where G_1 (G_2, G_3, respectively) is obtained from the path P_5, labeled consecutively by $v_1, \cdots, v_5$, by adding edges v_2v_4 (edge v_3v_5, edge v_2v_5 and v_3v_5, respectively), by direct calculation, we have $\Lambda_1(G) + \Lambda_1(\overline{G}) = 13.2750$, 13.5467, or 13.6754, and so (115) follows again. ■

3.4.2 Reciprocal distance spectral radius

Let $R\Lambda_1(G)$ be the maximum eigenvalue of the reciprocal distance matrix of G. In 2008, Zhou and Trianjstić [160] obtained Nordhaus–Gaddum type bounds for $R\Lambda_1(G)$ in terms of n only.

Theorem 3.26. [160] *Let $G \in \mathcal{G}(n)$ $(n \geq 4)$ be connected graph with a connected $\overline{G}$. Then*

$$n < R\Lambda_1(G) + R\Lambda_1(\overline{G}) < 2n - 3. \tag{116}$$

Improvements of the lower bound have then been given by Zhou, Cai, and Trianjstić [154] and by Das [25].

Theorem 3.27. [154] *Let $G \in \mathcal{G}(n)$ $(n \geq 4)$ be connected graph with a connected $\overline{G}$. Then*

$$R\Lambda_1(G) + R\Lambda_1(\overline{G}) > n - 1 + \frac{3}{n} + 2\sum_{i=3}^{n-1} \frac{1}{i}. \tag{117}$$

Zhou and Trianjstić [160] gave the following lower bound for $R\Lambda_1(G)$ in terms of n, m and d:

Lemma 3.20. [160] *Let $G \in \mathcal{G}(n,m)$ $(n \geq 2)$ be a connected graph with diameter d. Then*

$$R\Lambda_1(G) \geq \frac{2m}{n} + \frac{1}{d}\left(n - 1 - \frac{2m}{n}\right),$$

with equality holds if and only if G is a complete graph K_n or G is a regular graph of diameter 2.

By the above bound, Das [25] derived the following Nordhaus–Gaddum-type result.

Theorem 3.28. [25] *Let $G \in \mathcal{G}(n)$ $(n \geq 4)$ be connected graph with a connected $\overline{G}$. Then*

$$R\Lambda_1(G) + R\Lambda_1(\overline{G}) \geq (n-1)\left(1 + \frac{1}{k}\right), \tag{118}$$

where $k = \max\{diam(G), diam(\overline{G})\}$. Moreover, the second bound is reached if and only if both G and $\overline{G}$ are regular graphs of diameter 2.

Proof. From Lemma 3.20 we arrive at

$$R\Lambda_1(G) + R\Lambda_1(\overline{G}) \geq \frac{2m + 2\overline{m}}{n} + \frac{n(n-1) - 2m}{nd} + \frac{n(n-1) - 2\overline{m}}{n\overline{d}} \tag{119}$$

where $\overline{m}$ and $\overline{d}$ are, respectively, the number of edges and diameter of $\overline{G}$. Since $m + \overline{m} = \frac{n(n-1)}{2}$ and $k = \max\{d, \overline{d}\}$, we get (118) from (119). First part of the proof is over.

Now suppose that equality holds in (118). Then the equality holds in (119) and $k = d = \overline{d}$. From equality in (119), we get both G and $\overline{G}$ are regular graph of diameter 2, by Lemma 3.20. Hence both G and $\overline{G}$ are regular graph of diameter 2.

Conversely, let both G and $\overline{G}$ be regular graph of diameter 2. Then $R\Lambda_1(G) = \frac{n+r-1}{2}$ and $R\Lambda_1(\overline{G}) = \frac{2(n-1)-r}{2}$. Hence $R\Lambda_1(G) + R\Lambda_1(\overline{G}) = \frac{3}{2}(n-1)$. ■

For $G = C_5$, we have $R\Lambda_1(G) + R\Lambda_1(\overline{G}) = 6$, since complement of C_5 is also C_5.

Remark 3.9. [25] *It is easily see that our lower bound (118) is always better than (116) as* $2 \leq k \leq n-1$.

Das [25] obtained an upper bound of $R\Lambda_1$ in terms of the order, size, and minimum degree.

Lemma 3.21. [25] *Let* $G \in \mathcal{G}(n)$ $(n \geq 2)$ *be a connected graph with minimum vertex degree* δ. *Then*

$$R\Lambda_1(G) \leq \frac{1}{2}\sqrt{(n-1)^2 + 3(2m-\delta)}, \tag{120}$$

with equality if and only if G is a complete graph K_n.

A sharp upper bound using the minimum degree δ and the maximum degree Δ in addition to n has also been given by Das [25].

Theorem 3.29. [25] *Let* $G \in \mathcal{G}(n)$ $(n \geq 4)$ *be connected graph with a connected* $\overline{G}$. *Then*

$$R\Lambda_1(G) + R\Lambda_1(\overline{G}) \leq \sqrt{\frac{1}{2}[5(n-1)^2 + 3(\Delta - \delta)]}. \tag{121}$$

Proof. Using the inequality (120) from Lemma 3.21 we arrive at

$$\begin{aligned} R\Lambda_1(G) + R\Lambda_1(\overline{G}) &\leq \frac{1}{2}\sqrt{(n-1)^2 + 3(2m-\delta)} + \frac{1}{2}\sqrt{(n-1)^2 + 3(2\overline{m}-\overline{\delta})} \\ &= \frac{1}{2}\sqrt{(n-1)^2 + 3(2m-\delta)} + \frac{1}{2}\sqrt{4(n-1)^2 - 6m + 3\Delta} \qquad (122) \\ &\text{as } 2\overline{m} = n(n-1) - 2m \text{ and } \Delta = n-1-\overline{\delta}, \end{aligned}$$

where $\overline{m}$ and $\overline{\delta}$ are, respectively, the number of edges and the minimum vertex degree of $\overline{G}$. Now we consider a function

$$f(m) = \sqrt{(n-1)^2 + 3(2m-\delta)} + \sqrt{4(n-1)^2 - 6m + 3\Delta}.$$

It is easy to show that

$$f(m) \leq f\left(\frac{(n-1)^2 + \Delta + \delta}{4}\right) = 2\sqrt{\frac{1}{2}[5(n-1)^2 + 3(\Delta-\delta)]}. \tag{123}$$

From (122) and (123), we get the required result (121). ∎

Remark 3.10. [25] *In order to see that the upper bound (121) is always better than the upper bound (116) for any graphs, note that*

$$(2n-3)^2 \geq \frac{1}{2}[5(n-1)^2 + 3(\Delta - \delta)]$$

holds if and only if

$$\left(n - \frac{1}{3}\right)^2 + \frac{38}{9} - (\Delta - \delta) \geq 0$$

which, evidently, is always obeyed.

4. Distance–degree–based parameters

In chemical graph theory, distance-degree-based topological indices are expressions of the form

$$\sum_{u,v\in V(G)} F(deg_G(u), deg_G(v), d_G(u,v))$$

where F is a function, $deg_G(u)$ denotes the degree of u, and $d_G(u,v)$ denotes the distance between u and v.

The following Table 4.1 shows the authors contributing the Nordhaus–Gaddum problem for distance-degree-based parameters.

Distance-degree-based Parameters	Authors Contributing N-G Problem
Reciprocal molecular topological index	Zhou and Trinajstić [159]
Additive degree Kirchhoff index	Das, Yang, and Xu [36]
Multiplicative degree Kirchhoff index	Das, Yang, and Xu [36]
	Feng, Yu, and Liu [51]

Table 4.1. Distance–degree–based parameters

4.1 Reciprocal molecular topological index

In 1998, Schultz and Schultz [127] introduced the reciprocal molecular topological index $\mathrm{Sc}(G)$ of a connected graph $G=(V,E)$. It is defined by

$$\mathrm{RMTI}(G) = \sum_{v\in V}(d(v))^2 + \sum_{v\in V} d(v)\left(\sum_{u\in V-\{v\}} \frac{1}{d_G(u,v)}\right).$$

Zhou and Trinajstić [163] presented a relation between RMTI and the first Zagreb index M_1.

Lemma 4.1. [163] *Let $G\in\mathcal{G}(n,m)$ be a connected simple graph. Then*

$$\mathrm{RMTI}(G) \le \frac{3}{2}\mathrm{M}_1(G) + (n-1)m$$

with equality if and only if the diameter of G is at most two.

In the same paper, they [163] first give a Nordhaus–Gaddum type result for the first Zagreb index.

Lemma 4.2. [163] *Let $G\in\mathcal{G}(n)$ $(n\ge 4)$ be a connected graph with a connected $\overline{G}$. Then*

$$\mathrm{M}_1(G) + \mathrm{M}_1(\overline{G}) \le n^3 - 4n^2 + 3n + 8$$

with equality if and only if G or $\overline{G}$ is the graph S'_n, which is obtained by attaching a pendant vertex to a pendant vertex of the star S_{n-1}.

Next, Zhou and Trinajstić [159] proved the following theorem.

Theorem 4.1. [159] *If* $G \in \mathcal{G}(n)$ $(n \geq 4)$ *is a graph such that both* G *and* $\overline{G}$ *are connected, then*

$$\mathrm{RMTI}(G) + \mathrm{RMTI}(\overline{G}) < 2n^3 - 7n^2 + 5n + 12.$$

Proof. From Lemmas 4.1 and 4.2,

$$\begin{aligned}\mathrm{RMTI}(G) + \mathrm{RMTI}(\overline{G}) &\leq \frac{3}{2}[\mathrm{M}_1(G) + \mathrm{M}_1(\overline{G})] + \frac{1}{2}n(n-1)^2 \\ &\leq \frac{3}{2}(n^3 - 4n^2 + 3n + 8) + \frac{1}{2}n(n-1)^2 \\ &= 2n^3 - 7n^2 + 5n + 12.\end{aligned}$$

Note that if the upper bound in Lemma 4.2 is attained, then the diameter of G is 3. Hence the upper bound in Lemmas 4.1 and 4.2 cannot be achieved at the same time. The theorem is thus proved. ■

4.2 Additive degree Kirchhoff index

The *additive degree Kirchhoff index* was put forward in [64]. It is defined as

$$Kf^+(G) = \sum_{\{u,v\} \subseteq V(G)} (d(u) + d(v))\, R(u,v) = \sum_{i<j} (d_i + d_j)\, r_{ij}, \tag{124}$$

where d_i is the degree of vertex v_i for $i = 1, 2, \ldots, n$, and r_{ij} is the resistance distance between v_i and v_j.

To obtain the Nordhaus–Gaddum-type result for $Kf^+(G)$, the following two graph invariants are used. One is the inverse degree of G [21],

$$ID(G) = \sum_{v_i \in V(G)} \frac{1}{d_i};$$

the other is the modified second Zagreb index of G [33],

$$M_2^*(G) = \sum_{v_i v_j \in E(G)} \frac{1}{d_i d_j}. \tag{125}$$

Das, Yang, and Xu [36] studied $Kf(G)$, $Kf^+(G)$ and $Kf^*(G)$ (defined in the next subsection) in more detail, especially Nordhaus–Gaddum-type results for them, which are given in terms of the number of vertices, the number of edges, minimum and maximum vertex degree, the inverse degree and the modified second Zagreb index.

They first gave a lower bound for $Kf^+(G) + Kf^+(\overline{G})$ in terms of n only.

Theorem 4.2. [36] *Let* $G \in \mathcal{G}(n)$ *be a connected graph with connected complement* $\overline{G}$*. Then*

$$Kf^+(G) + Kf^+(\overline{G}) > 4n(n-2).$$

Proof. From (124),

$$
\begin{aligned}
& Kf^+(G) + Kf^+(\overline{G}) \\
= & \sum_{i<j}[(d_i+d_j)r_{ij} + (2n-d_i-d_j-2)\overline{r_{ij}}] \\
\geq & \sum_{v_iv_j\in E(G)} \left[\frac{(d_i+d_j-2)(d_i+d_j)}{d_id_j-1} + \left(\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}\right)(2n-d_i-d_j-2)\right] \\
& + \sum_{i<j,\ d_{ij}\geq 2} \left[\left(\frac{1}{d_i}+\frac{1}{d_j}\right)(d_i+d_j) + \frac{2n-d_i-d_j-4}{(n-d_i-1)(n-d_j-1)-1}(2n-d_i-d_j-2)\right] \\
& \text{by } (97) \\
> & \sum_{v_iv_j\in E(G)} \left[\frac{(d_i+d_j-2)(d_i+d_j)}{d_id_j} + \left(\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}\right)(2n-d_i-d_j-2)\right] \\
& + \sum_{i<j,\ d_{ij}\geq 2} \left[\left(\frac{1}{d_i}+\frac{1}{d_j}\right)(d_i+d_j) + \frac{2n-d_i-d_j-4}{(n-d_i-1)(n-d_j-1)-1}(2n-d_i-d_j-2)\right] \\
= & \sum_{v_iv_j\in E(G)} \left[\frac{d_i}{d_j}+\frac{d_j}{d_i}+2-2\left(\frac{1}{d_i}+\frac{1}{d_j}\right)+2+\left(\frac{n-d_j-1}{n-d_i-1}+\frac{n-d_i-1}{n-d_j-1}\right)\right] \\
& + \sum_{i<j,\ d_{ij}\geq 2} \left[\frac{d_i}{d_j}+\frac{d_j}{d_i}+2+\left(\frac{n-d_j-1}{n-d_i-1}+\frac{n-d_i-1}{n-d_j-1}+2\right)\right. \\
& \left. -2\left(\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}\right)\right] \geq 8m-2n+8\left(\frac{n(n-1)}{2}-m\right)-2n \\
= & 4n(n-2), \\
& \text{as } \frac{d_i}{d_j}+\frac{d_j}{d_i}\geq 2,\ \frac{n-d_j-1}{n-d_i-1}+\frac{n-d_i-1}{n-d_j-1}\geq 2 \text{ and } \sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)=n.
\end{aligned}
$$

This completes the proof. ■

Remark 4.1. [36] *If we choose G to be a conference graph on n vertices, then as proved in [142],*

$$Kf(G) = Kf(\overline{G}) = 2n.$$

Noticing that both G and $\overline{G}$ are $\frac{n-1}{2}$-regular, it follows that

$$Kf^+(G) + Kf^+(\overline{G}) = 2n(n-1) + 2n(n-1) = 4n(n-1),$$

which indicates that the lower bound obtained in Theorem 4.2 is asymptotically best.

In the same paper, they [36] also gave an upper bound for $Kf^+(G) + Kf^+(\overline{G})$ in terms of the order, size, maximum degree, and minimum degree.

Theorem 4.3. [36] *Let $G \in \mathcal{G}(n,m)$ be a connected graph, maximum degree Δ and minimum degree δ. Then*

$$\begin{aligned} Kf^+(G)+Kf^+(\overline{G}) &\le 2(n-1)(n-1+\Delta-\delta)+[n(n-1)-2m](n+3-2\delta)\Delta \\ &\quad +2(n-1-\delta)(2\Delta+5-n)m. \end{aligned}$$

Proof. By graph theoretic knowledge, it is easily seen that if $d_{ij} \ge 3$, then the length of any path connecting v_i and v_j must be less than or equal to $n+1-d_i-d_j$, thus

$$r_{ij} \le n+1-d_i-d_j.$$

Similarly, if $\overline{d}_{ij} \ge 3$, then

$$\overline{r}_{ij} \le n+1-\overline{d}_i-\overline{d}_j = d_i+d_j+3-n.$$

Using the above results, we get

$$\begin{aligned} & Kf^+(G)+Kf^+(\overline{G}) \\ = & \sum_{i<j}[(d_i+d_j)r_{ij}+(2n-d_i-d_j-2)\overline{r}_{ij}] \\ = & \sum_{v_iv_j\in E(G)}(d_i+d_j)r_{ij}+\sum_{v_iv_j\in E(\overline{G})}(2n-d_i-d_j-2)\overline{r}_{ij}+\sum_{d_{ij}=2}(d_i+d_j)r_{ij} \\ & +\sum_{\overline{d}_{ij}=2}(2n-d_i-d_j-2)\overline{r}_{ij}+\sum_{d_{ij}\ge 3}(d_i+d_j)r_{ij}+\sum_{\overline{d}_{ij}\ge 3}(2n-d_i-d_j-2)\overline{r}_{ij} \\ \le & 2(n-1)\Delta+2(n-\delta-1)(n-1)+2\sum_{d_{ij}=2}(d_i+d_j)+2\sum_{\overline{d}_{ij}=2}(2n-d_i-d_j-2) \\ & +\sum_{d_{ij}\ge 3}(d_i+d_j)(n+1-d_i-d_j)+\sum_{\overline{d}_{ij}\ge 3}(2n-d_i-d_j-2)(d_i+d_j+3-n) \\ \le & 2(n-1)\Delta+2(n-\delta-1)(n-1)+2\sum_{d_{ij}=2}(2\Delta)+2\sum_{\overline{d}_{ij}=2}(2n-2-2\delta) \\ & +\sum_{d_{ij}\ge 3}[2\Delta(n+1-2\delta)]+\sum_{\overline{d}_{ij}\ge 3}[(2n-2-2\delta)(2\Delta+3-n)]. \end{aligned}$$

Then the desired result can be derived by using the following inequalities

$$\sum_{d_{ij}=2}1 \le \frac{n(n-1)}{2}-m,\ \ \sum_{d_{ij}\ge 3}1 \le \frac{n(n-1)}{2}-m,\ \ \sum_{\overline{d}_{ij}=2}1 \le m,\ \ \sum_{\overline{d}_{ij}\ge 3} \le m.$$

■

If $\delta \le \frac{n-1}{2} \le \Delta$, we have $2 \le 2\Delta+3-n$ and $2 \le n+1-2\delta$. Therefore by the proof of Theorem 4.3, the following corollary can be easily obtained.

Corollary 4.1. [36] *Let $G \in \mathcal{G}(n,m)$ be a connected graph with maximum degree Δ and minimum degree δ such that $\delta \leq \frac{n-1}{2} \leq \Delta$. Then*

$$\begin{aligned} Kf^{+}(G)+Kf^{+}(\overline{G}) &\leq 2(n-1)(n-1+\Delta-\delta)+[n(n-1)-2m]\Delta(n+1-2\delta) \\ &\quad +m(2n-2-2\delta)(2\Delta+3-n). \end{aligned}$$

4.3 Multiplicative degree Kirchhoff index

A new index named *multiplicative degree Kirchhoff index* was put forward in [15]. It is defined as

$$Kf^{*}(G)=\sum_{\{u,v\}\subseteq V(G)} d(u)\,d(v)\,R(u,v)=\sum_{i<j} d_i\,d_j\,r_{ij}, \tag{126}$$

where d_i is the degree of vertex v_i for $i=1,2,\ldots,n$, and r_{ij} is the resistance distance between v_i and v_j.

Apparently, we can see that the multiplicative degree Kirchhoff index may be viewed as the resistance–distance analogue of the Gutman index.

In [17], Chung defined the *normalized Laplacian matrix* $\mathscr{L}(G)=(\mathscr{L}_{uv})_{n\times n}$ of a graph G as follows:

$$\mathscr{L}_{uv}=\begin{cases} 1 & \text{if } u=v, \\ -\frac{1}{\sqrt{deg_G(u)deg_G(v)}} & \text{if } u\sim v, \\ 0 & \text{otherwise.} \end{cases}$$

We call eigenvalues of $\mathscr{L}(G)$ the *normalized Laplacian eiganvalues* of G, and the eigenvalues of $\mathscr{L}(G)$ are ordered by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} > \lambda_n = 0$. One can find that $\mathscr{L}=D^{-1/2}LD^{-1/2}$.

A remarkable analogy between the Kirchhoff and multiplicative degree Kirchhoff indices is the formula [15]:

$$Kf^{*}(G)=2m\sum_{i=1}^{n-1}\frac{1}{\lambda_i}.$$

4.3.1 Nordhaus–Gaddum–type inequalities in $\mathcal{G}(n,m)$

Das, Yang, and Xu [36] gave lower bound for $Kf^{*}(G)+Kf^{*}(\overline{G})$ in terms of n, m, Δ and $M_2^{*}(G)$.

Theorem 4.4. [36] *Let $G \in \mathcal{G}(n,m)$ be a connected graph with maximum degree $\Delta < n-1$. Then*

$$Kf^{*}(G)+Kf^{*}(\overline{G}) > n(n^2-3n+4)-\frac{1}{(n-\Delta-1)^2}[n(n-1)-2m]-2M_2^{*}(G).$$

Proof. From (126),

$$
\begin{aligned}
& Kf^*(G)+Kf^*(\overline{G}) \\
= & \sum_{i<j}[d_id_jr_{ij}+(n-d_i-1)(n-d_j-1)\overline{r}_{ij}] \\
\geq & \sum_{v_iv_j\in E(G)}\left[\frac{d_i+d_j-2}{d_id_j-1}d_id_j+\left(\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}\right)(n-d_i-1)(n-d_j-1)\right] \\
& +\sum_{i<j,\ d_{ij}\geq 2}\left[\left(\frac{1}{d_i}+\frac{1}{d_j}\right)d_id_j+\frac{2n-d_i-d_j-4}{(n-d_i-1)(n-d_j-1)-1}(n-d_i-1)(n-d_j-1)\right] \\
= & \sum_{v_iv_j\in E(G)}\left[2n-4+\frac{d_i+d_j-2}{d_id_j-1}\right]+\sum_{i<j,\ d_{ij}\geq 2}\left[2n-4+\frac{2n-d_i-d_j-4}{(n-d_i-1)(n-d_j-1)-1}\right] \\
> & \sum_{i<j}(2n-4)+\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}\right) \\
& +\sum_{i<j,\ d_{ij}\geq 2}\left[\frac{1}{n-d_i-1}+\frac{1}{n-d_j-1}-\frac{2}{(n-d_i-1)(n-d_j-1)}\right] \\
= & n(n-1)(n-2)+2n-2\sum_{v_iv_j\in E(G)}\frac{1}{d_id_j}-2\sum_{i<j,\ d_{ij}\geq 2}\frac{1}{(n-d_i-1)(n-d_j-1)} \\
\geq & n(n^2-3n+4)-\frac{1}{(n-\Delta-1)^2}[n(n-1)-2m]-2M_2^*(G) \ \text{ as } \ \Delta\geq d_i.
\end{aligned}
$$

This completes the proof. ■

Remark 4.2. [36] *If we choose G to be a conference graph, then*

$$Kf^*(G)+Kf^*(\overline{G})=2n\cdot\frac{(n-1)^2}{4}+2n\cdot\frac{(n-1)^2}{4}=n(n-1)^2,$$

which indicates that the lower bound obtained in Theorem 4.4 is asymptotically best.

Similarly to Theorem 4.3, we obtain an upper bound for $Kf^*(G)+Kf^*(\overline{G})$ in terms of n, m, δ and Δ.

Theorem 4.5. [36] *Let $G\in\mathcal{G}(n,m)$ be a connected graph with minimum degree δ and maximum degree Δ. Then*

$$
\begin{aligned}
Kf^*(G)+Kf^*(\overline{G}) \leq & \left[\Delta^2+(n-\delta-1)^2\right](n-1)+\left[\frac{n(n-1)}{2}-m\right](n+3-2\delta)\Delta^2 \\
& +m(n-1-\delta)^2(2\Delta+5-n).
\end{aligned}
$$

Proof. Bearing in mind that

$$r_{ij}\leq n+1-d_i-d_j\leq n+1-2\delta \text{ for } d_{ij}\geq 3,$$

we have

$$
\begin{aligned}
& Kf^*(G) + Kf^*(\overline{G}) \\
= \; & \sum_{v_iv_j \in E(G)} d_id_jr_{ij} + \sum_{v_iv_j \in E(\overline{G})} (n-1-d_i)(n-1-d_j)\overline{r}_{ij} + \sum_{d_{ij}=2} d_id_jr_{ij} \\
& + \sum_{\overline{d}_{ij}=2} (n-1-d_i)(n-1-d_j)\overline{r}_{ij} + \sum_{d_{ij}\geq 3} d_id_jr_{ij} + \sum_{\overline{d}_{ij}\geq 3} (n-1-d_i)(n-1-d_j)\overline{r}_{ij} \\
\leq \; & \Delta^2(n-1) + (n-\delta-1)^2(n-1) + \sum_{d_{ij}=2} (2\Delta^2) + \sum_{\overline{d}_{ij}=2} 2(n-1-\delta)^2 \\
& + \sum_{d_{ij}\geq 3} \Delta^2(n+1-2\delta) + \sum_{\overline{d}_{ij}\geq 3} (n-1-\delta)^2(2\Delta+3-n) \\
\leq \; & [\Delta^2 + (n-\delta-1)^2](n-1) + \left[\frac{n(n-1)}{2} - m\right](n+3-2\delta)\Delta^2 \\
& + m(n-1-\delta)^2(2\Delta+5-n),
\end{aligned}
$$

as required. ■

Similarly as before, we can deduce the following corollary.

Corollary 4.2. [36] *Let $G \in \mathcal{G}(n,m)$ be a connected graph with minimum degree δ and maximum degree Δ such that $\delta \leq \frac{n-1}{2} \leq \Delta$. Then*

$$
\begin{aligned}
Kf^*(G) + Kf^*(\overline{G}) \;\leq\; & [\Delta^2 + (n-\delta-1)^2](n-1) + \left[\frac{n(n-1)}{2} - m\right](n+1-2\delta)\Delta^2 \\
& + m(n-1-\delta)^2(2\Delta+3-n).
\end{aligned}
$$

Feng, Yu, and Liu [51] obtained an upper bound for the multiplicative degree Kirchhoff index.

Lemma 4.3. [51] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected (molecular) graph with diameter d. Then*

$$Kf^*(G) \leq 4d(n-1)m^2.$$

By the upper bound, they [51] derived the Nordhaus–Gaddum-type result.

Theorem 4.6. [51] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected (molecular) graph with a connected complement $\overline{G}$. Then*

$$Kf^*(G) + Kf^*(\overline{G}) \leq 4(n-1)^2\left(m^2 + \left(\binom{n}{2} - m\right)^2\right).$$

Proof. Note that the diameter of any graph is at most $n-1$. From the result in Lemma 4.3, we have

$$Kf^*(G) + Kf^*(\overline{G}) \leq 4(n-1)^2\left(m^2 + \left(\binom{n}{2} - m\right)^2\right).$$

This implies the result. ■

4.3.2 Nordhaus–Gaddum–type inequalities in $\mathcal{G}(n)$

Feng, Yu, and Liu [51] first obtained some lower bounds for the degree Kirchhoff index.

Lemma 4.4. [51] *Let $G \in \mathcal{G}(n,m)$ $(n > 2)$ be a connected graph. Then*

$$\begin{aligned} Kf^*(G) &\geq 2m\left(n-2+\frac{1}{n}\right), \\ Kf^*(G) &\geq 2m\left(\frac{\Delta}{\Delta+1}+\frac{(n-2)^2}{n-1-\frac{1}{\Delta}}\right), \\ Kf^*(G) &\geq 2m\left(\frac{\chi}{\chi+1}+\frac{(n-2)^2}{n-1-\frac{1}{\chi}}\right). \end{aligned}$$

Each of the above equalities holds if and only if $G \cong K_n$.

By the lower bounds, they [51] derived the Nordhaus–Gaddum-type result for the degree Kirchhoff index.

Theorem 4.7. [51] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected (molecular) graph with a connected complement $\overline{G}$. Then*

$$Kf^*(G) + Kf^*(\overline{G}) \geq \frac{(n-1)^3}{2}.$$

Proof. From the result in Lemma 4.4, we have

$$\begin{aligned} Kf^*(G) + Kf^*(\overline{G}) &\geq 2m\left(n-2+\frac{1}{n}\right) + \left(\binom{n}{2} - 2m\right)\left(n-2+\frac{1}{n}\right) \\ &= \binom{n}{2}\left(n-2+\frac{1}{n}\right) = \frac{(n-1)^3}{2}. \end{aligned}$$

This implies the result. ■

Feng, Yu, and Liu [51] also got an upper bound for the multiplicative degree Kirchhoff index in terms of the order and maximum degree.

Lemma 4.5. [51] *Let $G \in \mathcal{G}(n)$ be a graph with maximum degree Δ. Then*

$$Kf^*(G) \leq \binom{n+1}{3}\Delta^3.$$

By Lemma 4.5, they derived the following result.

Theorem 4.8. [51] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected (molecular) graph with a connected complement $\overline{G}$. Then*

$$Kf^*(G) + Kf^*(\overline{G}) \leq \binom{n+1}{3}\left(\Delta^3 + (n-1-\delta)^3\right).$$

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The Vertex PI Index of Graphs

G. H. Fath–Tabar*, **F. Taghvaee**

Department of pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-51167, Iran

fathtabar@kashanu.ac.ir

Abstract

The vertex PI index of a graph G is the sum over all edges of the number of vertices which are not equidistant to u and v. In this chapter, we give lower and upper bound for the vertex PI index of graphs.

Contents

1. Introduction

In the theoretical chemistry molecular–graph based structure descriptors – also called topological indices – are used for modeling physico–chemical, pharmacologic, toxicologic, etc. properties of chemical compounds [14, 32]. There exist several types of such indices, reflecting different aspects of the molecular structure for instance Zagreb indices, atom–bond connectivity index, Szeged and GA index [7–9, 23, 27].

Khadikar [17] defined a topological index and called it Padmakar–Ivan index (PI). It is defined as $PI(G) = \sum_{e=uv\in E(G)}[m_u(e|G) + m_v(e|G)]$, where $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. This is the edge version of PI index and in [18, 19], the edge–PI index has been computed for some graphs. It is useful to mention that the PI index is a unique topological index related to parallelism of edges (we will make this more precise below) and it has been studied from many different points of view, see [1–4, 11, 16, 25, 37]. All topological indices mentioned have many chemical applications and it was shown that the PI index correlates well with the Wiener and Szeged indices and that they all correlate with the physico–chemical properties and biological activities of a large number of diverse and complex compounds. Recently, a new topological index, the vertex PI index, was introduced and some of its properties were studied [20, 21]. Its definition is similar to that of the (edge) PI index, in that it is additive, but now the distances of vertices (instead of edges) from edges is considered.

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between the vertices u and v of G is defined as the number of edges in a minimal path connecting them and is denoted by $d(u,v)$. The diameter of G is the greatest distance between two vertices of G denoted by $d(G)$. Denote by $d_G(v)$, the degree of the vertex $v \in V(G)$. Define $N_G(u)$ to be the set of all vertices adjacent to u. Let $e = uv$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that vertices equidistant to u and v are not counted. The vertex PI index of G is defined as:

$$PI_v(G) = \sum_{e=uv \in E(G)} [n_u(e) + n_v(e)] .$$

2. Extremal graphs with respect to the vertex PI index

In this section we present some formulas for computing the vertex PI index of a graph. Then we apply this formula to obtain the extremal graphs with respect to the vertex PI index. These results can be found in [29].

Lemma 2.1. *Let G be a n-vertex graph, $n \geq 4$. Then $PI_v(G) \leq |E(G)||V(G)|$ with equality if and only if G is bipartite.*

Lemma 2.2. *Let G be a connected graph. Then $PI_v(G) = \sum_{v \in V(G)} m_v(G)$, where $m_v(G) = |\{e = uv \in E(G); d(x,u) \neq d(x,v)\}|$.*

Theorem 2.1. *Let G be n-vertex graph, $n \geq 4$. Then $PI_v(G) \leq n \lfloor n/2 \rfloor \lceil n/2 \rceil$ with equality if and only if G is a complete bipartite graph with balanced bipartition.*

Suppose X_n is the set of all n-vertex graphs G with the property that if G has an even cycle $v_1, \ldots, v_{k-1}, v_1$, then there are unique integers s and t, $1 < s < t < k-1$, such that $v_s, \ldots, v_t$ are vertices of a layer which constitutes a clique, $v_i \in A_{i-1}, 1 \leq i \leq s$, and $v_{t+j} \in A_{s-j}, 1 \leq j \leq s$. Suppose $P_n, S_n,$ and, K_n denote the path,star and complete graphs with exactly n vertices. Then $X_3 = \{P_3, K_3\}$ and $X_4 = \{P_4, K_4, S_4\}$. The authors in [29] proved the following theorem.

Theorem 2.2. *Let G be n-vertex graph. Then $PI_v(G) \geq n(n-1)$ with equality if and only if $G \in X_n$.*

3. Lower and upper bounds on vertex PI index

In this section we consider some of bounds on the vertex PI index of a graph. For any n-vertex tree T and for the complete graph K_n it is easy to see that $PI_v(T) = PI_v(K_n) = n(n-1)$.

The authors in [6] found lower and upper bounds on vertex PI index of a graph as followings.

Theorem 3.1. *Let G be a connected graph on n vertices, m edges, and diameter d. Then*

$$PI_v(G) \geq 2m + d^2 - d$$

with equality holding if and only if $G \cong K_n$ or $G \cong P_n$.

Lemma 3.1. *Let G be a simple graph of order n, possessing $t(G)$ triangles. Then*

$$\sum_{uv \in E(G)} |N_u \cap N_v| = 3\,t(G)$$

where $|N_u \cap N_v|$ is the number of common neighbors of u and v.

The proof of this Lemma can be found in [6].

In the following by using above lemma we give an upper bound on the vertex PI index in terms of the number of vertices n, the number of edges m, and the number of triangles $t(G)$ in G.

Theorem 3.2. *Let G be a connected graph with $n > 2$ vertices and m edges. Also let $t(G)$ be the number of triangles of G. Then*

$$PI_v(G) \leq nm - 3t(G)$$

with equality holding if and only if G is a bipartite graph or $G \cong K_3$.

Theorem 3.3. *Let G be a connected graph on $n \geq 5$ vertices, diameter d, and with a connected complement $\overline{G}$. Then*

$$PI_v(G) + PI_v(\overline{G}) \geq n(n-1) + (d-1)(3d-4)$$

with equality holding if and only if $G \cong P_n$.

The proof of this theorem can be found in [6].

Suppose that G is a triangle free graph. Then the following result for the vertex PI index of G is obtained in [28].

Theorem 3.4. *Let G be a triangle free graph. Then*

$$PI_v(G) \geq \sum_{v \in V(G)} d_G(v)^2$$

where $d_G(v)$ is the degree of the vertex v and with equality if and only if $d_G(v) = 2$.

Shabani [31] calculated the PI_v index of a class of dendrimers where are parts of a group of macromolecules which is built from a starting atom, such as nitrogen, to which carbon and other elements are added by a repeating series of chemical reactions that produce a spherical branching structure. In a divergent synthesis of a dendrimer, one starts from the core (a multi connected atom or group of atoms) and growths out to the periphery. The following theorem is about of the PI_v index of tetrathiafulvalene dendrimers, denoted by $T = D[k]$.

Theorem 3.5. *The PI_v index of $T = D[k]$ is computed as follows*

$$PI_v(T) = 16368 \times 4^k - 19564 \times 2^k + 5806 \, .$$

Some authors discuss on the some operations of two graphs such as the corona product of two graphs, the Cartesian product of graphs and the join of graphs. In the following we consider these operations on graphs and we discuss the vertex PI index of them.

The corona product $G \circ H$ of two graphs G and H is defined as the graph obtained by taking one copy of G and $|V(G)|$ copies of H and joining the i-th vertex of G to every vertex in the i-th copy of H . Yarahmadi and Ashrafi [35, 36] computed some of indices such as the Szeged, vertex PI and the first and second Zagreb indices of corona product of two graphs G and H . We give the following results for the vertex PI index of the corona product of two graphs G and H .

Theorem 3.6. *Let G be a connected graph of order n and H be a graph with m vertices and q edges, then the vertex PI index of $G \circ H$ is given by*

$$PI_v(G \circ H) = (m+1)PI_v(G) + nM_1(H) + n^2m(m+1) - 2n(q+3t) \, ,$$

where t is the number of triangles of H and $M_1(H)$ is the first Zagreb index of H , that is defines as

$$M_1(H) = \sum_{u \in V(H)} d_H(u)^2$$

Corollary 3.1. *Suppose H is triangle–free graph with m vertices and q edges and G is a connected graph of order n . Then*

$$PI_v(G \circ H) = (m+1)PI_v(G) + nM_1(H) + n^2m(m+1) - 2nq \, .$$

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2 , [22].

Theorem 3.7. *Let G_i be graphs with adjacency matrix $A_i, 1 \leq i \leq n$, and $G = G_1 + G_2 + \cdots + G_n$. Then*

$$PI_v(G) = \sum_i |V_i| \left(\sum_{j \neq i} \left(|V_j|^2 - 2|E_j| \right) \right) + \sum_i \left(\left(A_i^2\right)_d \left(A_i^2\right)_d^t - \operatorname{tr}\left(A_i\right)^3 \right) \, .$$

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. If $G_1, G_2, \ldots, G_n$ are graphs then we denote $G_1 \times \cdots \times G_n$ by $\otimes_{i=1}^n G_i$. The vertex PI index of $\otimes_{i=1}^n G_i$ is as following [20].

Theorem 3.8. *Let $G_1, G_2, \ldots, G_n$ be connected graphs. Then*

$$PI_v\left(\overset{n}{\underset{i=1}{\otimes}} G_i \right) = \sum_{i=1}^n \left(\prod_{j=1, j \neq i}^n |V(G_j)|^2 \right) PI_v(G_i) \, .$$

By using the above theorem the following examples are obtained in [20].

Example 3.1. *Let C_n be a cycle graph with n vertices. Then $PI_v(C_n) = n^2$ if n is even and $PI_v(C_n) = n(n-1)$ if n is odd.*

Example 3.2. *Let $L_n = P_2 \times P_n$ be a ladder graph with $2n$ vertices. Then $PI_v(L_n) = 6n^2 - 4n$.*

Now consider the graph G whose vertices are the N-tuples $b_1 b_2 \dots b_N$ with $b_i \in \{0, 1, \dots, n_i - 1\}, n_i \geq 2$, and let two vertices be adjacent if the corresponding tuples differ in precisely one place. Such a graph is called a Hamming graph. It is well-known fact that a graph G is a Hamming graph if and only if it can be written in the form $\otimes_{i=1}^{n} K_{n_i}$. In the following example, the vertex and edge PI indices of a Hamming graph is computed.

Example 3.3. *Let G be a Hamming graph with above parameter. Then*

$$PI_v(G) = \prod_{i=1}^{N} n_i^2 \left(N - \sum_{i=1}^{N} \frac{1}{n_i} \right).$$

Example 3.4. *Let Q_n denote the hypercube of dimension n then $PI_v(Q_n) = n2^{2n-1}$.*

Let $H(n, w), w \leq n-1$ be the graph on n vertices consisting of a clique on w vertices and randomly connect $n - w$ pendent to arbitrary vertices of K_w. In [5] the authors obtained a lower bound on the vertex PI index of a connected graph G in terms of the number of vertices (n), edges (m), pendent vertices (p), and clique number (w), and characterize the extremal graphs as the following.

Theorem 3.9. *Let G be a connected graph with n vertices, m edges, p pendent vertices, and clique number $w (w \geq 3)$. Then*

$$PI_v(G) \geq 2m + (n-2)p + (n-w)(w-1),$$

with equality holding if and only if $G \cong K_n$ or $G \cong H(n, w)$.

Let $\{G_i\}_{i=1}^{d}$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The bridge graph $B(G_1, G_2, \dots, G_d) = B(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$ of $\{G_i\}_{i=1}^{d}$ with respect to the vertices $\{v_i\}_{i=1}^{d}$ is a graph obtained from the graphs $G_1, G_2, \dots, G_d$ by connecting the vertices v_i and v_{i+1} by an edge for $i = 1, 2, \dots, d-1$, see Figure 1. Let G be any graph and let v be a vertex of G. We denote the set of all edges $uu' \in E(G)$ such that $d(u, v) = d(u', v)$ by $M_v(G)$. The cardinality of $M_v(G)$ is denoted by $m_v(G)$. The following result was obtained in [26], for the vertex PI index of a bridge graph $B(G_1, G_2, \dots, G_d)$.

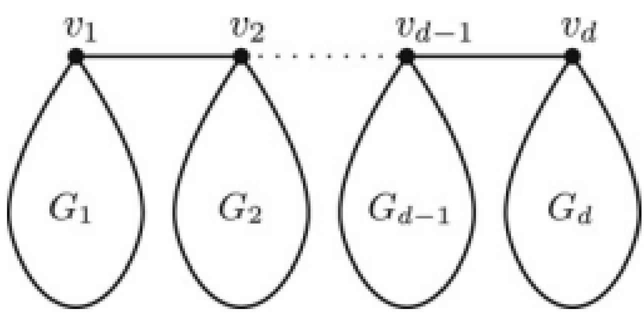

Figure 1. The bridge graph.

Theorem 3.10. *The vertex PI index of the bridge graph $B(G_1, G_2, \ldots, G_g)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is given by*

$$PI_v(G) = \sum_{i=1}^{d} PI_v(G_i) + (|E(G) - m(G))\,|V(G)| - ev(G) + mv(G)\,,$$

where

$$m(G) = \sum_{i=1}^{d} m_{v_i}(G_i),\ ev(G) = \sum_{i=1}^{d} |E(G)||V(G_i)|,\ mv(G) = \sum_{i=1}^{d} m_{v_i}(G_i)|V(G_i)|\,.$$

Corollary 3.2. *Let H be a graph with fixed vertex v. Then the vertex PI index of the bridge graph $G_d(H, v)$ is given by*

$$PI_v(G_d(H,v)) = dPI_v(H) + d(d-1)\,(|E(H)| + 1 - m_v(H))\,|V(H)|\,.$$

The fan molecular graph F_n is a graph obtained by join of the path P_n and a vertex v and the wheel graph W_n is a graph obtained by join the cycle C_n and a vertex v. The PI index of F_n and W_n is obtained as following [34].

Theorem 3.11.

$$PI_v(F_n) = n^2 + 3n - 4 \textit{ and } PI_v(W_n) = n^2 + 3n\,.$$

Let $\{G_i\}_{i=1}^d$ be the set of pairwise disjoint graphs with $v_i, w_i \in V(G_i)$. Then the chain graph $G = C(G_1, \ldots, G_d; v_1, w_1, \ldots, v_d, w_d)$ of $\{G_i\}_{i=1}^d$ with respect to $\{v_i, w_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, \ldots, G_d$ by identifying the vertex w_i and v_{i+1} for $i = 1, 2, \ldots, d-1$ as shown in Figure 2. The vertex PI index of $G = C(G_1, \ldots, G_d; v_1, w_1, \ldots, v_d, w_d)$ is obtained as following [24].

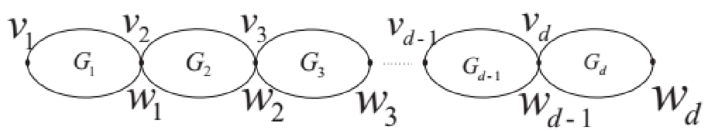

Figure 2. The chain graph.

Theorem 3.12. *Let $G = C(G_1, \ldots, G_d; v_1, w_1, \ldots, v_d, w_d)$ be a chain graph. Then*

$$PI_v(G) = \sum_{i=1}^{d} PI_v(G_i) + \sum_{i=2}^{d} (|E(G_i)| - |M_{v_i}(G_i)|)\,\alpha_i + \sum_{i=1}^{d-1} (|E(G_i)| - |M_{w_i}(G_i)|)\,\beta_i\,,$$

where $\alpha_i = \sum_{j=1}^{i-1} |V(G_j)|$ and $\beta_i = \sum_{j=i+1}^{d} |V(G_j)|$ and $M_v(G)$ is the set of all edges $xy \in E(G)$ such that $d(x,v) = d(y,v)$.

Suppose that v and w are two vertices of a graph H and let $G_i = H$ and $v_i = v, w_i = w$ for $i = 1, 2, \ldots, d$. Then by simple calculation the following result is obtained.

Corollary 3.3. *The vertex PI index of the chain graph $G = C(H, \ldots, H; v, w, \ldots, v, w)$ (d times) is given by*

$$PI_v(G) = dPI_v(H) + \binom{d}{2}(2|E(H)| - |M_v(H)| - |M_w(H)|) .$$

The fullerene ear was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, see [10] for more details. The well-known fullerene, the C_{60} molecule, is a closed cage carbon molecule with three–coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings. Let $p, h, n,$ and$m$ be the number of pentagons, hexagons carbon atoms and bounds between them in a given fullerene. One can see that a fullerene with n carbon atoms has 12 pentagonal, and $n/2 - 10$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20. The vertex PI polynomial of C_{12n+4} fullerenes are computed by Ghorbani [10] as the following.

Theorem 3.13. *The vertex PI polynomial of C_{12n+4} computed as*

$$PI_v(\mathrm{C}_{12n+4}, x) = (18n - 128)x^{12n+4} + 32x^{12n+3} + 48x^{12n+2} + 16x^{12n+1} + 8x^{12n} + 8x^{12n-4}$$
$$+ 8x^{12n-8} + 4x^{12n-20} + 8x^{37} + 2x^{34} .$$

4. The weighted vertex PI index

In order to increase diversity of the PI vertex index for graphs, the authors in [15] introduce weighted version defined as follows

$$PI_w(G) = \sum_{e=uv} (d_G(u) + d_G(v))(n_u(e) + n_v(e)) .$$

For bipartite graphs it holds $n_u(e) + n_v(e) = n$, and therefore the diversity of the original PI index is not satisfying.

The following inequality holds for a graph G with n vertices and m edges [21].

$$PI_v(G) \leq nm$$

with equality if and only if G is bipartite.

Assume that every edge $e = uv$ has weight $d_G(u) + d_G(v)$. Now, if G is a bipartite graph, then

$$PI_w(G) = n \sum_{v \in V(G)} d_G(v)^2 .$$

This means that the weighted vertex PI index is directly connected to the first Zagreb index. Furthermore, it follows that among bipartite graphs path P_n and complete bipartite graph $K_{\lfloor n/2 \rfloor \lceil n/2 \rceil}$ have the minimum and maximum value of weighted vertex PI index, respectively [12]. These values are

$$PI_w(P_n) = n(4n - 6),$$
$$PI_w\left(K_{\lfloor n/2 \rfloor \lceil n/2 \rceil}\right) = n^2 \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil .$$

In the following we give a formula for computing the weighted vertex PI index of a graph where is found in [15].

Lemma 4.1. *Let G be a connected graph. Then*

$$PI_w(G) = \sum_{x \in V} w_x(G) \,,$$

where

$$w_x = \sum_{e=uv \in E, d(x,v) \neq d(x,u)} [d_G(u) + d_G(v)] \ .$$

Also the authors in [15] are found lower and upper bounds for the weighted vertex PI index of a graph as following.

Theorem 4.1. *Let G be a connected graph on n vertices, m edges and diameter d. Then*

$$PI_w(G) \geq 4d^2 - 4d - 2 + 6m \,,$$

with equality if and only if $G \cong P_n$.

Theorem 4.2. *Let G be a connected graph on n vertices. Then*

$$PI_w(G) \geq n(4n-6) \,,$$

with equality if and only if $G \cong P_n$.

Let $e = uv$ be an arbitrary edge, such that it belongs to exactly $t(e)$ triangles. In this case, it easily follows

$$n_u(e) + n_v(e) \leq n - t(e) \,,$$
$$d_G(u) + d_G(v) \leq n + t(e) \ .$$

Therefore we have the following relation

$$PI_w(G) \leq \sum_{e \in E} (n - t(e))(n + t(e)) = n^2 m - \sum_{e \in E} t(e)^2 \ .$$

A complete multipartite graph $K_{n_1, n_2, \ldots, n_k}$ is a graph in which vertices are adjacent if and only if they belong to different partite sets. Let $T_{n,r}$ be the Turán graph which is a complete r-partite graph on n vertices whose partite sets differ in size by at most one. This famous graph appears in many extremal graph theory problems [33]. Nikiforov [30] established a lower bound on the minimum number of r-cliques in graphs with n vertices and m edges (for $r = 3$ and $r = 4$).

Theorem 4.3. *Let G be a connected graph on n vertices, m edges and t triangles. Then*

$$PI_w(G) \leq n^2 m - \frac{9t^2}{m} \,,$$

with equality if and only if $G \cong K_{a,b}$ for $t = 0$, and $G \cong T_{n,r}$ for $r | n$ and $t > 0$.

In the following we consider the Cartesian product of two graphs G and H and we characterize the weighted PI index of the Cartesian product of graphs. These formulas are found in [15].

Theorem 4.4. *Let G and H be two connected graphs. Then*

$$\begin{aligned} PI_w(G \times H) &= |V(G)|^2 PI_w(H) + |V(H)|^2 PI_w(G) \\ &= 4\left(|V(G)||E(G)|PI_v(H) + |V(H)||E(H)|PI_v(G)\right) . \end{aligned}$$

Let $\otimes_{i=1}^{n}(G_i)$ be the Cartesian product of graphs $G_1 \times G_2 \times \cdots \times G_n$ and let $|V(G_i)| = V_i$ and $|E(G_i)| = E_i$ for $i = 1, 2, \ldots, n$.

Theorem 4.5. *Let $G_1, G_2, \ldots, G_n$ be connected graphs. Then*

$$PI_w\left(\bigotimes_{i=1}^{n} G_i\right) = \sum_{i=1}^{n} PI_w(G_i) \prod_{j=1, j\neq i}^{n} V_j^2 + 4 \sum_{i,j=1, i\neq j}^{n} PI_v(G_i) V_j E_j \prod_{k=1, i\neq k\neq j}^{n} V_k^2 .$$

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Wiener Index of Digraphs

Martin Knor[a], **Riste Škrekovski**[b,c,d], **Aleksandra Tepeh**[b,e]

[a]*Slovak University of Technology in Bratislava, Faculty of Civil Engineering, Department of Mathematics, Bratislava, Slovakia*
[b]*Faculty of Information Studies, Novo mesto, Slovenia*
[c]*FMF, University of Ljubljana, Slovenia*
[d]*FAMNIT, University of Primorska, Slovenia*
[e]*Faculty of Electrical Engineering and Computer Science, University of Maribor, Slovenia*
knor@math.sk, skrekovski@gmail.com, aleksandra.tepeh@gmail.com

Abstract

Wiener index (i.e., the total distance or the transmission number), defined as the sum of distances between all unordered pairs of vertices in a graph, is one of the most popular molecular descriptors. Recently we extended this concept to directed graphs that are not necessarily strongly connected. In this chapter we survey our results, conjectures and problems on this topic.

Contents

1. Introduction

Wiener index of a graph G, $W(G)$, is defined as the sum of distances between all (unordered) pairs of vertices of G. It is one of the oldest and most important topological indices, and it was introduced by H. Wiener [29]. Wiener index not only correlates well with many physicochemical properties of organic compounds, it has wide application also outside chemistry, and it became the topic of countless studies also from mathematical point of view. Details can be found in some of many surveys [9, 10, 16, 20, 28].

While new results related to the Wiener index of a graph are constantly being reported, less attention has been devoted to the study of an analogous concept for digraphs, despite its application in sociometry, informetric studies etc. The first results on the Wiener index of digraphs are due to Harary [15], whose investigation was motivated by certain sociometric problems. Ng and Teh [23] found a strict lower bound for the Wiener index of digraphs. Plesník [24] found the lower bound in terms of the number of vertices and the diameter. As in the case of graphs, the Wiener index of digraphs was considered indirectly also through the study of the *average* (or *mean*) *distance*, defined as $\mu(D) = W(D)/n(n-1)$, see [6, 11].

A *directed graph* (or shortly *digraph*) D is given by a set of vertices $V(D)$ and a set of ordered pairs of vertices $A(D)$ called *directed edges* or *arcs*. A *(directed) path* in D is a sequence of vertices $v_0, v_1, \ldots, v_n$ such that $v_{i-1}v_i$ is an arc of D for every $i \in \{1, \ldots, n\}$. By adding the arc $v_n v_0$ to such a path we obtain *a (directed) cycle* $\overrightarrow{C}_n$. For $u \in V(D)$ we denote by $\mathrm{id}_D(u)$ and $\mathrm{od}_D(u)$ the in-degree and out-degree of u, respectively.

The *distance* $d_D(u, v)$ between vertices $u, v \in V(D)$ is the length of a shortest path from u to v, and if there is no such path then we assume

$$d_D(u, v) = 0. \tag{1}$$

For $u \in V(D)$, we will denote $w_D(u) = \sum_{v \in V(D)} d_D(u, v)$. We omit the index D when no confusion is likely.

In analogy to graphs, the Wiener index $W(D)$ of a digraph D is defined as the sum of all distances, where of course, each ordered pair of vertices has to be taken into account, since the distances $d_D(u, v)$ and $d_D(v, u)$ may be different. More precisely,

$$W(D) = \sum_{(u,v) \in V(D) \times V(D)} d_D(u, v) = \sum_{u \in V(D)} w_D(u).$$

In [17] we have the following simple observation.

Observation 1.1. *Let D be a digraph and let D^- be the reverse of D obtained by reversing the orientation of all arcs of D. Then $W(D) = W(D^-)$.*

Note that in real directed networks, there could be no path connecting some pairs of vertices. From theoretical point of view it is natural to define the distance between such a pair of vertices to be infinite and thus the study of the Wiener index of digraphs in pure mathematical papers is usually limited to *strongly connected* digraphs, i.e. digraphs for which a directed path between every pair of vertices exists. However, for practical purposes, the distance between two vertices in a digraph can be defined in a different way. For instance, Botafogo et al. [3] defined it as the number of vertices in the analyzed network, while Bonchev [1, 2] already assumed the condition (1).

Under the condition (1) several interesting properties of digraphs (general, not only strongly connected) can be proved. For instance, in Section 2 the famous Wiener theorem as well as a relation between the Wiener index and betweenness centrality is extended to digraphs. Thus, in this way, the Wiener index could be applicable in the topics of directed large networks, particularly because with this measure, one assigns finite values to the average distance and betweenness centrality of the nodes in a directed network. In next sections we summarize other interesting properties of the Wiener index of oriented graphs and open questions related to them. Details can be found in papers [17–19], which represent the basis of this chapter.

2. Wiener theorem and betweenness centrality relation

In [29], Wiener proved that for a tree T

$$W(T) = \sum_{e=ij\in E(T)} n_e(i)n_e(j),$$

where $n_e(i)$ and $n_e(j)$ are the orders of components of $T - ij$. The result is known as the Wiener theorem. An analogous statement for *directed trees*, i.e. digraphs whose underlying graphs are trees, was proved in [19]. Let $T(a)$ denote the set of vertices x with the property that there exists a directed path from x to a. Similarly, let $S(a)$ denote the set of vertices x with the property that there exists a directed path from a to x. Note that $a \in S(a)$ and $a \in T(a)$. Let $t(a) = |T(a)|$ and $s(a) = |S(a)|$.

Theorem 2.1. *Let T be a directed tree. Then*

$$W(T) = \sum_{ab\in A(T)} t(a)s(b).$$

White and Borgatti [30] generalized Freeman's geodesic centrality measures for betweenness on graphs to the case of digraphs. The *(directed) betweenness centrality* $B(x)$ of a vertex x in a digraph D is defined as

$$B(x) = \sum_{\substack{u,v\in V(D)\setminus\{x\}\\ u\neq v}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}},$$

where $\sigma_{u,v}$ denotes the number of all shortest directed paths in D from u to v and $\sigma_{u,v}(x)$ stands for the number of all shortest directed paths from u to v passing through the vertex x. Note that in the definition of $B(x)$ we consider only such ordered pairs (u, v) for which there exists a directed uv-path in D, i.e., for which $\sigma_{u,v} \neq 0$.

Gutman and Škrekovski [13] showed the following result.

Theorem 2.2. *For every connected graph G the following holds*

$$W(G) = \sum_{x\in V(G)} B(x) + \binom{n}{2}.$$

This formula shows that the Wiener index is related to the betweenness centrality. In [19] the above relation was extended to directed graphs. Let $P(D)$ denote the set of ordered pairs (u, v) such that there exists a directed path from u to v in D, and let $p(D) = |P(D)|$.

Theorem 2.3. *For any digraph D of order n*

$$W(D) = \sum_{x \in V(D)} B(x) + p(D).$$

Since in a strongly connected digraph there is a directed path between every ordered pair of vertices, we derive the following.

Corollary 2.1. *Let D be a strongly connected digraph of order n. Then*

$$W(D) = \sum_{x \in V(D)} B(x) + 2\binom{n}{2}.$$

3. Extremal values of Wiener index

It is obvious that the minimum possible value of the Wiener index of a digraph cannot be less than the number of edges in the underlying graph. This lower bound can always be achieved for bipartite graphs by orienting all edges of such a graph G so that the corresponding arcs go from one bipartition to the other. In such a case we obtain a digraph D with $W(D) = |E(G)|$. Thus the minimum value of Wiener index for a digraph on n vertices, such that the underlying graph is connected, is $n - 1$. Moreover, it is attained when the underlying graph is a tree. We further discuss digraphs with minimum Wiener index in Subsection 5.5.

Regarding the upper bound, Plesník [24] proved that for strongly connected digraphs D on n vertices the upper bound for the Wiener index is achieved if and only if D is a directed cycle. It can be observed that the same holds also when not restricted to strongly connected digraphs.

Proposition 3.1. *Let D be a directed graph (not necessarily strongly connected) on n vertices. Then*

$$W(D) \leq n\binom{n}{2}$$

with equality holding if and only if D is the directed cycle $\overrightarrow{C}_n$.

Proof. Observe that $w_D(u)$ is the greatest if all vertices are achievable from u and when there is a unique vertex at distance i from u, $1 \leq i \leq n-1$. That is, $w_D(u) \leq 1+2+\cdots+(n-1) = \binom{n}{2}$ for any $u \in V(D)$. This gives $W(D) \leq \binom{n}{2}n$ and if the equality is attained, then $\mathrm{od}_D(u) = 1$ for every vertex $u \in V(D)$. By Observation 1.1 we have $W(D^-) = W(D)$. Hence, if $W(D) = \binom{n}{2}n$, then also $W(D^-) = \binom{n}{2}n$, and so $\mathrm{od}_{D^-}(u) = 1$ for every $u \in V(D^-)$. This gives that if $W(D) = \binom{n}{2}n$, that is if the Wiener index is maximum possible in D, then $\mathrm{id}_D(u) = \mathrm{od}_D(u) = 1$ for every $u \in V(D)$, and so D is the directed cycle. ■

In [18] digraphs with the second maximum Wiener were considered. By $\overrightarrow{C}_n^+$ we denote a digraph obtained from $\overrightarrow{C}_n$ by adding the arc vu, where uv is an arc in $\overrightarrow{C}_n$ and by $\overleftrightarrow{P}_3$ we denote a digraph obtained from the undirected path on 3 vertices by replacing every edge by a pair of opposite arcs, see Figure 1.

Theorem 3.2. *Among all digraphs on $n \geq 4$ vertices, the digraph $\overrightarrow{C}_n^+$ is the unique digraph with the second maximum Wiener index and $W(\overrightarrow{C}_n^+) = \binom{n}{2}n - n + 2$.*

Regarding the case $n = 3$, two graphs, namely $\overrightarrow{C}_3^+$ and $\overleftrightarrow{P}_3$, attain the second maximum value. Note that both $\overrightarrow{C}_n^+$ and $\overleftrightarrow{P}_3$ contain pairs of opposite arcs. Therefore, these digraphs cannot be obtained as orientations of undirected simple graphs.

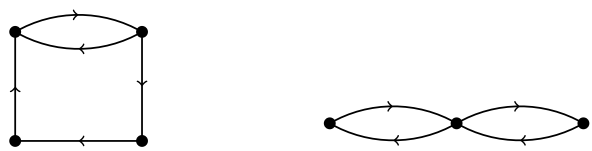

Figure 1. Two digraphs with opposite pairs of arcs.

Since the Wiener index in directed graphs is considered mainly for orientations of undirected simple graphs, in what follows we focus our attention to digraphs which do not contain opposite arcs. Such digraphs are called *antisymmetric*. To state our results for antisymmetric digraphs, we need to define orientations of so called theta-graphs.

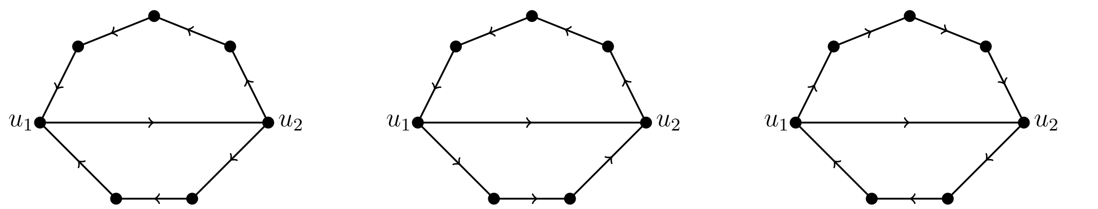

Figure 2. Orientations of theta-graph $\Theta_{3,1,0}$.

Let $a \geq b \geq c \geq 0$ and $b \geq 1$. By $\Theta_{a,b,c}$ we denote a *theta-graph*, a graph obtained when two vertices, say u_1 and u_2, are joined by three paths P_a, P_b, P_c of length $a+1$, $b+1$ and $c+1$, respectively. Then $\Theta_{a,b,c}$ has $a+b+c+2$ vertices. We consider three orientations of $\Theta_{a,b,c}$, namely $\overrightarrow{\Theta}_{a^-,b^-,c}$, $\overrightarrow{\Theta}_{a^-,b^+,c}$ and $\overrightarrow{\Theta}_{a^+,b^-,c}$. In all these orientations the path of length $c+1$ is directed from u_1 to u_2 and the other two paths are also directed. The superscript $+$ indicates that the corresponding path is directed from u_1 to u_2, while the superscript $-$ indicates that the corresponding path is directed from u_2 to u_1, see Figure 2 for $\overrightarrow{\Theta}_{3^-,2^-,0}$, $\overrightarrow{\Theta}_{3^-,2^+,0}$ and $\overrightarrow{\Theta}_{3^+,2^-,0}$ (displayed from left to right). In [18] we proved the following theorem.

Theorem 3.3. *Among all antisymmetric digraphs on $n \geq 6$ vertices, the digraph $\overrightarrow{\Theta}_{(n-3)^+,1^-,0}$ has the second maximum Wiener index and $W(\overrightarrow{\Theta}_{(n-3)^+,1^-,0}) = \binom{n}{2}n - 3n + 9$. Moreover, $\overrightarrow{\Theta}_{(n-3)^+,1^-,0}$ is the unique digraph with this property.*

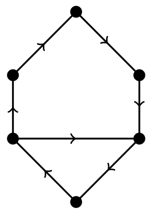

Figure 3. An orientation of $\Theta_{3^+,1^-,0}$.

In Figure 3 the unique digraph among antisymmetric digraphs on 6 vertices with the second maximal Wiener index is depicted. Regarding the cases $n = 4$ and $n = 5$ we have the following. If $n = 4$, then it turns out that there are two antisymmetric digraphs with the second maximum Wiener index, namely $\overrightarrow{\Theta}_{1^+,1^-,0}$ and $\overrightarrow{\Theta}_{1^-,1^-,0}$. If $n = 5$, then there are three antisymmetric digraphs with the second maximum Wiener index, namely $\overrightarrow{\Theta}_{2^+,1^-,0}$, $\overrightarrow{\Theta}_{2^-,1^+,0}$ and $\overrightarrow{\Theta}_{1^+,1^-,1}$.

4. Bounds on Wiener index for prescribed graphs

Let G be a given graph. Note that it has $2^{|E(G)|}$ orientations, and each one yields a digraph with some value of Wiener index. It is natural to ask what can be the maximum and the minimum of these values. Let $W_{\max}(G)$ and $W_{\min}(G)$ be the maximum possible and the minimum possible, respectively, Wiener index among all digraphs obtained by orienting the edges of G.

Figure 4. Two extremal orientations of a path on five vertices.

For example, in Figure 4, we have orientations of P_5 with the biggest and the smallest Wiener index $W_{\max}(P_5) = 20$ and $W_{\min}(P_5) = 4$. In [17], the following problems where posed.

Problem 4.1. *For a given graph G find* $W_{\max}(G)$ *and* $W_{\min}(G)$.

Problem 4.2. *For a given graph G, what is the complexity of finding* $W_{\max}(G)$ *(resp.* $W_{\min}(G)$*)? Are these problems NP-hard?*

The above problems have already been considered for strongly connected orientations. Plesník [24] proved that finding a strongly connected orientation of a given graph G that minimizes the Wiener index is NP-hard. Note that this does not solve the case for non-necessarily strongly connected digraphs.

In what follows we turn our attention to specific families of graphs. In a subsection about tournaments we will see that the orientation of a complete graph which attains the maximum value is strongly connected. The same was observed when searching for the maximum and second maximum Wiener index for digraphs on n vertices. However, using theta-graphs we described that this is not always the case. On the other hand, it is our strong conjecture that the minimum value of Wiener index must be attained for some acyclic orientation.

4.1 Tournaments

Transitive tournaments, i.e. acyclic orientations of complete graphs K_n, clearly yield the smallest possible Wiener index among all orientations of complete graphs. To see this, note that for any two vertices a an b in K_n we have

$$d_D(a,b) + d_D(b,a) \geq 1 \tag{2}$$

for any orientation D of K_n, and to obtain equality in (2) for all pairs a and b, D must be acyclic. Hence, $W_{\min}(K_n) = \binom{n}{2} = W(K_n)$.

Plesník [24] gave a sharp upper bound for the Wiener index of strongly connected tournaments. He proved that if T_n is a strongly connected tournament with $n \geq 3$ vertices, then $W(T_n) \leq \binom{n+2}{3} - 1$. In addition, he showed that the equality is achieved if and only if T_n is the tournament of diameter $n-1$. Note that for each $n \geq 3$ (up to isomorphism) there exists exactly one tournament of diameter $n-1$. We call it a *Hamiltonian-path* tournament and we denote it by H_n. It can be described as the digraph with vertices $v_1, v_2, \ldots, v_n$ in which $v_j v_i$ is an arc for every $i < j$ unless $j = i+1$ in which case H_n has the arc $v_i v_j$.

Moon [22] strengthened the result of Plesník by deriving a bound that involves an additional parameter which enabled him to characterize tournaments of order at least 5 with the second maximal Wiener index. These are two types of tournaments that can be obtained from H_n, $n \geq 5$, as follows: to obtain H_n^1, in H_n we reverse the direction of the arc $v_n v_{n-2}$, and to obtain H_n^2 we reverse the direction of the arcs $v_n v_3, v_n v_4, \ldots, v_n v_{n-2}$ (note that H_5^1 and H_5^2 are isomorphic). The result of Moon states that if T_n is a strongly connected tournament with $n \geq 5$ vertices and T_n is not isomorphic to a Hamiltonian-path tournament H_n, then $W(T_n) \leq \binom{n+2}{3} - n + 3$, where the equality is achieved exactly in the case of tournaments H_n^1 and H_n^2.

In [17] the results of Plesník and Moon were extended to the class of all tournaments (not necessarily strongly connected).

Theorem 4.3. *Let T_n be a tournament with at least 3 vertices which is not-necessary strongly connected. Then we have the following:*

- $W(T_n) \leq \binom{n+2}{3} - 1$ *and the equality is attained if and only if T_n is the Hamiltonian-path tournament H_n.*

- *if T_n has at least 5 vertices and is not isomorphic to a Hamiltonian-path tournament, then $W(T_n) \leq \binom{n+2}{3} - n + 3$ with equality holding only if T_n is isomorphic to H_n^1 or H_n^2.*

4.2 Theta–graphs

As mentioned above, the motivation for studying theta-graphs originally comes from an intuition that orientations of digraphs which achieve the maximum Wiener index should be strongly connected. In such orientations P_a must be a directed path and the same holds for P_b and P_c. By symmetry (also by Observation 1.1), we can fix the orientation of P_c, say from u_1 towards u_2 and consequently we obtain only three orientations of $\Theta_{a,b,c}$ which are strongly connected, namely $\overrightarrow{\Theta}_{a^-,b^-,c}$, $\overrightarrow{\Theta}_{a^-,b^+,c}$ and $\overrightarrow{\Theta}_{a^+,b^-,c}$, considered already in Section 3. Observe that if $a = b$ then $\overrightarrow{\Theta}_{a^-,b^+,0}$ and $\overrightarrow{\Theta}_{a^+,b^-,0}$ are isomorphic, hence we do not distinguish them in the next theorems. In [17] the orientation with the maximum Wiener index among strongly connected orientations of $\Theta_{a,b,c}$ was identified.

Theorem 4.4. *Among strongly connected orientations of* $\Theta_{a,b,c}$, $\overrightarrow{\Theta}_{a^+,b^-,c}$ *has the maximum Wiener index unless* $a \neq b$ *and* $ab - c(a+b) - c^2 - 2c - 2 < 0$ *in which case the maximum Wiener index is attained by* $\overrightarrow{\Theta}_{a^-,b^+,c}$.

Next theorem shows that the orientation of a theta-graph $\Theta_{a,b,c}$ that attains maximum value is strongly connected if $c = 0$.

Theorem 4.5. *Let* $\overrightarrow{\Theta}_{a,b,0}$ *be an orientation of* $\Theta_{a,b,0}$. *Then* $W(\overrightarrow{\Theta}_{a,b,0}) \leq W(\overrightarrow{\Theta}_{a^+,b^-,0})$. *Moreover, if* $W(\overrightarrow{\Theta}_{a,b,0}) = W(\overrightarrow{\Theta}_{a^+,b^-,0})$, *then* $\overrightarrow{\Theta}_{a,b,0}$ *is strongly connected.*

However, already for $c = 1$ it turns out that the orientation yielding the maximum Wiener index need not be strongly connected. By reversing the orientation of u_1z_1 in $\overrightarrow{\Theta}_{a^+,b^-,1}$, we obtain a specific orientation which we denote by $\overrightarrow{\Theta}^+_{a,b,1}$ (in Figure 5, $\overrightarrow{\Theta}^+_{3,2,1}$ is depicted). Obviously, $\overrightarrow{\Theta}^+_{a,b,1}$ is not strongly connected since z_1 is its source. Nevertheless, for some values of a and b this orientation achieves the maximum Wiener index.

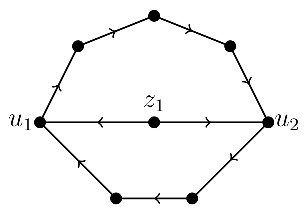

Figure 5. An orientation of $\Theta_{3,2,1}$.

Theorem 4.6. *Let* $\overrightarrow{\Theta}_{a,b,1}$ *be a non-strongly-connected orientation of* $\Theta_{a,b,1}$ *which is different from* $\overrightarrow{\Theta}^+_{a,b,1}$ *and also from* $(\overrightarrow{\Theta}^+_{a,b,1})^-$. *Then* $W(\overrightarrow{\Theta}_{a,b,1}) < W(\overrightarrow{\Theta}^+_{a,b,1})$ *or* $W(\overrightarrow{\Theta}_{a,b,1}) < W(\overrightarrow{\Theta}_{a^+,b^-,1})$.

Thus in several cases still strongly connected orientation has the maximum Wiener index. However, if $b \geq a^{1/2+\varepsilon}$ for fixed $\varepsilon > 0$, then for a big enough, non-strongly-connected orientation $\overrightarrow{\Theta}^+_{a,b,1}$ attains the maximum. More precisely, we obtained the following characterization.

Corollary 4.1. *The orientation of* $\Theta_{a,b,1}$ *which results in the maximum Wiener index is not strongly connected if and only if*

(a) $ab^2 - a^2 - ab - 2b^2 - 5a - 10b - 10 > 0$*, or*

(b) $ab^2 - a^2 - ab - 2b^2 - 5a - 10b - 10 = 0$ *and the orientation of* $\Theta_{a,b,1}$ *is not isomorphic to* $\overrightarrow{\Theta}_{a^+,b^-,1}$.

An interested reader is referred to [17] for more detailed description how orientations and parameters a, b influence the value of the Wiener index of a directed graph whose underlying graph is $\Theta_{a,b,1}$.

Similarly, it can be shown that if a is big comparing to c and $b \geq a^{1/2+\varepsilon}$, then the orientation of $\Theta_{a,b,c}$ which achieves the maximum Wiener index is not strongly connected if $c \geq 2$. The reason is that for a and b satisfying these conditions the strongly connected orientation of $\Theta_{a,b,c}$ with maximum Wiener index is $\overrightarrow{\Theta}_{a^+,b^-,c}$ (see Theorem 4.4) and $2W(\overrightarrow{\Theta}_{a^+,b^-,c}) = a^3 + 3a^2b + 2ab^2 + b^3 + (2c+5)a^2 + (4c+7)ab + (3c+5)b^2 + (2c^2+8c+6)a + (3c^2+10c+8)b + c^3 + 5c^2 + 8c + 4$. However, if we orient the u_1u_2-paths of lengths $a+1$ and $b+1$ to obtain a directed cycle and the u_1u_2-path of length $c+1$ to obtain a subdigraph, not isomorphic to a directed path, then for the resulting digraph $\overrightarrow{\Theta}^+_{a,b,c}$ we have $2W(\overrightarrow{\Theta}^+_{a,b,c}) \geq 2(a+b+2)\binom{a+b+2}{2} = a^3 + 3a^2b + 3ab^2 + b^3 + 5a^2 + 10ab + 5b^2 + 8a + 8b + 4$. Now comparing the coefficients at the highest powers of a and b gives the result. Thus the orientation of $\Theta_{a,b,c}$ which achieves the maximum Wiener index is not strongly connected if $c \geq 2$.

5. Some conjectures

In what follows we will state several conjectures about Wiener index of directed graphs. This research area is rich with problems as even for a given graph one has many orientations and to find the one with the maximum or minimum Wiener index can be a real challenge. All these problems bring us the following metahypotheses:

- orientations with large Wiener index should have long cycles or/and paths,
- orientations with small Wiener index should not have cycles, and directed paths should be short.

5.1 Theta–graphs conjecture

As we pointed out before, the maximum Wiener index of theta-graphs is not necessarily obtained for a strongly connected orientation. However, we believe it must contain the longest possible cycle.

Conjecture 5.1. *Let* $a \geq b \geq c$*. Then* $W_{\max}(\Theta_{a,b,c})$ *is attained by an orientation of* $\Theta_{a,b,c}$ *in which the union of the* u_1u_2*-paths of lengths* $a+1$ *and* $b+1$ *forms a directed cycle.*

Analogous statement possibly holds also for other graphs which are not very dense and which admit an orientation with one huge directed cycle without “shortcuts”, that is without directed paths shortening the cycle.

5.2 No–zig–zag conjecture

A vertex v in a directed tree T is *core* if for every vertex u of T, there exists either a directed path from u to v or a directed path from v to u. Notice that then in each component C of $T - v$ all edges point in the direction towards v or all edges point in the direction from v. See Figure 6 for an example of a directed tree with two core vertices and a directed tree that does not contain any core vertex. A different view of the very same notion can be described as follows. An orientation of a tree is called *no-zig-zag* if there is no subpath in which edges change the orientation twice. Note that a directed tree has a core vertex if and only if its orientation is no-zig-zag.

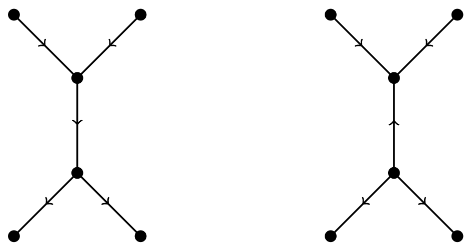

Figure 6. The graph on the left has two core vertices, while the right one has no core vertex.

In [19] we have the following conjecture.

Conjecture 5.2. *Let T be a tree. Then every orientation of T achieving the maximum Wiener index is no-zig-zag.*

This conjecture is valid for

- trees on at most 10 vertices,
- subdivision of stars,
- $T_{a,b,c}$ trees - obtained from two stars $K_{1,a}$ and $K_{1,b}$, central vertices of which are connected by a path of length c.

5.3 Chordal graphs conjecture

Theta-graphs have long induced cycles and low connectivity. Examples with higher connectivity can easily be derived from theta-graphs, by the lexicographic product

$$L(a, k) = \Theta_{a,a,2}[K_k]$$

with $a >> k$. The graph $L(a, k)$ is $2k$-connected, and in a similar way as for theta-graphs, one can show that $W_{\max}(L(a, k))$ is attained for a non-strongly connected orientation. On the other hand, we were not able to find examples without long induced cycles which makes us wonder if the following holds.

Conjecture 5.3. *Let G be a 2-connected chordal graph. Then $W_{\max}(G)$ is attained by an orientation which is strongly connected.*

5.4 Ladder graphs conjecture

Our intuition about long cycles and paths tells us that the following conjecture may hold. Of course it would be even more interesting to consider it for meshes of order $m \times n$, and not only of order $2 \times n$ (i.e. so called ladder graphs).

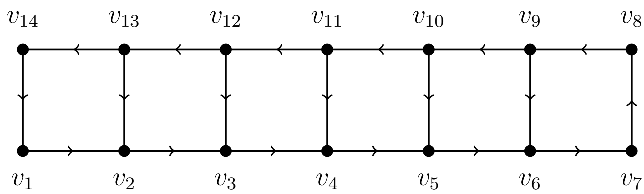

Figure 7. An orientation of the ladder graph $P_2 \Box P_7$ with large Wiener index.

Conjecture 5.4. *Let $G = P_2 \Box P_n$ be a ladder graph. Then $W_{\max}(G)$ is attained by an orientation that has a hamiltonian cycle $v_1 v_2 \cdots v_{2n}$, and every other remaining edge $v_i v_{2n+1-i}$, where $1 < i < n$, is oriented from v_{2n+1-i} to v_i.*

In Figure 7 we have an orientation of $P_2 \Box P_7$ described in the above conjecture.

5.5 Acyclic orientations conjecture

Another problem is to find an orientation of a graph that yields the minimum possible Wiener index. As already mentioned in the introduction, Plesník [24] proved that this problem is NP-hard for strongly connected orientations of graphs. However, one might consider the following conjecture from [19].

Conjecture 5.5. *For every graph G, the value $W_{\min}(G)$ is achieved for some acyclic orientation of G.*

This conjecture is valid for

- bipartite graphs,
- unicyclic graphs,
- the Petersen graph,
- prisms.

5.6 Chromatic conjecture

Our next conjecture is motivated by the following well-known Gallai-Hasse-Roy-Vitaver theorem.

Theorem 5.1. *Let G be a graph. A number k is the smallest number of colors admitting a proper coloring of G if and only if k is the largest number for which every orientation of G contains a simple directed path with k vertices. The orientations for which the longest path has the minimum length always include at least one acyclic orientation.*

In other words, the chromatic number $\chi(G)$ is one plus the length of a longest path in a special orientation of the graph which minimizes the length of a longest path.

A graph orientation is called *k-coloring-induced*, if it is obtained from some proper k-coloring by orienting every edge from the vertex with the bigger color to the vertex with the smaller color.

Conjecture 5.6. *$W_{\min}(G)$ is achieved for a $\chi(G)$-coloring-induced orientation.*

This conjecture is valid for the same graphs for which the acyclic Conjecture 5.5 is confirmed. In fact, the chromatic conjecture implies the acyclic conjecture.

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An Overview on Randić (Normalized Laplacian) Spread

Enide Andrade[a], **Maria Aguieiras A. de Freitas**[b],
María Robbiano[c], **B. San Martín**[c]

[a]*CIDMA – Center for Research and Development in Mathematics and Applications, Department of Mathematics, University of Aveiro, 3810-193 Aveiro, Portugal*

[b]*Instituto de Matemática and COPPE/Produção Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil*

[c]*Departamento de Matemáticas, Universidad Católica del Norte, Av. Angamos, 0610 Antofagasta, Chile*

enide@ua.pt, maguieiras@im.ufrj.br, mrobbiano@ucn.cl

Abstract

The definition of Randić matrix comes from a molecular structure descriptor introduced by Milan Randić in 1975, known as Randić index. The plethora of chemical and pharmacological applications of the Randić index, as well as numerous mathematical investigations are well known and presented in the literature. In spite of its connection with Randić index this matrix seems to have not been much studied in mathematical chemistry however, some graph invariants related with this matrix such as Randić energy (the sum of the absolute values of the eigenvalues of the Randić matrix), the concept of Randić spread (that is, the maximum difference between two eigenvalues of the Randić matrix, disregarding the spectral radius) were recently introduced and some of their properties were established. We review some topics related with the graph invariant Randić spread, such as bounds that were obtained from matrix and/or numerical inequalities establishing relations between this spectral parameter and some structural parameters of the underlying graph. Moreover, some new bounds for the Randić spread are obtained. Comparisons with some upper bounds for the Randić spread of regular graphs are done. Finally, a possible relation between Randić spread and Randić energy is established.

Contents

1. Randić index and Randić matrix

The aim of this paper is to present an outline of previously established bounds for the *Randić spread* known in literature as *normalized Laplacian spread* ([27]). This concept is related with the so-called graph matrix *Randić matrix*. We describe briefly how this matrix appeared but, firstly we recall the concept of Randić index.

In Chemistry, some molecular properties depend on their shape and vary in a regular way within a series of similar components. The degree of branching of a molecular skeleton is a critical factor. The boiling points of the hydrocarbon molecules and the retention volumes or the retention times obtained from the chromatographic studies are typical factors for this kind of correlation. Therefore, the degree of branching and the molecular size are related with the magnitude of this correlation. The molecular topology is important to characterize some of these chemical experimental quantities. Therefore, in order to develop a procedure that can characterize in a quantitatively way the degree of a molecular branching of a carbon-atom skeleton of saturated hydrocarbons, in 1975 Milan Randić [45] invented a molecular structure descriptor (topological index) that the author called "branching index" (the name came from the previous purpose), and which later became known under the name "connectivity index" or "Randić index". In many references in the contemporary mathematical and mathematical–chemical literature, the Randić index is usually denoted by R (see [16, 21–23, 34, 35, 37]) however, we will use this symbol for the Randić matrix and therefore we return here to Randić's original notation χ [45]. For a (chemical) graph $G = (V(G), E(G))$ the Randić index is defined as the sum over all edges $ij \in E(G)$ of $\frac{1}{\sqrt{d_i\, d_j}}$, where d_i denotes the degree of a vertex i, that is:

$$\chi = \chi(G) = \sum_{ij \in E(G)} \frac{1}{\sqrt{d_i\, d_j}}\,. \tag{1}$$

For a regular graph G with n vertices, it is easily checked that

$$\chi(G) = \frac{n}{2}. \tag{2}$$

The chemical and pharmacology applications of this graph invariant are known and very well documented and the reader must be referred, for instance, to [22, 33–35, 37, 46] and the references cited therein.

The Randić index happens to be the first in a long series of vertex–degree based structure descriptors encountered and studied in contemporary mathematical chemistry; for details the readers must be referred to [16, 21, 23].

It is worth to mention some applications to medicine of this topological index, see for instance, J. Aguiló, A. Figueras, A. Freire, F. Martín, C. R. Munteanu, A. Pazos. Nuevas Fronteras Tecnológicas. Redes Nanoroadmap e IBERO-NBIC 2010, in [42]. Nowadays, the cancer can be theoretical predictable using the sequence of graphs obtained from the proteins and the studies of the mass protein spectrum. In fact, the Randić index can be used in studies that predict the colorectal and breast cancer. This molecular descriptor was used in the statistical methods to find classification models that can predict if a new protein is related with the two previous type of cancers.

Back to Eq. (1), a graph matrix $\mathbf{R} = \mathbf{R}(G) = (r_{ij})$, where $r_{ij} = 1/\sqrt{d_i\, d_j}$ if $ij \in E(G)$, and zero otherwise was conceived. The matrix $\mathbf{R}$ was called Randić matrix, terminology justified by the previous relation. If $\mathbf{D} = \mathbf{D}(G)$ is the diagonal matrix of the vertex degrees of a graph G without singletons, the diagonal matrix $\mathbf{D}^{-1/2}$ is well defined and the Randić matrix (see e.g. [7, 8]) satisfies

$$\mathbf{R}(G) = \mathbf{D}^{-1/2}\mathbf{A}\,(G)\,\mathbf{D}^{-1/2}, \tag{3}$$

where $\mathbf{A}\,(G)$ stands for the adjacency matrix of G. But this matrix (without any name and without any mention to the Randić Index) was found already in the seminal book by Cvetković, Doob and Sachs [12] (p. 26).

The matrix

$$\mathcal{L} = \mathcal{L}(G) = \mathbf{D}^{-1/2}\,\mathbf{L}(G)\,\mathbf{D}^{-1/2},$$

where $\mathbf{L}(G)$ denotes the Laplacian matrix of G, is the "normalized Laplacian matrix" For comprehensive literature of the mathematical properties of this matrix see the book F. Chung, *Spectral Graph Theory*, Am. Math. Soc., Providence, 1997, [11].

It is easy to see that

$$\mathcal{L}(G) = \mathbf{I}_n - \mathbf{R}(G), \tag{4}$$

establishing a relation between the eigenvalues of the Randić matrix and those of the normalized Laplacian matrix. We list here some known facts concerning these matrices.

Facts:

1. λ is a Randić eigenvalue of G if and only if $1 - \lambda$ is a normalized Laplacian eigenvalue of G.

2. The normalized Laplacian matrix is positive semidefinite (see [11]). This implies that for graphs with at least one edge, $\lambda = 1$ is the greatest Randić eigenvalue.

3. The vector $\mathbf{w} = \mathbf{D}^{1/2}\,\mathbf{e}$, where $\mathbf{e}$ is the all ones vector, is an eigenvector of the Randić matrix for the eigenvalue $\lambda = 1$ and also of the normalized Laplacian matrix for eigenvalue $\lambda = 0$.

4. For connected graphs G, $\mathbf{R}(G)$ is a nonnegative irreducible matrix.

5. For an arbitrary graph G, the multiplicity of $1 \in \sigma(\mathbf{R}(G))$, where $\sigma(\mathbf{R}(G))$ denotes the set of eigenvalues of $\mathbf{R}(G)$, corresponds to the number of connected components of G which are not singletons.

6. For bipartite graphs, the Randić spectra is union of sets $\{\lambda, -\lambda\}$ with λ being real.

In connection with the Randić index, the matrix $\mathbf{R}$ seems to be first time used in 2005 by Rodríguez, who referred to it as the "weighted adjacency matrix" [47] and the "degree adjacency matrix" [48]. The matrix was regarded as an adjacency matrix where the weight of the edge ij is $\frac{1}{\sqrt{d_i d_j}}$, justifying then the terminology used.

In 2010, the new concept of *Randić energy* [7, 8], equals to the sum of absolute values of the eigenvalues of $\mathbf{R}$, appeared and was motivated from a systematic study of spectral properties of the Randić matrix, [5–8,10,15,28–30,49]. Independently, based on the matrix $\mathcal{L}$, the "normalized Laplacian energy" appeared in [10], which is exactly the same as the Randić energy.

2. The Randić spread. Definition

We start this section recalling the definition of the spread, $s\left(\mathbf{M}\right)$, of an $n \times n$ complex matrix $\mathbf{M}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$:

$$s(\mathbf{M}) = \max_{i,j} |\lambda_i - \lambda_j|, \tag{5}$$

where the maximum is taken over all pairs of eigenvalues of $\mathbf{M}$.

This parameter appears in literature in many references, see for instance [3, 32, 39, 40, 44]. The following upper bound for the spread of a square matrix $\mathbf{M}$ was given in [40]

$$s^2\left(\mathbf{M}\right) \leq 2\left|\mathbf{M}\right|^2 - \frac{2}{n}\left|\text{trace}\left(\mathbf{M}\right)\right|^2, \tag{6}$$

with $|\mathbf{M}|^2 = \text{trace}(\mathbf{M}^*\mathbf{M})$, where $\mathbf{M}^*$ is the transconjugate of $\mathbf{M}$. In [18] it was introduced the concept of *Randić spread*. Therefore, considering the definition in (5), the definition of the spread of a graph was defined as the spread of its adjacency matrix [20]. However, in the particular case of the Randić matrix and normalized Laplacian matrix, the Randić spread of the graph was not considered as the spread of the Randić matrix (analogously, the concept of normalized Laplacian spread was modified) attending to the following facts from [18].

Facts:

1. For the Laplacian and normalized Laplacian matrices, the smallest eigenvalue is always equal to zero.

2. For the Randić matrix of a graph with at least one edge, the greatest eigenvalue is always equal to unity.

3. Using the concept (5), $s(\mathbf{L})$ and $s(\mathcal{L})$ are equal to the spectral radii of the respective matrices and in the literature there are many results on the greatest eigenvalues of $\mathbf{L}$ and $\mathcal{L}$, i.e., on their spectral radii, especially upper bounds (see for instance [50, 52]).

4. $s(\mathbf{R})$ is equal to 1 minus the smallest Randić eigenvalue, and, in addition, is equal to $s(\mathcal{L})$.

5. For all bipartite graphs, $s(\mathbf{R}) = 2$.

Note that, using the definition of spread for these matrices, this concept becomes trivial and uninteresting. In order to address these difficulties, the concepts of $s(\mathbf{L})$, $s(\mathcal{L})$ and $s(\mathbf{R})$, were modified.

Taking into account that the smallest eigenvalue of the Laplacian matrix of a graph G is zero, and that the second smallest eigenvalue is the algebraic connectivity of G (which is an important algebraic measure of the connectivity of a graph [2, 14]), the "Laplacian spread" was defined in [13]

$$spr_{\mathbf{L}}(G) = \max\left\{|\lambda_i(\mathbf{L}) - \lambda_j(\mathbf{L})| : \lambda_i(\mathbf{L}), \lambda_j(\mathbf{L}) \in \sigma(\mathbf{L}(G)) \setminus \{0\}\right\}. \tag{7}$$

In an analogous manner, [27], the normalized Laplacian spread of G is

$$spr_{\mathcal{L}}(G) = \max\left\{|\lambda_i(\mathcal{L}) - \lambda_j(\mathcal{L})| : \lambda_i(\mathcal{L}), \lambda_j(\mathcal{L}) \in \sigma(\mathcal{L}(G)) \setminus \{0\}\right\}. \tag{8}$$

In parallel with definitions (7) and (8), the Randić spread was defined in [18] as

$$spr_{\mathbf{R}}(G) = \max\left\{|\lambda_i(\mathbf{R}) - \lambda_j(\mathbf{R})| : \lambda_i(\mathbf{R}), \lambda_j(\mathbf{R}) \in \sigma(\mathbf{R}(G)) \setminus \{1\}\right\}. \tag{9}$$

¿From (8) and (9) it follows that for graphs G having no singletons, $spr_{\mathbf{R}}(G)$ coincides with $spr_{\mathcal{L}}(G)$, (see [18]). For instance, if $G \cong K_n$, then

$$\sigma(\mathbf{R}(K_n)) = \left\{1, \left(-\frac{1}{n-1}\right)^{(n-1)}\right\} \qquad \text{and} \qquad \sigma(\mathcal{L}(K_n)) = \left\{\left(\frac{n}{n-1}\right)^{(n-1)}, 0\right\}.$$

Therefore, $spr_{\mathbf{R}}(K_n) = spr_{\mathcal{L}}(K_n) = 0$.

In 1998 Bollobás and Erdös, [4], introduced the graph parameter

$$R_\alpha(G) = \sum_{ij \in E(G)} (d_i d_j)^\alpha$$

for a real number $\alpha \neq 0$. Note that the Randić Index in (1) is a particular case of the previous one considering $\alpha = -1/2$. Most of the research concerned with bounds for $R_\alpha(G)$ focus on the case $|\alpha| \leq 1$. In [38], the authors investigate bounds for $R_\alpha(G)$ considering $|\alpha| > 1$. In [37] it was shown that a graph G without singletons with minimum vertex degree δ and maximum vertex degree Δ,

$$\frac{n}{2\Delta} \leq R_{-1}(G) \leq \frac{n}{2\delta}, \tag{10}$$

where the equality holds if and only if G is a regular graph.

In [10] some known results for the graph invariant $R_{-1}(G)$ are highlighted and the authors provided upper and lower bounds for the energy of a simple graph with respect to the normalized Laplacian eigenvalues (defined as the sum of its absolute values), and called normalized Laplacian energy, $E_{\mathcal{L}}(G)$. An upper bound for $R_{-1}(G)$ known for trees was also extended by these authors to connected graphs. Also, in [10] for a graph G of order n without singletons it was proved that

$$2R_{-1}(G) \leq E_{\mathcal{L}}(G) \leq \sqrt{2nR_{-1}(G)},$$

and this shows the relevant importance of $R_{-1}(G)$ when related with $E_{\mathcal{L}}(G)$.

The next theorem is due to Brauer [9] and relates the eigenvalues of a matrix and the matrix resulting from a rank-one additive perturbation.

Theorem 2.1. *[9] Let* $\mathbf{M}$ *be an arbitrary* $n \times n$ *matrix with eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_n$*. Let* x_k *be an eigenvector of* $\mathbf{M}$ *associated with the eigenvalue* λ_k*, and let* $\mathbf{q}$ *be any* n*-dimensional vector. Then the matrix* $\mathbf{M} + \mathbf{x}_k\,\mathbf{q}^t$ *has eigenvalues*

$$\lambda_1, \ldots, \lambda_{k-1}\,,\; \lambda_k + \mathbf{x}_k^t\,\mathbf{q}\,,\; \lambda_{k+1}, \ldots, \lambda_n\,.$$

Using this theorem, in [18], a rank-one additive perturbation on Randić matrix was done in order to obtain a matrix with spread equals to the Randić spread of the graph. The following facts can be found in [18].

Facts:

1. Let suppose that the vertices p and q of a graph G are adjacent, then the Randić matrix associated to this edge, $\mathbf{R}_{pq}$, is a principal submatrix of order 2 of $\mathbf{P}\,\mathbf{R}(G)\,\mathbf{P}^t$, where

$$\mathbf{R}_{pq} = \begin{pmatrix} 0 & (d_p\,d_q)^{-1/2} \\ (d_p\,d_q)^{-1/2} & 0 \end{pmatrix}$$

   and $\mathbf{P}$ is an appropriated permutation matrix of order n.

2. $\lambda_{pq} = -1/\sqrt{d_p\,d_q}$ is the smallest eigenvalue of $\mathbf{R}_{pq}$ and, by the Cauchy Interlacing Theorem, we have

$$\lambda_n(\mathbf{R}(G)) \le \tfrac{-1}{\sqrt{d_p d_q}} \le \lambda_2(\mathbf{R}(G)).$$

3. In consequence, the average of these values $\frac{1}{m}\sum\limits_{p\sim q} \frac{-1}{\sqrt{d_p d_q}} = -\frac{\chi(G)}{m}$ also has the property

$$\lambda_n(\mathbf{R}(G)) \le -\frac{\chi(G)}{m} \le \lambda_2(\mathbf{R}(G))$$

   or equivalently

$$-m\lambda_2(\mathbf{R}(G)) \le \chi(G) \le -m\lambda_n(\mathbf{R}(G)).$$

4. The vector $\mathbf{w} = D^{1/2}\mathbf{e} = \left(\sqrt{d_1}, \ldots, \sqrt{d_n}\right)^t$, where $\mathbf{e}$ is the all ones vector, is an eigenvector corresponding to the Randić eigenvalue 1.

5. Let $\beta_{pq} = \frac{-1}{2m}\left(1 + \frac{1}{\sqrt{d_p\,d_q}}\right)$. By Brauer's Theorem, $\mathbf{B}_{pq} = \mathbf{R}(G) + \beta_{pq}\,\mathbf{w}\,\mathbf{w}^t$ has spectrum

$$\sigma(\mathbf{B}_{pq}) = \sigma(\mathbf{R}(G)) \setminus \{1\} \cup \left\{ \frac{-1}{\sqrt{d_p\,d_q}} \right\}.$$

6. Furthermore, if $\mathbf{B} = \mathbf{R}(G) + \gamma\,\mathbf{w}\,\mathbf{w}^t$, where $\gamma = \frac{-1}{2m}\left(\frac{\chi(G)}{m} + 1\right)$ and $\mathbf{w}$ as before, by Brauer's Theorem, the matrix $\mathbf{B}$ has spectrum

$$\sigma(\mathbf{B}) = \sigma(\mathbf{R}(G)) \setminus \{1\} \cup \left\{ -\frac{\chi\,(G)}{m} \right\}.$$

7. By 2. and 3. (first inequality) it is concluded that $spr_{\mathbf{R}}(G) = s(\mathbf{B}) = s\left(\mathbf{B}_{pq}\right)$.

8. Note that for an arbitrary γ the entries of $\mathbf{B} = \mathbf{R}(G) + \gamma\, \mathbf{w}\, \mathbf{w}^t = (b_{ij})$ are given by

$$b_{ij} = \begin{cases} \gamma\sqrt{d_i d_j}, & \text{if } ij \notin E(G) \\ \frac{1}{\sqrt{d_i d_j}} + \gamma\sqrt{d_i d_j} & \text{if } ij \in E(G). \end{cases}$$

3. Lower bounds for the Randić spread

We start this section recalling that the normalized Laplacian eigenvalues and the Randić eigenvalues can be related in the following way:

$$\lambda_i(\mathcal{L}) = 1 - \lambda_{n+1-i}(\mathbf{R}), i \in \{1, \ldots, n\}$$

In [11] it was proved the following result.

Theorem 3.1. *[11, Lemma 1.7] Let $0 = \lambda_n(\mathcal{L}) \leq \lambda_{n-1}(\mathcal{L}) \leq \ldots \leq \lambda_1(\mathcal{L})$ be the normalized Laplacian eigenvalues of a graph G, then*

$$\lambda_{n-1}(\mathcal{L}) \leq 1 + \frac{1}{n-1}$$

with equality holding if and only if G is the complete graph with n vertices. Also for a graph G without isolated vertices we have

$$\lambda_1(\mathcal{L}) \geq 1 + \frac{1}{n-1}.$$

Remark 1. *[18] By Theorem 2.1, and in a more general way, for any given value ς such that $\lambda_n(\mathbf{R}(G)) \leq \varsigma \leq \lambda_2(\mathbf{R}(G))$, the equality*

$$spr_{\mathbf{R}}(G) = s(\mathbf{B}_\varsigma)$$

holds, where

$$\mathbf{B}_\varsigma = \mathbf{R}(G) + \beta\, \mathbf{w}\, \mathbf{w}^t$$

with

$$\beta = \frac{1}{2m}\,(\varsigma - 1).$$

In [31] it was proved:

Theorem 3.2. *[31, Theorem 6] Let $\mathbf{M} = (m_{ij})$ be an $n \times n$ Hermitian matrix. Then*

$$s\left(\mathbf{M}\right) \geq \max_{\Upsilon} \frac{2}{\sqrt{|\Upsilon|}} \sqrt{\sum_{\substack{i \in \Upsilon \\ j \notin \Upsilon}} |m_{ij}|^2}, \tag{11}$$

where $\emptyset \neq \Upsilon \subset \{1, 2, \ldots, n\}$ and $|\Upsilon| \leq \frac{n}{2}$, where $|\cdot|$ stands the cardinality of sets.

In [18] the following definition was given.

Definition 1. *[18] Let G be an arbitrary (n, m)-graph with list of vertex degrees $d_1, \ldots, d_n$ such that $d_i \neq 0$ for all $1 \leq i \leq n$. For the i-th vertex of G, define*

$$\Gamma(i) = \sum_{s \sim i} \frac{1}{d_s}. \tag{12}$$

Clearly, if G is a k-regular graph then $\Gamma(i) = 1$, for all $1 \leq i \leq n$.

The next lower bound, presented in [18], depends on the degrees of the vertices and the number of edges.

Theorem 3.3. *[18] Let G be an arbitrary graph with n vertices and m edges. Then*

$$spr_{\mathbf{R}}(G)^2 \geq \max_{i \leq j} \left\{ 4\beta\,(d_j + d_i)(1 + \beta m) - \beta^2\,(d_j + d_i)^2 + \frac{2}{d_j}\,\Gamma(j) + \frac{2}{d_i}\,\Gamma(i) \right\} \tag{13}$$

where β is either

$$\beta_1 = \frac{-1}{2m}\left(1 + \frac{1}{\sqrt{d_p\, d_q}}\right), \tag{14}$$

or

$$\beta_2 = \frac{-1}{2m}\left(1 + \frac{\chi\,(G)}{m}\right). \tag{15}$$

Remark 2. *Using Lemma 3.1, the parameter*

$$\beta_3 = \frac{-1}{2m}\left(\frac{n}{n-1}\right). \tag{16}$$

can be included in the above list also. This parameter β_3 was not considered in the previous works.

The next lemma was proved in [18].

Lemma 3.4. *[18] Let G be a connected graph of order n. Then $\lambda_2(\mathbf{R}(G)) < 0$ if and only if $G \cong K_n$.*

Remark 3. *If $G \ncong K_n$ is a connected graph, by Lemma 3.4, $\lambda_n(\mathbf{R}(G)) \leq 0 \leq \lambda_2(\mathbf{R}(G))$ which implies that*

$$\beta_0 = -\frac{1}{2m} \tag{17}$$

satisfies the condition in Remark 1 and can be chosen as a different parameter rather than β in Theorem 3.5 and Remark 2.

Remark 4. *Note that, for an arbitrary graph G with m edges, it is easily checked*

$$\sum_{j \in V(G) \setminus \{i\}} d_j = 2m - d_i.$$

Now we apply the Theorem 3.2 to the next result.

Theorem 3.5. *Let G be an arbitrary graph with n vertices and m edges. Let Υ be a subset of vertices of G, where $|\Upsilon| \leq \frac{n}{2}$.*

$$\begin{aligned} spr_{\mathbf{R}}(G) &\geq \frac{2}{\sqrt{|\Upsilon|}} \sqrt{\sum_{i \in \Upsilon} \left(\frac{\Gamma(i)}{d_i} + 2\beta d_i + \sum_{j \in V(G) \setminus \{i\}} \beta^2 d_i d_j \right)} \\ &= \frac{2}{\sqrt{|\Upsilon|}} \sqrt{\sum_{i \in \Upsilon} \left(\frac{\Gamma(i)}{d_i} + 2\beta d_i + \beta^2 d_i (2m - d_i) \right)}. \end{aligned}$$

where β is defined either as in (14) or (15) or (16) and, in the case of $G \ncong K_n$ as in (17).

Proof. Let Υ be a subset of vertices of G. We apply the lower bound (11) to a matrix $\mathbf{B}_\zeta$ in Remark 1 and we use Item 8 in latter **Facts** to obtain:

$$\begin{aligned} s(\mathbf{B}_\zeta) &= spr_{\mathbf{R}}(G) \geq \frac{2}{\sqrt{|\Upsilon|}} \sqrt{\sum_{i \in \Upsilon} \left(\sum_{ij \in E(G)} \left(\frac{1}{d_i d_j} + 2\beta + \beta^2 d_i d_j \right) + \sum_{ij \notin E(G)} \beta^2 d_i d_j \right)}. \\ &= \frac{2}{\sqrt{|\Upsilon|}} \sqrt{\sum_{i \in \Upsilon} \left(\frac{1}{d_i} \Gamma(i) + 2\beta d_i + \beta^2 d_i \sum_{ij \in E(G)} d_j + \sum_{ij \notin E(G)} \beta^2 d_i d_j \right)} \\ &= \frac{2}{\sqrt{|\Upsilon|}} \sqrt{\sum_{i \in \Upsilon} \left(\frac{1}{d_i} \Gamma(i) + 2\beta d_i + \beta^2 d_i \sum_{j \in V(G) \setminus \{i\}} d_j \right)}. \end{aligned}$$

■

Taking $|\Upsilon| = 1$ in the lower bound given in Theorem 3.5 we obtain

Theorem 3.6. *Let G be an arbitrary graph with n vertices and m edges, then*

$$spr_{\mathbf{R}}(G) \geq \max_{i \in V(G)} 2 \sqrt{\frac{\Gamma(i)}{d_i} + 2\beta d_i + \beta^2 d_i (2m - d_i)}, \tag{18}$$

where β is defined either as in (14) or (15) or (16) and, in the case of $G \ncong K_n$ as in (17).

If G is a k-regular graph then

$$\begin{aligned} &\beta_0 = -\tfrac{1}{nk}, \quad \beta_1 = \beta_2 = \tfrac{-(k+1)}{nk^2}, \quad \beta_3 = \tfrac{-1}{(n-1)k} \\ &\Gamma(j) = 1, \text{ for all, } j = 1, 2 \ldots, n. \end{aligned} \tag{19}$$

For a k regular graph G, replacing the parameter β in (18), by β_0, β_1 and β_3, in (19), respectively we obtain the next corollaries.

Corollary 3.1. *[1] Let $G \ncong K_n$ be a k-regular graph of order n. Then*

$$spr_{\mathbf{R}}(G) \geq 2\sqrt{\frac{1}{k} - \frac{1}{n} - \frac{1}{n^2}}$$

Corollary 3.2. *[18, Remark 3] Let G be a k-regular graph of order n. Then*

$$spr_{\mathbf{R}}(G) \geq \frac{2}{nk}\sqrt{(n-1-k)(kn+k+1)}.$$

Corollary 3.3. *Let G be a k-regular graph of order n. Then*

$$spr_{\mathbf{R}}(G) \geq 2\sqrt{\frac{1}{k}-\frac{1}{n-1}}.$$

Remark 5. *The lower bound in Corollary 3.3 is new and improves the lower bound in [18] given by*

$$spr_{\mathbf{R}}(G) \geq \frac{1}{k}-\frac{1}{n-1}.$$

Now we introduce the following notation that will be used in the next results. For a square matrix H, $tr\,(H)$ stands for the trace of H. The sum $\sum\limits_{i_1=1}^{n}\sum\limits_{i_2=1}^{n}\cdots\sum\limits_{i_s=1}^{n} f\,(i_1, i_2, \ldots, i_s)$ will be denoted by $\sum\limits_{i_1,i_2,\ldots,i_s=1}^{n} f\,(i_1, i_2, \ldots, i_s)\,.$

The following lemma was proved in [1].

Lemma 3.7. *[1]Let $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_{n-1} \geq \gamma_n = 0$ be the normalized Laplacian eigenvalues of a graph G. Let $A = (a_{ij})$ be the adjacency matrix of G whose degrees sequence is $d_1, d_2, \ldots, d_n$. Then,*

1. $\sum\limits_{i=1}^{n-1}\gamma_i^2 = n + 2R_{-1};$
2. $\sum\limits_{i=1}^{n-1}\gamma_i^4 = n + 6\sum\limits_{i_1,i_2=1}^{n}\frac{a_{i_1i_2}a_{i_2i_1}}{d_{i_1}d_{i_2}} - 4\sum\limits_{i_1,i_2,i_3=1}^{n}\frac{a_{i_1i_2}a_{i_2i_3}a_{i_3i_1}}{d_{i_1}d_{i_2}d_{i_3}} + \sum\limits_{i_1,i_2,i_3,i_4=1}^{n}\frac{a_{i_1i_2}a_{i_2i_3}a_{i_3i_4}a_{i_4i_1}}{d_{i_1}d_{i_2}d_{i_3}d_{i_4}}.$

On the same way, using a numerical inequality, see [41, *Complementary Inequalities (12.3)*] together with the previous lemma were obtained the following results.

Theorem 3.8. *[1] Let $A = (a_{ij})$ be the adjacency matrix of a graph G whose degrees sequence is $d_1, d_2, \ldots, d_n$. Then,*

$$s_{\mathcal{L}}\,(G) = s_R\,(G) \geq$$

$$\left(\frac{n+6\sum\limits_{i_1,i_2=1}^{n}\frac{a_{i_1i_2}a_{i_2i_1}}{d_{i_1}d_{i_2}}-4\sum\limits_{i_1,i_2,i_3=1}^{n}\frac{a_{i_1i_2}a_{i_2i_3}a_{i_3i_1}}{d_{i_1}d_{i_2}d_{i_3}}+\sum\limits_{i_1,i_2,i_3,i_4=1}^{n}\frac{a_{i_1i_2}a_{i_2i_3}a_{i_3i_4}a_{i_4i_1}}{d_{i_1}d_{i_2}d_{i_3}d_{i_4}}.}{n+2R_{-1}}-\frac{n+2R_{-1}}{n-1}\right)^{1/2}.$$

Applying Theorem 3.8, for a k-regular graph G it was obtained.

Corollary 3.4. *[1] . Let $A = (a_{ij})$ be the adjacency matrix of a k regular graph G. Then*

$$s_{\mathcal{L}}\,(G) = s_R\,(G) \geq \left(\frac{nk + (1/k^3)\,tr\,(6k^2A^2 - 4kA^3 + A^4)}{n\,(k+1)} - \frac{n\,(k+1)}{k\,(n-1)}\right)^{1/2}. \tag{20}$$

Using another numerical inequality in [41, *Complementary Inequalities (12.4)*] the following result was presented.

Theorem 3.9. *[1] Let G be a connected graph with $n \geq 2$ vertices. Then*

$$s_R(G) = s_{\mathcal{L}}(G) \geq \tfrac{2}{n-1}\sqrt{2(n-1)R_{-1} - n}. \tag{21}$$

Corollary 3.5. *[1] Let G be a connected graph with $n \geq 2$ vertices and maximum vertex degree Δ. Then*

$$s_R(G) = s_{\mathcal{L}}(G) \geq \tfrac{2}{n-1}\sqrt{\frac{n(n-1)}{\Delta} - n}.$$

Moreover, if G is k-regular $(k \geq 2)$, then

$$s_R(G) = s_{\mathcal{L}}(G) \geq \tfrac{2}{(n-1)k}\sqrt{nk(n-1-k)}. \tag{22}$$

Remark 6. *For circulant graphs, see [17], we present results obtained with MATLAB comparing the lower bound in (20) with the lower bound in (22). For short we present only the first row of the adjacency matrix of our graphs. As shows the following table both lower bounds (22) and (20) are efficient to approximate the $s_R(G)$. The following table gives the first row of the adjacency matrix of a circulant graph G, the Randić spread of G and the lower bounds in (22) and (20), respectively.*

G	$s_R(G)$	*(22)*	*(20)*
$\begin{pmatrix}0&0&0&1&1&1&1&1&0&0\end{pmatrix}$	0.8944	0.6285	**0.6733**
$\begin{pmatrix}0&0&1&1&0&0&0&1&1&0\end{pmatrix}$	1.1180	0.7857	**0.8724**
$\begin{pmatrix}0&0&1&0&0&0&0&0&1&0\end{pmatrix}$	1.8090	**1.3147**	1.1180
$\begin{pmatrix}0&0&0&1&1&1&1&0&0\end{pmatrix}$	0.9698	0.7500	**0.7945**
$\begin{pmatrix}0&1&1&1&0&0&1&1&1\end{pmatrix}$	0.5686	**0.4330**	0.4315
$\begin{pmatrix}0&1&0&0&1&0&1&0&1&0&0&1\end{pmatrix}$	0.9464	0.6900	**0.7644**
$\begin{pmatrix}0&1&1&0&1&1&1&1&1&0&1&1\end{pmatrix}$	0.4444	0.2969	**0.2971**
$\begin{pmatrix}0&1&0&1&1&1&1&1&1&1&0&1\end{pmatrix}$	0.4444	**0.2969**	0.2967
$\begin{pmatrix}0&0&0&0&0&1&0&0&0&0&1&0&0&0&0\end{pmatrix}$	1.500	**1.3553**	0.8018
$\begin{pmatrix}0&1&1&0&1&0&0&1&1&0&0&1&0&1&1\end{pmatrix}$	0.6250	0.4792	**0.5012**

4. Upper bounds for the Randić spread

In what follows we present upper bounds for the Randić spread and discuss the equality cases. The first one uses a known upper bound for the spread of a matrix due to D. Scott [51], which can be proven by Gershgorin circle theorem (see the proof of Theorem 3.1 in [3]). Let $\mathbf{M} = (m_{ij})$ be a square matrix. Then

$$s(\mathbf{M}) \leq \max_{i \neq j}\left\{|m_{ii} - m_{jj}| + \sum_{k \neq i}|m_{ik}| + \sum_{k \neq j}|m_{jk}|\right\}. \tag{23}$$

Using (23) it was established the next theorem.

Theorem 4.1. *[18] Let G be a graph on n vertices and m edges whose degrees sequence is $d_1, d_2, \ldots,$ d_n and $\mathbf{B}_\varsigma$ be the matrix defined in Remark 1, with $\lambda_n(\mathbf{R}(G)) \leq \varsigma \leq \lambda_2(\mathbf{R}(G))$. Then*

$$s(\mathbf{B}_\varsigma) \leq \max_{i<j}\left\{\left(\tfrac{1-\varsigma}{2m}\right)|d_i - d_j| + \sum_{l \sim i}\left|\tfrac{1}{\sqrt{d_i d_l}} - \left(\tfrac{1-\varsigma}{2m}\right)\sqrt{d_i d_l}\right| + \tfrac{(1-\varsigma)}{2m}\sum_{l \not\sim i}\sqrt{d_i d_l} + \sum_{l \sim j}\left|\tfrac{1}{\sqrt{d_j d_l}} - \left(\tfrac{1-\varsigma}{2m}\right)\sqrt{d_j d_l}\right| + \tfrac{(1-\varsigma)}{2m}\sum_{l \not\sim i}\sqrt{d_j d_l}\right\}. \tag{24}$$

On the other hand, if $G \ncong K_n$ is a connected graph, by Lemma 3.4, $\lambda_n(\mathbf{R}(G)) \leq 0 \leq \lambda_2(\mathbf{R}(G))$, which implies that $\varsigma = 0$ satisfies the condition in Remark 1. Thus the next upper bound follows from (24) .

Corollary 4.1. *Let $G \ncong K_n$ be a connected graph with n vertices and m edges whose degrees sequence is $d_1, d_2, \ldots, d_n$. Then*

$$spr_{\mathcal{L}}(G)=spr_{\mathbf{R}}(G)\leq \max_{i<j}\left\{\frac{\left|d_i-d_j\right|}{2m}+\sum_{l\sim i}\left|\frac{1}{\sqrt{d_i d_l}}-\frac{\sqrt{d_i d_l}}{2m}\right|+\sum_{l\sim j}\left|\frac{1}{\sqrt{d_j d_l}}-\frac{\sqrt{d_j d_l}}{2m}\right|+\sum_{l\nsim j}\frac{\sqrt{d_j d_l}}{2m}+\sum_{l\nsim i}\frac{\sqrt{d_i d_l}}{2m}\right\}. \tag{25}$$

Moreover, if G is k-regular with $k \neq n-1$, then

$$spr_{\mathcal{L}}(G) = spr_{\mathbf{R}}(G) \leq 4 - \frac{2(2k+1)}{n}.$$

More recently, the authors in [27] obtained the following upper bound for $spr_{\mathcal{L}}(G)$.

Theorem 4.2. *[27, Theorem 4] Let G be an undirected simple connected graph with $n \geq 3$ vertices. Then*

$$spr_{\mathcal{L}}(G) = spr_{\mathbf{R}}(G) \leq \sqrt{\frac{2}{n-1}}\sqrt{2(n-1)R_{-1} - n}. \tag{26}$$

Equality holds if and only if $G \cong K_n$.

By the above result together with the upper bound in (10) the following result is obtained.

Corollary 4.2. *Let G be an undirected simple connected graph with $n \geq 3$ vertices. with ordered list of vertex degrees, $d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. Then*

$$spr_{\mathcal{L}}(G) = spr_{\mathbf{R}}(G) \leq \sqrt{\frac{2n(n-1-\delta)}{(n-1)\delta}}.$$

Equality holds if and only if $G \cong K_n$.

The next corollary, presented in [27], is a particular case of Theorem 4.2.

Corollary 4.3. *[27, Corollary 7] Let G be a k-regular connected graph with n vertices $(n \geq 3)$. Then*

$$spr_{\mathcal{L}}(G) = spr_{\mathbf{R}}(G) \leq \sqrt{2n\left(\frac{1}{k} - \frac{1}{n-1}\right)}. \tag{27}$$

Equality holds if and only if $G \cong K_n$.

In what follows, using the suggestion in Remark 1, we deduce some upper bounds for the Randić spread (and for the spread of a rank one perturbed Randić matrix). By using inequality in (6) the following results were obtained.

Theorem 4.3. *[19] Let G be a graph on n vertices and m edges and $\mathbf{B}_\varsigma$ be the matrix defined in Remark 1. Then*

$$s(\mathbf{B}_\varsigma) \leq \sqrt{4R_{-1}(G) + \frac{2(\varsigma-1)}{n}(1 + n + \varsigma(n-1))}. \tag{28}$$

Corollary 4.4. *[19] Let $G \ncong K_n$ be a connected graph with n vertices Then*

$$spr_{\mathbf{R}}(G) \leq \sqrt{4R_{-1}(G) - \frac{2(1+n)}{n}}. \tag{29}$$

Moreover, if G is k-regular $k \neq n-1$, then

$$spr_{\mathbf{R}}(G) \leq \sqrt{\frac{2n^2 - 2k(1+n)}{nk}} = \sqrt{2n\left(\frac{1}{k} - \frac{1}{n} - \frac{1}{n^2}\right)}. \tag{30}$$

The following result is obtained by setting $\varsigma = -\frac{\chi(G)}{m}$ in (28).

Corollary 4.5. *[19] Let G be a graph with n vertices and m edges. Then*

$$spr_{\mathbf{R}}(G) \leq \sqrt{4R_{-1}(G) - \frac{2(\chi(G)+m)(m(1+n) - \chi(G)(n-1))}{nm^2}}. \tag{31}$$

Moreover, if G is a k-regular graph,

$$spr_{\mathbf{R}}(G) \leq \sqrt{\frac{2n^2k - 2(k^2-1)n - 2(k+1)^2}{nk^2}}. \tag{32}$$

5. Some conclusions

In this section, for a connected k-regular graph G, we compare the lower bound given in (27) with its counterparts in (30) and (32).

Proposition 5.1. *Let $G \ncong K_n$ be a connected k-regular graph. Then the upper bound given in (30) is an improvement of the upper bound given in (27).*

Proof. This proof is based on the equivalence

$$\frac{2n(n-1-k)}{k(n-1)} \geq \frac{2n^2 - 2k(1+n)}{nk}$$

if and only if

$$\begin{aligned} \frac{n(n-1-k)}{n-1} &\geq \frac{n^2 - k(1+n)}{n} \Leftrightarrow \\ n^3 - n^2 - n^2k &\geq (n-1)\left(n^2 - k - kn\right) \\ &= n^3 - nk - n^2k - n^2 + k + kn \end{aligned}$$

if and only if

$$0 \geq k,$$

which is false. ∎

Proposition 5.2. *Let $G \ncong K_n$ be a connected k-regular graph. Then, the upper bound given in (30) is an improvement of the upper bound given in (32) if and only if*

$$n \geq 2k+1.$$

Proof. This proof is based on the equivalence

$$\begin{aligned} \frac{2n^2k - 2\left(k^2-1\right)n - 2\left(k+1\right)^2}{nk^2} &\geq \frac{2n^2 - 2k\left(1+n\right)}{nk} \Leftrightarrow \\ n^2k - k^2n + n - k^2 - 2k - 1 &\geq n^2k - k^2 - k^2n \Leftrightarrow \\ n - 2k - 1 &\geq 0 \end{aligned}$$

if and only if

$$n \geq 2k+1.$$

■

6. Relations between the Randić spread and the Randić energy

The concept of matrix energy was conceived by analogy with graph energy [43]. For details on graph energy see for instance the papers [24, 25] and the book [36]. According to Nikiforov, for an arbitrary (not necessarily square) matrix $\mathbf{M}$ with singular values $s_1(\mathbf{M}),\ s_2(\mathbf{M}), \ldots$, its energy $E(\mathbf{M})$ is equal to $s_1(\mathbf{M}) + s_2(\mathbf{M}) + \cdots$. In the special case when $\mathbf{M}$ is symmetric with eigenvalues $\lambda_1(\mathbf{M}), \lambda_2(\mathbf{M}), \ldots,$ $\lambda_n(\mathbf{M})$, then its energy is given by

$$E(\mathbf{M}) = \sum_{i=1}^{n} \left|\lambda_i\left(\mathbf{M}\right)\right| .$$

In addition to the ordinary graph energy, namely the energy of the adjacency matrix, a variety of other energies based on other graph matrices have been introduced [26, 36]. Recently, the concept of *Randić energy*, $E_{\mathbf{R}}$, was introduced in [7], equal to the sum of absolute values of the eigenvalues of the Randić matrix:

$$E_{\mathbf{R}}(G) = \sum_{i=1}^{n} |\rho_i| .$$

For further study on this graph invariant the reader is referred to [5–8, 29, 30, 49]. Independently, for graphs without isolated vertices, and based on the matrix $\mathcal{L}$, the *normalized Laplacian energy* was defined in [10]

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\gamma_i - 1|$$

which is exactly same as the Randić energy, that is, $E_{\mathcal{L}}(G) = E_{\mathbf{R}}(G)$.

In [10] it was shown that $E_{\mathcal{L}}(G)$ can be bounded in terms of the graph invariant $R_{-1}(G)$.

Lemma 6.1. *[10] Let G be a graph of order n with no isolated vertices. Then*

$$2\,R_{-1}(G) \leq E_{\mathcal{L}}(G) \leq \sqrt{2n\,R_{-1}(G)}\ .$$

Moreover, it was shown that

$$2 \leq E_{\mathcal{L}}(G) \leq \left\lfloor \frac{n}{2} \right\rfloor$$

and the graphs attaining these bounds were characterized [10]. If G is connected, then the upper bound can be improved to $E_{\mathcal{L}}(G) < \sqrt{\frac{15}{28}}\,(n+1)$. The authors in [10] also provide a class of connected graphs for which $E_{\mathcal{L}}(G) = \frac{n}{\sqrt{2}} + O(1)$ and the question if this class has maximal $E_{\mathcal{L}}(G)$ was considered.

The next result was proven in [27].

Theorem 6.2. *[27]Let G be a graph with $n \geq 2$ vertices. Then*

$$(n-1)\,(n+2R_{-1}) - n^2 \leq \left(\frac{n-1}{2}\right) spr_{\mathbf{R}}\,(G)\, E_{\mathbf{R}}(G). \tag{33}$$

By combining the upper bound in (26) with the inequality in (33) the authors propose the following lower bound.

Theorem 6.3. *[27, Theorem 5] Let G be an undirected simple and connected graph with $n \geq 3$, vertices and m edges. Then*

$$E_{\mathcal{L}}(G) = E_{\mathbf{R}}(G) \geq \sqrt{\frac{2}{n-1}}\sqrt{2\,(n-1)\,R_{-1} - n}.$$

As a corollary and by using the right hand inequality in (10) we derive.

Corollary 6.1. *Let G be an undirected simple and connected graph with $n \geq 3$ vertices and largest vertex degree Δ. Then*

$$E_{\mathcal{L}}(G) = E_{\mathbf{R}}(G) \geq \sqrt{\frac{2n}{(n-1)\,\Delta}}\sqrt{n-1-\Delta}.$$

Moreover, if G is a k-regular graph,

$$E_{\mathcal{L}}(G) = E_{\mathbf{R}}(G) \geq \sqrt{\frac{2n}{k}}\sqrt{\frac{n-1-k}{n-1}}. \tag{34}$$

On the other hand a classical lower bound for the energy of a n-vertex graph G with m edges, see [36], is given by the inequality

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

For a k-regular graph G with n vertices, from the above lower bound we obtain

$$E\,(G) \geq 2\sqrt{\frac{nk}{2}}.$$

¿From the equality (3), for a k-regular graph G with n vertices it is derived

$$E_{\mathbf{R}}(G) \geq \frac{2}{k}\sqrt{\frac{nk}{2}} = \sqrt{\frac{2n}{k}}. \tag{35}$$

It is clear that the lower bound (34) is worse than the one presented in (35).

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On the Co-PI Energy

Ezgi Kaya[a], A. Dilek Maden[b]

[a]*Department of Mathematics–Computers, Faculty of Science and Literature, Igdir University, Igdir, Turkey*

[b] *Department of Mathematics, Faculty of Science, Selçuk University, Campus, 42075, Konya, Turkey*

ezgi.kaya@igdir.edu.tr, aysedilekmaden@selcuk.edu.tr

Contents

1. Introduction

Let G be a finite, connected, simple graph with $n = |V|$ vertices and $m = |E|$ edges. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between u and v in G. The diameter $diam(G)$ is the greatest distance between two vertices of G. The degree $\deg_G(v)$ of a vertex v is the number of edges incident with it in G. The maximum degree of a graph of G is denoted by $d_{\max}$. Let $e = uv$ be an edge connecting vertices u and $v \in G$. Define the sets:

$$\begin{aligned} N_u(e) &= \{z \in V \,|d_G(z,u) < d_G(z,v)\} \\ N_v(e) &= \{z \in V \,|d_G(z,v) < d_G(z,u)\} \end{aligned}$$

which are sets consisting of vertices lying closer to u than to v and those lying closer to v than to u, respectively. The number of such vertices are denoted by

$$n_u = n_u(e) = |N_u(e)| \text{ and } n_v = n_v(e) = |N_v(e)|.$$

Other terminology and notations needed will be introduced as it naturally occurs in the following and we use [1, 3, 4, 16] for those not defined here.

A topological index is a number related to graph which is invariant under graph isomorphism. In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modeling physicochemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [9]. There exist several types of such indices, especially those based on vertex and edge distances. One of the most intensively studied topological indices is the Wiener index W, defined as the sum of distances between all pairs of vertices of the molecular graph [30]. In a molecular graph, each vertex represented an atom of the molecule and bond between atoms are represented by edges between corresponding edges.

The vertex PI index [22], Szeged index [10] and the first Zagreb index [7], defined as follows:

$$\begin{aligned} PI_v &= \sum_{e=uv\in E(G)} n_u(e)+n_v(e) \\ Sz(G) &= \sum_{e=uv\in E(G)} n_u(e)n_v(e) \\ M_1(G) &= \sum_{v\in V(G)} \deg^2(v)\,. \end{aligned}$$

Recently, Hassani et al. introduced a new topological index similar to the vertex version of PI index [14]. This index is called the $Co-PI_v$ index of G and defined as:

$$Co-PI_v(G)=\sum_{e=uv\in E(G)} |n_u(e)-n_v(e)|\,.$$

Here the summation goes over all edges of G.

Hassani et al. computed Co-PI index for $TUC_4C_8(R)$ nanotubes in [15]. Su et al. presented an equivalent definition of $Co-PI_v$ index and established further mathematical properties of the $Co-PI_v$ index [29]. They computed the $Co-PI_v$ index of Cartesian product graphs as in the following.

Theorem 1.1. *[29] Let $G=G_1\square G_2$ be the Cartesian product of two graphs G_1 and G_2. Then*

$$Co-PI_v(G_1\square G_2)=|V_1|^2\,Co-PI_v(G_2)+|V_2|^2\,Co-PI_v(G_1).$$

Theorem 1.2. *[29] Let G_1,G_2, ...,G_n be n graphs on at least two vertices. Then*

$$Co-PI_v\left(\bigotimes_{i=1}^{n} G_i\right)=\sum_{i=1}^{n}\left(Co-PI_v(G_i)\prod_{j\neq i}^{n}|V_j|^2\right).$$

Kaya et al. established the following results for the $Co-PI_v$ index of graphs [19].

Theorem 1.3. *[19] Let G be a connected graph with $n\geq 2$ vertices and m edges. Then,*

$$Co-PI_v(G)\leq m(n-2)$$

with equality if and only if G is isomorphic to S_n.

The following two upper bounds over $Co-PI_v$ index are in terms of n, m and *Szeged* index.

Theorem 1.4. *[19] Let G be a connected graph with $n\geq 2$ vertices and m edges. Then,*

$$Co-PI_v(G)\leq\sqrt{m}\sqrt{m(n^2-2n+2)-2Sz(G)}$$

with equality if and only if G is isomorphic to S_n.

Theorem 1.5. *[19] Let G be a connected graph with $n \geq 2$ vertices and m edges. Then,*

$$Co - PI_v(G) \leq \sqrt{m(n^2 - 2n + 2) - 2Sz(G) + m(m-1)(n-2)^2}$$

with equality if and only if G is isomorphic to S_n.

Now we present a lower bound on $Co - PI_v$ index of graphs.

Theorem 1.6. *[19] Let G be a connected graph with $n \geq 2$. Then,*

$$Co - PI_v(G) \geq \sqrt{|(n^2 - 2n + 2) - 2Sz(G)|}.$$

Equality holds if and only if G is isomorphic to K_2.

Using the Ozeki inequality [18] in the following theorem, it was obtained an upper bound for the $Co - PI_v$ index.

Theorem 1.7. *[19] Let G be a connected graph with $n \geq 2$. Then,*

$$Co - PI_v(G) \leq \sqrt{\frac{m^2}{3}(n-2)^2 + PI_v^2(G) - 4mSz(G)}.$$

Equality holds if and only if G is isomorphic to the K_2 .

Now we give an upper bound on $Co - PI_v$ index in terms of m, first Zagreb index and maximum degree.

Theorem 1.8. *[19] Let G be a connected graph with diameter 2. Then,*

$$Co - PI_v(G) \leq \sqrt{mM_1(d_{\max} - 2)}$$

inequality holds.

Corollary 1.1. *[19] Let T be a tree with n vertices. Then,*

$$2\,(n-2) \leq Co - PI_v(T) \leq (n-1)\,(n-2)\,.$$

Lower bound holds if and only if T is isomorphic to K_2 and upper bound holds if and only if T is isomorphic to S_n.

Su et al. [29] introduced the Co-PI matrix and the Laplacian Co-PI matrix of a graph in this way:

The adjacent matrix $A(G) = [a_{ij}]_{n \times n}$ of G is the integer matrix with rows and columns indexed by its vertices, such that the $ij-$th-entry is equal to the number of edges connecting i and j. Let the weight of the edge $e = uv$ be a non-negative integer $|n_u(e) - n_v(e)|$, we can define a weight function: $w : E \to$

$R^{+} \cup \{0\}$ on E, which is said to be the $Co-PI\ weighting$ of G. The adjacency matrix of G weighted by the Co-PI weighting is said to be its $Co-PI\ matrix$ and denoted by $M_{CPI}(G) = [c_{ij}]_{n\times n}$ .That is,

$$c_{ij} = \begin{cases} \left|n_{v_i}(e) - n_{v_j}(e)\right|, \ e = v_i v_j \\ 0 \qquad\qquad\qquad\quad , otherwise \end{cases} .$$

The eigenvalues of M_{CPI} are said to be the Co-PI eigenvalues of G and denoted by $\lambda_k^*(G)$ for $k = 1, 2, ..., |V|$.

The Laplacian matrix of G is defined as $\mathbf{L}(G) = \mathbf{D}(G)^T - \mathbf{A}(G)$, where $D(G)$ is the vector of degrees of its vertices. Such matrix weighted by the Co-PI weighting is said to be the Laplacian Co-PI matrix and denoted by $\mathbf{LM_{CPI}}(G)$. Its eigenvalues are the Laplacian Co-PI eigenvalues and we denote them by $\mu_k^*(G)$ for $k = 1, 2, ..., |V|$. Easy verification shows that the Co-PI index of G can be expressed as one half of the sum of all entries of $M_{CPI}(G)$, i.e.,

$$Co - PI_v(G) = \frac{1}{2}\sum_{i=1}^{n} M_{CPI_i}(G)$$

where M_{CPI_i} is the sum of i-th row of the matrix M_{CPI}.

Since Co-PI matrix is symmetric, all its eigenvalues λ_i^*, $k = 1, 2, ..., |V|$, are real and can be labeled so that $\lambda_1^* \geq \lambda_2^* ... \geq \lambda_n^*$. The greatest eigenvalue λ_1^* will be called the Co-PI spectral radius of G. Research on spectral radius of graphs is nowadays very active, as seen from recent papers [5, 6, 17, 19, 20, 26, 27, 32].

In the following two theorems Su et al. [29] characterized the Co-PI spectra of Cartesian product graphs as in the following.

Theorem 1.9. *[29] Let $G = G_1 \Box G_2$ be the Cartesian product of two graphs G_1 and G_2. Then*
(i) $\lambda_{kl}^*(G_1 \Box G_2) = |V_1|\, \lambda_l^*(G_2) + |V_2|\, \lambda_k^*(G_1)$ for $k = 1, 2, ..., |V_1|$ and $l = 1, 2, ..., |V_2|$.
(ii) $\mu_{kl}^*(G_1 \Box G_2) = |V_1|\, \mu_l'(G_2) + |V_2|\, \mu_k^*(G_1)$ for $k = 1, 2, ..., |V_1|$ and $l = 1, 2, ..., |V_2|$.

Theorem 1.10. *[29] Let G_1,G_2, ...,G_n be n graphs on at least two vertices. Then*
(i) $\lambda_{i_1 i_2 ... i_n}^*\left(\bigotimes_{i=1}^{n} G_i\right) = \prod_{i=1}^{n} |V_i| \left(\sum_{j=1}^{n} \frac{\lambda_{k_j}^*(G_i)}{|V_j|}\right)$ for $1 \leq i_j \leq |V_j|$.
(ii) $\mu_{i_1 i_2 ... i_n}^*\left(\bigotimes_{i=1}^{n} G_i\right) = \prod_{i=1}^{n} |V_i| \left(\sum_{j=1}^{n} \frac{\mu_{k_j}^*(G_i)}{|V_j|}\right)$ for $1 \leq i_j \leq |V_j|$.

Let $P(G; x) = x^n + c_1 x^{n-1} + ... + c_{n-1} x + c_n$ be the characteristic polynomial of G. N. Biggs proved that all coeffіcents of $P(G; x)$ can be expressed in terms of the principle minors of $\mathbf{A}(G)$, where a principle minor is the determinant of a submatrix obtained by taking a subset of the rows and that of columns. This leads to the following result.

Theorem 1.11. *[1] The coefficents of the characteristic polynomial $P(G; x)$ of a connected graph G satisfy: $c_1 = 0$, $-c_2$ is the number of edges and $-c_3$ is twice the number of triangles of G.*

Let $\mathbf{A}$ be the adjacency matrix of a graph G. It is well known that the $(i,j)-$th element $a_{ij}^{(k)}$ of the power matrix $\mathbf{A}^k$, $k \geq 1$, represents the number of walks of length k from the vertex u_i to the vertex u_j. Therefore, Su et al. [29] deduced bounds on the second and third Co-PI spectral moment of a graph G as in the following.

Theorem 1.12. *[29] Let G be a connected graph with order $n \geq 3$, size m and t triangles. Then,*

$$2m \leq \lambda_1^{*^2} + \lambda_2^{*^2} + ... + \lambda_n^{*^2} \leq 2m(n-2)^2 \tag{1}$$

and

$$6t \leq \lambda_1^{*^3} + \lambda_2^{*^3} + ... + \lambda_n^{*^3} \leq 6t(n-2)^3.$$

Kaya et al. [19] obtained following bounds for Co-PI spectral radius.

Theorem 1.13. *[19] Let G be a connected graph with $n \geq 2$. Then,*

$$\sqrt{\frac{\sum_{i=1}^{n} M_{CPI_i}^2}{n}} \leq \lambda_1^* \leq \max_{1 \leq j \leq n} \sum_{i=1}^{n} M_{CPI_{ij}} \sqrt{\frac{M_{CPI_j}}{M_{CPI_i}}}$$

where M_{CPI_i} is the sum of i-th row of the matrix M_{CPI}. Equality holds if and only if $M_{CPI_1} = M_{CPI_2} = ... = M_{CPI_n}$.

Note that $trace\,[M_{CPI}] = 0$ and denote by S the trace of M_{CPI}^2. Therefore, the eigenvalues λ_i^* for $i = 1, 2, ..., n$ of M_{CPI} satisfy the relations

$$\sum_{i=1}^{n} \lambda_i^* = 0 \tag{2}$$

,

$$\sum_{i=1}^{n} \lambda_i^{*2} = 2\sum_{i<j}^{n} (c_{ij})^2 = S \tag{3}$$

Let Γ be the class of connected graphs whose Co-PI matrices have exactly one positive eigenvalue. In the following, Kaya et al. [19] presented upper and lower bounds for λ_1^* of graphs in the class Γ in terms of n and S.

Theorem 1.14. *[19] Let $G \in \Gamma$ with $n \geq 2$ vertices. Then,*

$$\lambda_1^* \leq \sqrt{\frac{n-1}{n} S} \tag{4}$$

inequality holds.

Theorem 1.15. *[19] Let $G \in \Gamma$ with $n \geq 2$ vertices. Then,*

$$\lambda_1^* \geq \sqrt{\frac{S}{2}} \tag{5}$$

inequality holds.

From the (1),(4) and (5), we arrive at the Nordhous-Gaddum type inequalities for the largest Co-PI eigenvalue of G.

Theorem 1.16. *[19] Let G be a connected graph on $n > 2$ vertices, m edges. Further, assume that $G \in \Gamma$ has a connected complement $\overline{G}$ with $\overline{m}$ edges. Then,*

$$\lambda_1^*(G) + \lambda_1^*(\overline{G}) \leq \sqrt{\frac{n-1}{n}} \left[\sqrt{2m(n-2)^2} + \sqrt{(n(n-1)-2m)\,(n-2)^2} \right]$$

and

$$\lambda_1^*(G) + \lambda_1^*(\overline{G}) \geq \sqrt{m} + \sqrt{\frac{(n(n-1)-2m)}{2}}$$

inequalities hold.

Let G be a graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and Co-PI matrix M_{CPI}. Then, the Co-PI degree of v_i, M_{CPI_i}, is given by $M_{CPI_i} = \sum_{j=1}^{n} c_{ij}$. Let $\{M_{CPI_1}, M_{CPI_2}, .., M_{CPI_n}\}$ be the Co-PI degree sequence. Then, the second Co-PI degree of v_i, denoted by MT_{CPI_i}, is given by $MT_{CPI_i} = \sum_{j=1}^{n} c_{ij} M_{CPI_j}$. If $\{M_{CPI_1}, M_{CPI_2}, .., M_{CPI_n}\}$ is the Co-PI degree sequence, then G is a k-Co-PI regular graph if $M_{CPI_i} = k$, for all i. If G has the Co-PI degree sequence and second Co-PI degree sequence $\{M_{CPI_1}, M_{CPI_2}, .., M_{CPI_n}\}$ and $\{MT_{CPI_1}, MT_{CPI_2}, ..., MT_{CPI_n}\}$ respectively, then G is pseudo k-Co-PI regular graph if $\frac{MT_{CPI_i}}{M_{CPI_i}} = k$, for all i.

Using the Co-PI degree sequence, following results are obtained by Kaya et al. in [19,20].

Theorem 1.17. *[19] Let G be a connected graph with $n \geq 2$. Then,*

$$\lambda_1^* \geq \frac{2Co - PI_v(G)}{n}$$

with equality holding if and only if $M_{CPI_1} = M_{CPI_2} = ... = M_{CPI_n}$.

In order to obtain a different lower bound for the Co-PI energy of graphs, for each $i = 1, 2, ..., n$, we define the sequence $C_i^{(1)}, C_i^{(2)}, ..., C_i^{(t)}, ...$ as follows: For a fixed $\alpha \in \mathbb{R}$, let $C_i^{(1)} = M_{CPI_i}^{\alpha}$ and, for each $t \geq 2$, let $C_i^{(t)} = \sum_{i=1}^{n} c_{ij} C_j^{(t-1)}$.

Theorem 1.18. *[20] Let G be a connected graph, $\alpha \in \mathbb{R}$ and $t \in \mathbb{Z}$. Thus,*

$$\lambda_1^* \geq \sqrt{\frac{\sum_{i=1}^{n} \left(C_i^{(t+1)}\right)^2}{\sum_{i=1}^{n} \left(C_i^{(t)}\right)^2}}.$$

For a special case, if we take $\alpha = 1$ and $t = 1$, we obtained the following result.

Corollary 1.2. *[20] Let G be a graph with first and second Co-PI degree sequences*

$$\{M_{CPI_1}, M_{CPI_2}, .., M_{CPI_n}\} \text{ and } \{MT_{CPI_1}, MT_{CPI_2}, ..., MT_{CPI_n}\},$$

respectively. Then,

$$\lambda_1^* \geq \sqrt{\frac{\sum_{i=1}^{n} (MT_{CPI_i})^2}{\sum_{i=1}^{n} (M_{CPI_i})^2}}.$$

Equality holds if and only if, for a constant k, G is a pseudo k-Co-PI regular.

Theorem 1.19. *[20] Let G be a graph with Co-PI degree sequence* $\{M_{CPI_1}, M_{CPI_2}, .., M_{CPI_n}\}$*. Then,*

$$\lambda_1^* \geq \sqrt{\frac{M_{CPI_1}^2 + M_{CPI_2}^2 + ... + M_{CPI_n}^2}{n}}$$

with equality holding if and only if G is Co-PI regular.

The following bounds are related to the second Co-PI spectral moment.

Theorem 1.20. *[21] Let G be a graph with n vertices and m edges. Then,*

$$\begin{aligned} \frac{2}{m} Co - PI_v^2(G) \quad \leq \quad & \sum_{i=1}^{n} \lambda_i^{*^2} \leq \min\{2(n-2)Co - PI_v(G), \\ & 2m(n^2 - 2n + 2) - 4Sz(G)\}. \end{aligned} \tag{6}$$

The left equaliy (6) holds if and only if $G \cong K_2$ *and the right one if and only if* $G \cong S_n$*.*

The next theorem is related to upper bound for λ_1^*.

Theorem 1.21. *[21] Let G be a graph with n vertices and m edges. Then,*

$$\lambda_1^* \leq \min \left\{ \begin{array}{c} \sqrt{\frac{2(n-1)(n-2)Co-PI_v(G)}{n}}, \\ \sqrt{\frac{(n-1)}{n}} \sqrt{2m(n^2 - 2n + 2) - 4Sz(G)} \end{array} \right\}.$$

On one of the most remarkable chemical applications of spectral graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of $\pi-$electrons in conjugated hydrocarbons. For the Hüchkel molecular orbital approximation, the total $\pi-$electron energy in conjugated hydrocarbons is given by the sum of absolute values of the eigenvalues corresponding to the molecular graph G in which the maximum degree is not more than four in general. The notation of the energy of a graph was introduced by Ivan Gutman in [8] as

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

λ_i, $i = 1, ..., n$ are the eigenvalues of adjacency matrix of G. Details and more information on graph energy can be found in the recent papers [11–13, 23–25, 28, 31].

In a similar way, the Co-PI energy of a graph G,

$$Co - PIE(G) = \sum_{i=1}^{n} |\lambda_i^*| \tag{7}$$

was defined by Kaya et al. in [21].

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present some lower and upper bounds on Co-PI energy for graphs.

2. Known results

In this section, we shall list previously known results that will be related with Co-PI energy of graphs.

Theorem 2.1. *[21] Let G be a connected graph. Then,*

$$Co - PIE(G) \leq \sqrt{2n \sum_{e=v_iv_j} \left| n_{v_i} - n_{v_j} \right|^2} \tag{8}$$

Equality holds (8) if and only if G is empty. Moreover,

$$Co - PIE(G) \leq \sqrt{n\alpha}$$

in which

$$\alpha = \min \left\{ \sqrt{n}\sqrt{2(n-2)Co - PI_v(G)}, \sqrt{n}\sqrt{2m(n^2 - 2n + 2) - 4Sz(G)} \right\}.$$

Theorem 2.2. *[21] Let G be a connected graph, $\alpha \in \mathbb{R}$ and $t \in \mathbb{Z}$. Thus,*

$$Co - PIE(G) \leq \sqrt{\frac{\sum_{i=1}^{n} \left(C_i^{(t+1)}\right)^2}{\sum_{i=1}^{n} \left(C_i^{(t)}\right)^2}} + \sqrt{(n-1)\left[S - \frac{\sum_{i=1}^{n} \left(C_i^{(t+1)}\right)^2}{\sum_{i=1}^{n} \left(C_i^{(t)}\right)^2}\right]} \tag{9}$$

where S is the sum of the squares of entries in the Co-PI matrix. Equality holds in (9) if and only if G is a connected graph satisfying

$$\frac{C_1^{(t+1)}}{C_1^{(t)}} = \frac{C_2^{(t+1)}}{C_2^{(t)}} = ... = \frac{C_n^{(t+1)}}{C_n^{(t)}} = k \geq \sqrt{\frac{S}{n}}$$

with three distinct eigenvalues $\left(k, \sqrt{\frac{S-k^2}{n-1}}, -\sqrt{\frac{S-k^2}{n-1}}\right)$.

For a special case, if we take $\alpha = 1$ and $t = 1$, we get the following result.

Corollary 2.1. *[21] Let G be a graph with first and second Co-PI degree sequences* $\{M_{CPI_1}, M_{CPI_2}, \ldots, M_{CPI_n}\}$ *and* $\{MT_{CPI_1}, MT_{CPI_2}, ..., MT_{CPI_n}\}$*, respectively. Then,*

$$Co-PIE(G) \leq \sqrt{\frac{\sum_{i=1}^{n}\left(MT_{CPI_i}\right)^2}{\sum_{i=1}^{n}\left(M_{CPI_i}\right)^2}} + \sqrt{(n-1)\left[S - \frac{\sum_{i=1}^{n}\left(MT_{CPI_i}\right)^2}{\sum_{i=1}^{n}\left(M_{CPI_i}\right)^2}\right]} \tag{10}$$

where S is the sum of the squares of entries in the Co-PI matrix. Equality holds in (10) if and only if for a constant k, G is a pseudo k- Co-PI regular with three distinct eigenvalues $\left(k, \sqrt{\frac{S-k^2}{n-1}}, -\sqrt{\frac{S-k^2}{n-1}}\right)$.

3. New bounds for Co-PI energy

In this section, we present some new lower and upper bounds on Co-PI energy.

Let $a_1, a_2, ..., a_r$ be positive real numbers. For a positive number k among the values $1 \leq k \leq r$, let us suppose that each P_k is defined as in the following:

$$\begin{aligned} P_1 &= \frac{a_1 + a_2 + ... + a_r}{r}, \\ P_2 &= \frac{a_1a_2 + a_1a_3 + ... + a_1a_r + a_2a_3 + ... + a_{r-1}a_r}{\frac{1}{2}r(r-1)}, \\ &\vdots \\ P_{r-1} &= \frac{a_1a_2...a_{r-1} + a_1a_2...a_{r-2}a_r + ... + a_2a_3...a_{r-1}a_r}{r} \\ P_r &= a_1a_2...a_r \end{aligned}$$

Hence the arithmetic mean is simply P_1 while the geometric mean is $P_r^{1/r}$. In fact the following lemma gives a relationship among them.

Lemma 3.1. *[2, Maclaurin's symmetric mean inequality] For* $a_1, a_2, ..., a_r \in \mathbb{R}^+$*, it is true that*

$$P_1 \geq P_2^{1/2} \geq P_3^{1/3} \geq ... \geq P_r^{1/r}. \tag{11}$$

Equality among them holds if and only if $a_1 = a_2 = ... = a_r$.

After all above material, we are ready to present our main results.

Theorem 3.2. *Let G be a connected graph with n vertices and let* Δ *be the absolute value of the determinant of the Co-PI matrix and S be the sum of the squares of entries in the Co-PI matrix of G. Then,*

$$Co-PIE(G) \geq \sqrt{S + n(n-1)\Delta^{\frac{2}{n}}}.$$

Equality holds if and only if $|\lambda_1^*| = |\lambda_2^*| = ... = |\lambda_n^*|$.

Proof. Taking $r = n$, $a_i = |\lambda_i^*|$, $i = 1, 2, ..., n$, by Lemma 3.1, we have

$$P_2^{1/2} \geq P_{n-1}^{1/n-1} \tag{12}$$

where

$$\begin{aligned} P_2 &= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} |\lambda_i^*| \left|\lambda_j^*\right| \quad (13) \\ &= \frac{1}{n(n-1)} \left[\left(\sum_{i=1}^{n} |\lambda_i^*| \right)^2 - \sum_{i=1}^{n} |\lambda_i^*|^2 \right] \\ &= \frac{1}{n(n-1)} \left[Co - PIE(G)^2 - S \right], \ \text{ as } \sum_{i=1}^{n} |\lambda_i^*|^2 = S \end{aligned}$$

and

$$\begin{aligned} P_{n-1} &= \frac{\sum\limits_{i=1}^{n} \prod\limits_{\substack{j=1 \\ j \neq n-i+1}}^{n} |\lambda_i^*|}{n} \quad (14) \\ &= \frac{\prod\limits_{i=1}^{n} |\lambda_i^*|}{n} \sum_{i=1}^{n} \frac{1}{|\lambda_i^*|} \\ &\geq \prod_{i=1}^{n} |\lambda_i^*| \left(\prod_{i=1}^{n} \frac{1}{|\lambda_i^*|} \right)^{1/n} \end{aligned}$$

by the arithmetic-geometric mean inequality. Therefore, by (12), (13), (14) and Lemma 3.1 , we get

$$\frac{1}{n(n-1)} \left[Co - PIE(G)^2 - S \right] \geq \Delta^{2/n}$$

i.e.,

$$Co - PIE(G) \geq \sqrt{S + n(n-1)\Delta^{\frac{2}{n}}}.$$

From Lemma 3.1, the equality holds if and only if $|\lambda_1^*| = |\lambda_2^*| = ... = |\lambda_n^*|$. ■

Theorem 3.3. *Let G be a connected graph with n vertices and let S be the sum of the squares of entries in the Co-PI matrix of G. Then,*

$$Co - PIE(G) \leq \sqrt{nS} \tag{15}$$

Equality holds if and only if $|\lambda_1^*| = |\lambda_2^*| = ... = |\lambda_n^*|$.

Proof. If we take $r = n$ and $a_i = |\lambda_i^*|$ for $i = 1, 2, ..., n$ by Lemma 3.1, then we have

$$P_1 \geq P_2^{1/2} \tag{16}$$

$$P_1 = \frac{\sum\limits_{i=1}^{n} |\lambda_i^*|}{n} = \frac{Co - PIE(G)}{n} \tag{17}$$

and

$$\begin{aligned} P_2 &= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ i \neq j}}^{n} |\lambda_i^*| \, |\lambda_j^*| \quad (18) \\ &= \frac{1}{n(n-1)} \left[\left(\sum_{i=1}^{n} |\lambda_i^*| \right)^2 - \sum_{i=1}^{n} |\lambda_i^*|^2 \right] \\ &= \frac{1}{n(n-1)} \left((Co - PIE(G))^2 - S \right). \end{aligned}$$

Therefore, by (16), (17), (18) and Lemma 3.1 we get the result. From Lemma 3.1, the equality holds if and only if $|\lambda_1^*| = |\lambda_2^*| = ... = |\lambda_n^*|$. ■

Remark 3.4. *Note that in Theorem 3.3, we recover the same result in Theorem 2.1 in the paper [21], through a different approach and equality condition.*

Theorem 3.5. *Let G be a connected graph with n vertices and let S be the sum of the squares of entries in the Co-PI matrix of G. Then,*

$$Co - PIE(G) \leq \frac{S}{n} + \sqrt{(n-1) \left[S - \left(\frac{S}{n} \right)^2 \right]}. \quad (19)$$

Proof. Our proof follows the ideas of Koolen and Moulton [23, 24], who obtained an analogous upper bound for ordinary graph energy $E(G)$.

By applying the Cauchy-Schwartz inequality to the two $(n-1)$ vectors $(1, 1, ..., 1)$ and $(|\lambda_2^*|, |\lambda_3^*|, \ldots, |\lambda_n^*|)$, we get

$$\begin{aligned} \left(\sum_{i=2}^{n} |\lambda_i^*| \right)^2 &\leq (n-1) \left(\sum_{i=2}^{n} \lambda_i^{*2} \right) \\ (Co - PIE(G) - \lambda_1^*)^2 &\leq (n-1) \left(S - \lambda_1^{*2} \right) \\ Co - PIE(G) &\leq \lambda_1^* + \sqrt{(n-1)(S - \lambda_1^{*2})}. \end{aligned}$$

Now consider the following function

$$f(x) = x + \sqrt{(n-1)(S - x^2)}.$$

From

$$\sum_{i=1}^{n} \lambda_i^{*2} = S$$

we get

$$x^2 = \lambda_1^{*2} \leq S.$$

Therefore,

$$x \leq \sqrt{S}.$$

Now, $f'(x) = 0$ implies $x = \sqrt{\frac{S}{n}}$. Therefore $f(x)$ is a decreasing function in the interval $\sqrt{\frac{S}{n}} \leq x \leq 2\sqrt{\frac{S}{2}}$ and $\sqrt{\frac{S}{n}} \leq \frac{S}{n} \leq \lambda_1^*$. Hence $f(\lambda_1^*) \leq f\left(\frac{S}{n}\right)$ and inequality (19) holds. ■

Example 3.6. *Let us consider $K_{p,q}$ complete bipartite graph. Since $M_{CPI}(K_{p,q}) = |p-q|\, A(K_{p,q})$ and $K_{p,q}$ has eigenvalues $\sqrt{pq}, -\sqrt{pq}, 0$ with respective multiplicities $1, 1, p+q-2$,*

$$Co - PIE(G) = |p-q|\, E(G) = 2\,|p-q|\, \sqrt{pq}.$$

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Bounds on Multiplicative Zagreb Indices of Graph Operations and Subdivision Operators

Mahdieh Azari[a], **Ali Iranmanesh**[b,*]

[a]*Department of Mathematics, Kazerun Branch, Islamic Azad University, P. O. Box: 73135-168, Kazerun, Iran*

[b]*Department of Pure Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P. O. Box: 14115-137, Tehran, Iran*

azari@kau.ac.ir, iranmanesh@modares.ac.ir

Abstract

In this chapter, we review our recent results on computing bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the most important graph operations and subdivision operators.

Contents

1. Introduction

Chemical graphs, particularly *molecular graphs*, are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. Physico-chemical or biological properties of molecules can be predicted by using the information encoded in the molecular graphs, eventually translated in the adjacency or connectivity matrix associated to these graphs. This paradigm is achieved by considering various *graph theoretical invariants* of molecular graphs (also known as *topological indices* or *structural descriptors/measures*) and evaluating how strongly are they correlated with various molecular properties. A topological index is any function calculated on a chemical/molecular graph irrespective of the labeling of its vertices. Several hundreds of different invariants have been employed to date with various degrees of success in QSAR/QSPR studies [9, 18, 27]. Topological indices based on end-vertex-degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in QSPR/QSAR studies. Two of the oldest and most thoroughly investigated are *Zagreb indices* introduced by Gutman and Trinajstić [19] in 1972. These indices have since been used to study molecular complexity, chirality, ZE-isomerism, and hetero-systems. For details on their theory and applications see [2, 3, 6, 7, 10, 20, 23, 24, 32, 33]. Let G be a simple graph with the vertex set $V(G)$ and the edge set $E(G)$. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively, and defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 \quad \textit{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v),$$

where $d_G(u)$ denotes the degree of the vertex u in G. The first Zagreb index can also be expressed as a sum over edges of G,

$$M_1(G) = \sum_{\mathrm{uv} \in E(G)} [d_G(u) + d_G(v)].$$

Multiplicative versions of Zagreb indices were introduced by Todeschini and Consonni [26] in 2010. The first and second *multiplicative Zagreb indices* of G are denoted by $\Pi_1(G)$ and $\Pi_2(G)$, respectively, and defined as

$$\Pi_1(G) = \prod_{u \in V(G)} d_G(u)^2 \quad \textit{and} \quad \Pi_2(G) = \prod_{uv \in E(G)} d_G(u) d_G(v).$$

The second multiplicative Zagreb index can also be expressed as a product over vertices of G [17],

$$\Pi_2(G) = \prod_{u \in V(G)} d_G(u)^{d_G(u)}.$$

In 2012, Eliasi et al. [13] introduced another multiplicative version of the first Zagreb index called *multiplicative sum Zagreb index*. The multiplicative sum Zagreb index of G is denoted by $\Pi_1^*(G)$ and defined as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} \big[d_G(u) + d_G(v)\big].$$

We refer the reader to [8, 11, 12, 15, 16, 21, 22, 25, 28–31] for mathematical properties and applications of the multiplicative Zagreb indices and multiplicative sum Zagreb index.

In this chapter, we review our recent results on computing bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the most important graph operations and subdivision operators. The chapter is organized as follows. In Sect. 2, we present lower bounds on the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of several graph operations such as union, join, corona product, composition, direct product, Cartesian product, and strong product in terms of the order, size, multiplicative Zagreb indices, and multiplicative sum Zagreb index of their components. In Sect. 3, we give some upper and/or lower bounds on the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of subdivision operators in terms of the order, size, first Zagreb index, multiplicative Zagreb indices, and multiplicative sum Zagreb index of the primary graph.

2. Lower bounds on multiplicative versions of Zagreb indices of graph operations

In this section, we present lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of several graph operations such as union, join, corona product, composition, direct product, Cartesian product, and strong product in terms of the order, size, multiplicative Zagreb indices, and multiplicative sum Zagreb index of their components. All considered operations are binary. Hence, we will usually deal with two finite and simple graphs G_1 and G_2. For a given graph G_i, its vertex and edge sets will be denoted by $V(G_i)$ and $E(G_i)$, and its order and size by n_i and m_i, respectively, where $i \in \{1, 2\}$. Throughout the section, we assume that G_1 and G_2 have no isolated vertices. Most of the results of this section, have been taken from [1,4,14].

At first, we recall two well-known inequalities.

Lemma 2.1. *(AM-GM inequality) Let $x_1, x_2 \dots, x_n$ be nonnegative numbers. Then*

$$\frac{x_1 + x_2 + \cdots + x_n}{n} \geq \sqrt[n]{x_1 x_2 \dots x_n},$$

with equality if and only if $x_1 = x_2 = \ldots = x_n$.

Lemma 2.2. *Let $x_1, x_2 \dots, x_n, y_1, y_2, \dots, y_n$ be positive numbers and for every $1 \leq i \leq n$, $x_i \geq y_i$. Then*

$$x_1 x_2 \dots x_n \geq y_1 y_2 \dots y_n,$$

with equality if and only if for every $1 \leq i \leq n$, $x_i = y_i$.

2.1 Union

The *union* $G_1 \cup G_2$ of graphs G_1 and G_2 with disjoint vertex sets $V(G_1)$ and $V(G_2)$ is a graph with the vertex set $V(G_1) \cup V(G_2)$ and the edge set $E(G_1) \cup E(G_2)$. The degree of a vertex u of $G_1 \cup G_2$ is equal to the degree of u in the component $G_i,\ i \in \{1, 2\}$ that contains it.

In the following theorems, exact formulae for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the union of G_1 and G_2 are presented. The proofs follow easily from the definition of the union of graphs, so are omitted.

Theorem 2.3. *The first multiplicative Zagreb index of $G_1 \cup G_2$ is given by*

$$\Pi_1(G_1 \cup G_2) = \Pi_1(G_1)\Pi_1(G_2).$$

Theorem 2.4. *The second multiplicative Zagreb index of $G_1 \cup G_2$ is given by*

$$\Pi_2(G_1 \cup G_2) = \Pi_2(G_1)\Pi_2(G_2).$$

Theorem 2.5. *The multiplicative sum Zagreb index of $G_1 \cup G_2$ is given by*

$$\Pi_1^*(G_1 \cup G_2) = \Pi_1^*(G_1)\Pi_1^*(G_2).$$

It is clear from Theorems 2.3, 2.4, and 2.5 that we can restrict our attention to connected graphs. Since for a graph with several connected components its first and second multiplicative Zagreb indices and multiplicative sum Zagreb index are equal to the product of the indices of its components.

2.2 Join

The *join* $G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets $V(G_1)$ and $V(G_2)$ is a graph union $G_1 \cup G_2$ together with all the edges joining $V(G_1)$ and $V(G_2)$. The join of two graphs is also known as their *sum*. The degree of a vertex u of $G_1 + G_2$ is given by

$$d_{G_1+G_2}(u) = \begin{cases} d_{G_1}(u) + n_2 & u \in V(G_1), \\ d_{G_2}(u) + n_1 & u \in V(G_2). \end{cases}$$

In the following theorems, lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the join of G_1 and G_2 are presented.

Theorem 2.6. *The first multiplicative Zagreb index of $G_1 + G_2$ satisfies the following inequality:*

$$\Pi_1(G_1 + G_2) > 4^{n_1+n_2} {n_1}^{n_2} {n_2}^{n_1} \sqrt{\Pi_1(G_1)\Pi_1(G_2)}.$$

Proof. Let $G = G_1 + G_2$. By definition of the first multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\begin{aligned}\Pi_1(G) = \prod_{u\in V(G)} d_G(u)^2 &= \prod_{u\in V(G_1)} \left(d_{G_1}(u) + n_2\right)^2 \times \prod_{u\in V(G_2)} \left(d_{G_2}(u) + n_1\right)^2 \\ &> \prod_{u\in V(G_1)} \left(2\sqrt{d_{G_1}(u) \times n_2}\right)^2 \times \prod_{u\in V(G_2)} \left(2\sqrt{d_{G_2}(u) \times n_1}\right)^2 \\ &= 4^{n_1+n_2} {n_1}^{n_2} {n_2}^{n_1} \sqrt{\Pi_1(G_1)\Pi_1(G_2)}.\end{aligned}$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u \in V(G_1)$, $d_{G_1}(u) + n_2 = 2\sqrt{d_{G_1}(u) \times n_2}$ and for every $u \in V(G_2)$, $d_{G_2}(u) + n_1 = 2\sqrt{d_{G_2}(u) \times n_1}$. By Lemma 2.1, this implies that for every $u \in V(G_1)$, $d_{G_1}(u) = n_2$ and for every $u \in V(G_2)$, $d_{G_2}(u) = n_1$, which is a contradiction. ■

Theorem 2.7. *The second multiplicative Zagreb index of $G_1 + G_2$ satisfies the following inequality:*

$$\begin{aligned}\Pi_2(G_1 + G_2) > {} & 4^{m_1+m_2+n_1 n_2} {n_1}^{m_2} {n_2}^{m_1} \left(\sqrt{n_1 n_2}\right)^{n_1 n_2} \sqrt[4]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}} \\ & \times \sqrt{\Pi_2(G_1)\Pi_2(G_2)}.\end{aligned}$$

Proof. Let $G = G_1 + G_2$. By definition of the second multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\begin{aligned}
\Pi_2(G) &= \prod_{uv\in E(G)} d_G(u)d_G(v) \\
&= \prod_{uv\in E(G_1)} \big(d_{G_1}(u)+n_2\big)\big(d_{G_1}(v)+n_2\big) \\
&\quad \times \prod_{uv\in E(G_2)} \big(d_{G_2}(u)+n_1\big)\big(d_{G_2}(v)+n_1\big) \\
&\quad \times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} \big(d_{G_1}(u)+n_2\big)\big(d_{G_2}(v)+n_1\big) \\
&> \prod_{uv\in E(G_1)} \big(2\sqrt{d_{G_1}(u)\times n_2}\big)\big(2\sqrt{d_{G_1}(v)\times n_2}\big) \\
&\quad \times \prod_{uv\in E(G_2)} \big(2\sqrt{d_{G_2}(u)\times n_1}\big)\big(2\sqrt{d_{G_2}(v)\times n_1}\big) \\
&\quad \times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} \big(2\sqrt{d_{G_1}(u)\times n_2}\big)\big(2\sqrt{d_{G_2}(v)\times n_1}\big) \\
&= 4^{m_1+m_2+n_1n_2} {n_1}^{m_2} {n_2}^{m_1} (\sqrt{n_1n_2})^{n_1n_2} \sqrt[4]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}} \sqrt{\Pi_2(G_1)\Pi_2(G_2)}.
\end{aligned}$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u \in V(G_1)$ and $v \in V(G_2)$, $d_{G_1}(u) + n_2 = 2\sqrt{d_{G_1}(u) \times n_2}$ and $d_{G_2}(v) + n_1 = 2\sqrt{d_{G_2}(v) \times n_1}$. By Lemma 2.1, this implies that for every $u \in V(G_1)$ and $v \in V(G_2)$, $d_{G_1}(u) = n_2$ and $d_{G_2}(v) = n_1$, which is a contradiction. ■

Theorem 2.8. *The multiplicative sum Zagreb index of $G_1 + G_2$ satisfies the following inequality:*

$$\begin{aligned}
\Pi_1^*(G_1+G_2) >& (2\sqrt{2})^{m_1+m_2} \sqrt{{n_2}^{m_1}{n_1}^{m_2}} (3\sqrt[3]{n_1+n_2})^{n_1n_2} \sqrt[6]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}} \\
&\times \sqrt{\Pi_1^*(G_1)\Pi_1^*(G_2)}.
\end{aligned}$$

Proof. Let $G = G_1 + G_2$. By definition of the multiplicative sum Zagreb index, we have

$$\begin{aligned}
\Pi_1^*(G) &= \prod_{uv\in E(G)} \big[d_G(u)+d_G(v)\big] = \prod_{uv\in E(G_1)} \big[\big(d_{G_1}(u)+n_2\big)+\big(d_{G_1}(v)+n_2\big)\big] \\
&\quad \times \prod_{uv\in E(G_2)} \big[\big(d_{G_2}(u)+n_1\big)+\big(d_{G_2}(v)+n_1\big)\big] \\
&\quad \times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} \big[\big(d_{G_1}(u)+n_2\big)+\big(d_{G_2}(v)+n_1\big)\big] \\
&= \prod_{uv\in E(G_1)} \big[\big(d_{G_1}(u)+d_{G_1}(v)\big)+2n_2\big] \\
&\quad \times \prod_{uv\in E(G_2)} \big[\big(d_{G_2}(u)+d_{G_2}(v)\big)+2n_1\big] \\
&\quad \times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} \big[d_{G_1}(u)+d_{G_2}(v)+(n_1+n_2)\big].
\end{aligned}$$

Now by Lemmas 2.1 and 2.2, we have

$$\begin{aligned}\Pi_1^*(G) >& \prod_{uv\in E(G_1)} 2\sqrt{\big(d_{G_1}(u)+d_{G_1}(v)\big)\times 2n_2}\\ &\times \prod_{uv\in E(G_2)} 2\sqrt{\big(d_{G_2}(u)+d_{G_2}(v)\big)\times 2n_1}\\ &\times \prod_{u\in V(G_1)}\prod_{v\in V(G_2)} 3\sqrt[3]{d_{G_1}(u)\times d_{G_2}(v)\times(n_1+n_2)}\\ =&(2\sqrt{2})^{m_1+m_2}\sqrt{{n_2}^{m_1}{n_1}^{m_2}}\,(3\sqrt[3]{n_1+n_2})^{n_1n_2}\sqrt[6]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}\sqrt{\Pi_1^*(G_1)\Pi_1^*(G_2)}.\end{aligned}$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u\in V(G_1)$ and $v\in V(G_2)$, $d_{G_1}(u)+d_{G_2}(v)+(n_1+n_2)=3\sqrt[3]{d_{G_1}(u)\times d_{G_2}(v)\times(n_1+n_2)}$. By Lemma 2.1, this implies that for every $u\in V(G_1)$ and $v\in V(G_2)$, $d_{G_1}(u)=d_{G_2}(v)=n_1+n_2$, which is a contradiction. ■

2.3 Corona product

The *corona product* $G_1\circ G_2$ of graphs G_1 and G_2 is a graph obtained by taking one copy of G_1 and n_1 copies of G_2 and joining the $i-$th vertex of G_1 to every vertex in $i-$th copy of G_2 for $1\le i\le n_1$. We denote the $i-$th copy of G_2 by $G_{2,i}$, $1\le i\le n_1$. The degree of a vertex u of $G_1\circ G_2$ is given by

$$d_{G_1\circ G_2}(u)=\begin{cases} d_{G_1}(u)+n_2 & u\in V(G_1),\\ d_{G_2}(u)+1 & u\in V(G_{2,i}).\end{cases}$$

In the following theorems, lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the corona product $G_1\circ G_2$ are presented.

Theorem 2.9. *The first multiplicative Zagreb index of $G_1\circ G_2$ satisfies the following inequality:*

$$\Pi_1(G_1\circ G_2)\ge 4^{n_1(n_2+1)}(n_2)^{n_1}\sqrt{\Pi_1(G_1)\Pi_1(G_2)^{n_1}},$$

with equality if and only if G_1 is an n_2-regular graph and G_2 is a $1-$regular graph.

Proof. Let $G=G_1\circ G_2$. By definition of the first multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\begin{aligned}\Pi_1(G)=\prod_{u\in V(G)} d_G(u)^2 =& \prod_{u\in V(G_1)}\big(d_{G_1}(u)+n_2\big)^2\times\Big[\prod_{u\in V(G_2)}\big(d_{G_2}(u)+1\big)^2\Big]^{n_1}\\ \ge& \prod_{u\in V(G_1)}\big(2\sqrt{d_{G_1}(u)\times n_2}\big)^2\times\Big[\prod_{u\in V(G_2)}\big(2\sqrt{d_{G_2}(u)}\big)^2\Big]^{n_1}\\ =&4^{n_1(n_2+1)}(n_2)^{n_1}\sqrt{\Pi_1(G_1)\Pi_1(G_2)^{n_1}}.\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u\in V(G_1)$, $d_{G_1}(u)+n_2=2\sqrt{d_{G_1}(u)\times n_2}$ and for every $u\in V(G_2)$, $d_{G_2}(u)+1=2\sqrt{d_{G_2}(u)}$. By Lemma 2.1, this implies that for every $u\in V(G_1)$, $d_{G_1}(u)=n_2$ and for every $u\in V(G_2)$, $d_{G_2}(u)=1$. So, the equality holds if and only if G_1 is an n_2-regular graph and G_2 is a $1-$regular graph. ■

Theorem 2.10. *The second multiplicative Zagreb index of $G_1 \circ G_2$ satisfies the following inequality:*

$$\Pi_2(G_1 \circ G_2) \geq 4^{m_1+n_1m_2+n_1n_2}(\sqrt{n_2})^{n_1n_2+2m_1}\sqrt[4]{\Pi_1(G_1)^{n_2}\ \Pi_1(G_2)^{n_1}}\sqrt{\Pi_2(G_1)\Pi_2(G_2)^{n_1}},$$

with equality if and only if G_1 is an n_2-regular graph and G_2 is a $1-$regular graph.

Proof. Let $G = G_1 \circ G_2$. By definition of the second multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\begin{aligned}\Pi_2(G) = \prod_{uv\in E(G)} d_G(u)d_G(v) = &\prod_{uv\in E(G_1)} \big(d_{G_1}(u)+n_2\big)\big(d_{G_1}(v)+n_2\big)\\ &\times\Big[\prod_{uv\in E(G_2)}\big(d_{G_2}(u)+1\big)\big(d_{G_2}(v)+1\big)\Big]^{n_1}\\ &\times\prod_{u\in V(G_1)}\prod_{v\in V(G_2)}\big(d_{G_1}(u)+n_2\big)\big(d_{G_2}(v)+1\big)\\ \geq &\prod_{uv\in E(G_1)}\big(2\sqrt{d_{G_1}(u)\times n_2}\big)\big(2\sqrt{d_{G_1}(v)\times n_2}\big)\\ &\times\Big[\prod_{uv\in E(G_2)}\big(2\sqrt{d_{G_2}(u)}\big)\big(2\sqrt{d_{G_2}(v)}\big)\Big]^{n_1}\\ &\times\prod_{u\in V(G_1)}\prod_{v\in V(G_2)}\big(2\sqrt{d_{G_1}(u)\times n_2}\big)\big(2\sqrt{d_{G_2}(v)}\big)\\ =&4^{m_1+n_1m_2+n_1n_2}(\sqrt{n_2})^{n_1n_2+2m_1}\sqrt[4]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}\\ &\times\sqrt{\Pi_2(G_1)\Pi_2(G_2)^{n_1}}.\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $uv \in E(G_1)$, $d_{G_1}(u) + n_2 = 2\sqrt{d_{G_1}(u)\times n_2}$, $d_{G_1}(v) + n_2 = 2\sqrt{d_{G_1}(v)\times n_2}$, for every $uv \in E(G_2)$, $d_{G_2}(u) + 1 = 2\sqrt{d_{G_2}(u)}$, $d_{G_2}(v) + 1 = 2\sqrt{d_{G_2}(v)}$, and for every $u \in V(G_1)$, $v \in V(G_2)$, $d_{G_1}(u) + n_2 = 2\sqrt{d_{G_1}(u)\times n_2}$, $d_{G_2}(v) + 1 = 2\sqrt{d_{G_2}(v)}$. By Lemma 2.1, this implies that for every $u \in V(G_1)$, $d_{G_1}(u) = n_2$ and for every $v \in V(G_2)$, $d_{G_2}(v) = 1$. So, the equality holds if and only if G_1 is an n_2-regular graph and G_2 is a $1-$regular graph. ■

Theorem 2.11. *The multiplicative sum Zagreb index of $G_1 \circ G_2$ satisfies the following inequality:*

$$\begin{aligned}\Pi_1^*(G_1 \circ G_2) >&(2\sqrt{2})^{m_1+n_1m_2}(\sqrt{n_2})^{m_1}(3\sqrt[3]{n_2+1})^{n_1n_2}\sqrt[6]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}\\ &\times\sqrt{\Pi_1^*(G_1)\Pi_1^*(G_2)^{n_1}}.\end{aligned}$$

Proof. Let $G = G_1 \circ G_2$. By definition of the multiplicative sum Zagreb index, we have

$$\begin{aligned}\Pi_1^*(G) &= \prod_{uv\in E(G)}\big[d_G(u)+d_G(v)\big]\\ &= \prod_{uv\in E(G_1)}\big[\big(d_{G_1}(u)+n_2\big)+\big(d_{G_1}(v)+n_2\big)\big]\end{aligned}$$

$$
\begin{aligned}
&\times \Big[\prod_{uv\in E(G_2)} \big[\big(d_{G_2}(u)+1\big)+\big(d_{G_2}(v)+1\big)\big]\Big]^{n_1}\\
&\times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} \big[\big(d_{G_1}(u)+n_2\big)+\big(d_{G_2}(v)+1\big)\big]\\
= &\prod_{uv\in E(G_1)} \big[\big(d_{G_1}(u)+d_{G_1}(v)\big)+2n_2\big]\\
&\times \Big[\prod_{uv\in E(G_2)} \big[\big(d_{G_2}(u)+d_{G_2}(v)\big)+2\big]\Big]^{n_1}\\
&\times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} \big[d_{G_1}(u)+d_{G_2}(v)+(n_2+1)\big].
\end{aligned}
$$

Now by Lemmas 2.1 and 2.2, we have

$$
\begin{aligned}
\Pi_1^*(G) > &\prod_{uv\in E(G_1)} 2\sqrt{\big(d_{G_1}(u)+d_{G_1}(v)\big)\times 2n_2}\\
&\times \Big[\prod_{uv\in E(G_2)} 2\sqrt{\big(d_{G_2}(u)+d_{G_2}(v)\big)\times 2}\Big]^{n_1}\\
&\times \prod_{u\in V(G_1)} \prod_{v\in V(G_2)} 3\sqrt[3]{d_{G_1}(u)\times d_{G_2}(v)\times (n_2+1)}\\
=&(2\sqrt{2})^{m_1+n_1m_2}(\sqrt{n_2}\,)^{m_1}(3\sqrt[3]{n_2+1})^{n_1n_2}\sqrt[6]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}\sqrt{\Pi_1^*(G_1)\Pi_1^*(G_2)^{n_1}}.
\end{aligned}
$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u \in V(G_1)$ and $v \in V(G_2)$, $d_{G_1}(u)+d_{G_2}(v)+(n_2+1) = 3\sqrt[3]{d_{G_1}(u)\times d_{G_2}(v)\times (n_2+1)}$. By Lemma 2.1, this implies that for every $u \in V(G_1)$ and $v \in V(G_2)$, $d_{G_1}(u) = d_{G_2}(v) = n_2+1$, which is a contradiction. ■

2.4 Composition

The *composition* $G_1[G_2]$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1)\times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if $u_1v_1 \in E(G_1)$ or [$u_1 = v_1$ and $u_2v_2 \in E(G_2)$]. The composition of two graphs is also known as their *lexicographic product*. The degree of a vertex $u = (u_1, u_2)$ of $G_1[G_2]$ is given by

$$d_{G_1[G_2]}(u) = n_2 d_{G_1}(u_1) + d_{G_2}(u_2).$$

In the following theorems, lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the composition $G_1[G_2]$ are presented.

Theorem 2.12. *The first multiplicative Zagreb index of $G_1[G_2]$ satisfies the following inequality:*

$$\Pi_1(G_1[G_2]) > (4n_2)^{n_1n_2}\sqrt{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}.$$

Proof. Let $G = G_1[G_2]$. By definition of the first multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\Pi_1(G) = \prod_{(u_1,u_2)\in V(G)} d_G((u_1,u_2))^2 = \prod_{u_1\in V(G_1)} \prod_{u_2\in V(G_2)} \big(n_2 d_{G_1}(u_1) + d_{G_2}(u_2)\big)^2$$

$$
\begin{aligned}
&> \prod_{u_1\in V(G_1)} \prod_{u_2\in V(G_2)} \left(2\sqrt{n_2 d_{G_1}(u_1)\times d_{G_2}(u_2)}\right)^2\\
&=(4n_2)^{n_1 n_2}\sqrt{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}.
\end{aligned}
$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$, $n_2 d_{G_1}(u_1) + d_{G_2}(u_2) = 2\sqrt{n_2 d_{G_1}(u_1) \times d_{G_2}(u_2)}$. By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$, $n_2 d_{G_1}(u_1) = d_{G_2}(u_2)$, which is a contradiction. ■

Theorem 2.13. *The second multiplicative Zagreb index of $G_1[G_2]$ satisfies the following inequality:*

$$\Pi_2(G_1[G_2]) > (4n_2)^{n_1 m_2 + n_2^2 m_1}\sqrt{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1 n_2}}\sqrt{\Pi_2(G_1)^{n_2^2}\Pi_2(G_2)^{n_1}}.$$

Proof. Let $G = G_1[G_2]$. By definition of the second multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$
\begin{aligned}
\Pi_2(G) &= \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} d_G((u_1,u_2))d_G((v_1,v_2))\\
&= \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \left(n_2 d_{G_1}(u_1) + d_{G_2}(u_2)\right)\left(n_2 d_{G_1}(u_1) + d_{G_2}(v_2)\right)\\
&\quad\times \prod_{u_1v_1\in E(G_1)} \prod_{u_2\in V(G_2)} \prod_{v_2\in V(G_2)} \left(n_2 d_{G_1}(u_1) + d_{G_2}(u_2)\right)\left(n_2 d_{G_1}(v_1) + d_{G_2}(v_2)\right)\\
&> \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \left(2\sqrt{n_2 d_{G_1}(u_1)\times d_{G_2}(u_2)}\right)\left(2\sqrt{n_2 d_{G_1}(u_1)\times d_{G_2}(v_2)}\right)\\
&\quad\times \prod_{u_1v_1\in E(G_1)} \prod_{u_2\in V(G_2)} \prod_{v_2\in V(G_2)} \left(2\sqrt{n_2 d_{G_1}(u_1)\times d_{G_2}(u_2)}\right)\left(2\sqrt{n_2 d_{G_1}(v_1)\times d_{G_2}(v_2)}\right)\\
&=(4n_2)^{n_1 m_2 + n_2^2 m_1}\sqrt{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1 n_2}}\sqrt{\Pi_2(G_1)^{n_2^2}\Pi_2(G_2)^{n_1}}.
\end{aligned}
$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$, $n_2 d_{G_1}(u_1) + d_{G_2}(u_2) = 2\sqrt{n_2 d_{G_1}(u_1) \times d_{G_2}(u_2)}$ and $n_2 d_{G_1}(u_1) + d_{G_2}(v_2) = 2\sqrt{n_2 d_{G_1}(u_1) \times d_{G_2}(v_2)}$. By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$, $n_2 d_{G_1}(u_1) = d_{G_2}(u_2) = d_{G_2}(v_2)$, which is a contradiction. ■

Theorem 2.14. *The multiplicative sum Zagreb index of $G_1[G_2]$ satisfies the following inequality:*

$$
\begin{aligned}
\Pi_1^*(G_1[G_2]) >&(2\sqrt{2})^{n_1 m_2} 3^{n_2^2 m_1}(\sqrt[6]{n_2})^{3n_1 m_2 + 2n_2^2 m_1}\sqrt[12]{\Pi_1(G_1)^{3m_2}\Pi_1(G_2)^{4m_1 n_2}}\\
&\times\sqrt[6]{\Pi_1^*(G_1)^{2n_2^2}\Pi_1^*(G_2)^{3n_1}}.
\end{aligned}
$$

Proof. Let $G = G_1[G_2]$. By definition of the multiplicative sum Zagreb index, we have

$$
\begin{aligned}
\Pi_1^*(G) &= \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} \left[d_G((u_1,u_2)) + d_G((v_1,v_2))\right]\\
&= \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \left[\left(n_2 d_{G_1}(u_1) + d_{G_2}(u_2)\right) + \left(n_2 d_{G_1}(u_1) + d_{G_2}(v_2)\right)\right]
\end{aligned}
$$

$$\times \prod_{u_1v_1\in E(G_1)} \prod_{u_2\in V(G_2)} \prod_{v_2\in V(G_2)} \left[\left(n_2 d_{G_1}(u_1) + d_{G_2}(u_2)\right) + \left(n_2 d_{G_1}(v_1) + d_{G_2}(v_2)\right)\right]$$
$$= \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \left[2n_2 d_{G_1}(u_1) + \left(d_{G_2}(u_2) + d_{G_2}(v_2)\right)\right]$$
$$\times \prod_{u_1v_1\in E(G_1)} \prod_{u_2\in V(G_2)} \prod_{v_2\in V(G_2)} \left[n_2\left(d_{G_1}(u_1) + d_{G_1}(v_1)\right) + d_{G_2}(u_2) + d_{G_2}(v_2)\right].$$

Now by Lemmas 2.1 and 2.2, we have

$$\Pi_1^*(G) > \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} 2\sqrt{2n_2 d_{G_1}(u_1) \times \left(d_{G_2}(u_2) + d_{G_2}(v_2)\right)}$$
$$\times \prod_{u_1v_1\in E(G_1)} \prod_{u_2\in V(G_2)} \prod_{v_2\in V(G_2)} 3\sqrt[3]{n_2\left(d_{G_1}(u_1) + d_{G_1}(v_1)\right) \times d_{G_2}(u_2) \times d_{G_2}(v_2)}$$
$$=(2\sqrt{2})^{n_1m_2} 3^{n_2^2 m_1} (\sqrt[6]{n_2})^{3n_1m_2+2n_2^2m_1} \sqrt[12]{\Pi_1(G_1)^{3m_2}\Pi_1(G_2)^{4m_1n_2}}$$
$$\times \sqrt[6]{\Pi_1^*(G_1)^{2n_2^2}\Pi_1^*(G_2)^{3n_1}}.$$

The above inequality is strict. Since if the equality holds then by Lemma 2.2, for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$,

$$2n_2 d_{G_1}(u_1) + \left(d_{G_2}(u_2) + d_{G_2}(v_2)\right) = 2\sqrt{2n_2 d_{G_1}(u_1) \times \left(d_{G_2}(u_2) + d_{G_2}(v_2)\right)}.$$

By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$, $d_{G_2}(u_2) + d_{G_2}(v_2) = 2n_2 d_{G_1}(u_1)$, which is a contradiction. ■

2.5 Direct product

The *direct product* $G_1 \times G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$. The direct product of two graphs is also known as their *tensor product*, *Kronecker product*, *categorical product*, *cardinal product*, *relational product* or *conjunction*. The degree of a vertex $u = (u_1, u_2)$ of $G_1 \times G_2$ is given by

$$d_{G_1\times G_2}(u) = d_{G_1}(u_1)d_{G_2}(u_2).$$

In the following theorems, exact formulae for the first and second multiplicative Zagreb indices of the direct product $G_1 \times G_2$ and a lower bound for its multiplicative sum Zagreb index are presented.

Theorem 2.15. *The first multiplicative Zagreb index of $G_1 \times G_2$ satisfies the following inequality:*

$$\Pi_1(G_1 \times G_2) = \Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}.$$

Proof. Let $G = G_1 \times G_2$. By definition of the first multiplicative Zagreb index, we have

$$\Pi_1(G) = \prod_{(u_1,u_2)\in V(G)} d_G((u_1,u_2))^2 = \prod_{u_1\in V(G_1)} \prod_{u_2\in V(G_2)} \left(d_{G_1}(u_1)d_{G_2}(u_2)\right)^2$$
$$=\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}.$$

■

Theorem 2.16. *The second multiplicative Zagreb index of $G_1 \times G_2$ satisfies the following inequality:*

$$\Pi_2(G_1 \times G_2) = \Pi_2(G_1)^{2m_2}\Pi_2(G_2)^{2m_1}.$$

Proof. Let $G = G_1 \times G_2$. By definition of the second multiplicative Zagreb index, we have

$$\begin{aligned}
\Pi_2(G) =& \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} d_G((u_1,u_2))d_G((v_1,v_2)) \\
=& \prod_{u_1v_1\in E(G_1)} \prod_{u_2v_2\in E(G_2)} \big[\big(d_{G_1}(u_1)d_{G_2}(u_2)d_{G_1}(v_1)d_{G_2}(v_2)\big) \\
& \times \big(d_{G_1}(u_1)d_{G_2}(v_2)d_{G_1}(v_1)d_{G_2}(u_2)\big)\big] \\
=& \prod_{u_1v_1\in E(G_1)} \prod_{u_2v_2\in E(G_2)} \big(d_{G_1}(u_1)d_{G_1}(v_1)\big)^2\big(d_{G_2}(u_2)d_{G_2}(v_2)\big)^2 \\
=&\Pi_2(G_1)^{2m_2}\Pi_2(G_2)^{2m_1}.
\end{aligned}$$

■

Theorem 2.17. *The multiplicative sum Zagreb index of $G_1 \times G_2$ satisfies the following inequality:*

$$\Pi_1^*(G_1 \times G_2) \geq 4^{m_1m_2}\Pi_2(G_1)^{m_2}\Pi_2(G_2)^{m_1},$$

with equality if and only if G_1 and G_2 are regular graphs.

Proof. Let $G = G_1 \times G_2$. By definition of the multiplicative sum Zagreb index, we have

$$\begin{aligned}
\Pi_1^*(G) =& \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} \big[d_G((u_1,u_2)) + d_G((v_1,v_2))\big] \\
=& \prod_{u_1v_1\in E(G_1)} \prod_{u_2v_2\in E(G_2)} \big[\big(d_{G_1}(u_1)d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(v_2)\big) \\
& \times \big(d_{G_1}(u_1)d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(u_2)\big)\big].
\end{aligned}$$

Now by Lemmas 2.1 and 2.2, we have

$$\begin{aligned}
\Pi_1^*(G) \geq& \prod_{u_1v_1\in E(G_1)} \prod_{u_2v_2\in E(G_2)} \big[2\sqrt{d_{G_1}(u_1)d_{G_2}(u_2) \times d_{G_1}(v_1)d_{G_2}(v_2)} \\
& \times 2\sqrt{d_{G_1}(u_1)d_{G_2}(v_2) \times d_{G_1}(v_1)d_{G_2}(u_2)}\big] \\
=& \prod_{u_1v_1\in E(G_1)} \prod_{u_2v_2\in E(G_2)} 4\big[d_{G_1}(u_1)d_{G_1}(v_1) \times d_{G_2}(u_2)d_{G_2}(v_2)\big] \\
=&4^{m_1m_2}\Pi_2(G_1)^{m_2}\Pi_2(G_2)^{m_1}.
\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$,

$$d_{G_1}(u_1)d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(v_2) = 2\sqrt{d_{G_1}(u_1)d_{G_2}(u_2) \times d_{G_1}(v_1)d_{G_2}(v_2)}$$

and

$$d_{G_1}(u_1)d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(u_2) = 2\sqrt{d_{G_1}(u_1)d_{G_2}(v_2) \times d_{G_1}(v_1)d_{G_2}(u_2)}.$$

By Lemma 2.1, this implies that for every $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$,

$$d_{G_1}(u_1)d_{G_2}(u_2) = d_{G_1}(v_1)d_{G_2}(v_2)$$

and

$$d_{G_1}(u_1)d_{G_2}(v_2) = d_{G_1}(v_1)d_{G_2}(u_2),$$

which clearly implies that G_1 and G_2 must be regular graphs. ■

2.6 Cartesian product

The *Cartesian product* $G_1 \Box G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if [$u_1 = v_1$ and $u_2v_2 \in E(G_2)$] or [$u_2 = v_2$ and $u_1v_1 \in E(G_1)$]. The degree of a vertex $u = (u_1, u_2)$ of $G_1 \Box G_2$ is given by

$$d_{G_1 \Box G_2}(u) = d_{G_1}(u_1) + d_{G_2}(u_2).$$

In the following theorems, lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the Cartesian product $G_1 \Box G_2$ are presented.

Theorem 2.18. *The first multiplicative Zagreb index of $G_1 \Box G_2$ satisfies the following inequality:*

$$\Pi_1(G_1 \Box G_2) \geq 4^{n_1n_2}\sqrt{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}},$$

with equality if and only if G_1 and G_2 are regular graphs with the same regularities.

Proof. Let $G = G_1 \Box G_2$. By definition of the first multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\begin{aligned}\Pi_1(G) = \prod_{(u_1,u_2)\in V(G)} d_G((u_1,u_2))^2 &= \prod_{u_1\in V(G_1)}\prod_{u_2\in V(G_2)} \big(d_{G_1}(u_1) + d_{G_2}(u_2)\big)^2 \\ &\geq \prod_{u_1\in V(G_1)}\prod_{u_2\in V(G_2)} \Big(2\sqrt{d_{G_1}(u_1) \times d_{G_2}(u_2)}\Big)^2 \\ &= 4^{n_1n_2}\sqrt{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}}.\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$,

$$d_{G_1}(u_1) + d_{G_2}(u_2) = 2\sqrt{d_{G_1}(u_1)d_{G_2}(u_2)}.$$

By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$, $d_{G_1}(u_1) = d_{G_2}(u_2)$. This clearly implies that G_1 and G_2 must be regular graphs with the same regularities. ■

Theorem 2.19. *The second multiplicative Zagreb index of $G_1 \Box G_2$ satisfies the following inequality:*

$$\Pi_2(G_1 \Box G_2) \geq 4^{n_1m_2+n_2m_1}\sqrt{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1}\Pi_2(G_1)^{n_2}\Pi_2(G_2)^{n_1}},$$

with equality if and only if G_1 and G_2 are regular graphs with the same regularities.

Proof. Let $G = G_1 \square G_2$. By definition of the second multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\begin{aligned}
\Pi_2(G) =& \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} d_G((u_1,u_2))d_G((v_1,v_2)) \\
=& \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \big(d_{G_1}(u_1)+d_{G_2}(u_2)\big)\big(d_{G_1}(u_1)+d_{G_2}(v_2)\big) \\
&\times \prod_{u_2\in V(G_2)} \prod_{u_1v_1\in E(G_1)} \big(d_{G_1}(u_1)+d_{G_2}(u_2)\big)\big(d_{G_1}(v_1)+d_{G_2}(u_2)\big) \\
\geq& \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \big(2\sqrt{d_{G_1}(u_1)\times d_{G_2}(u_2)}\big)\big(2\sqrt{d_{G_1}(u_1)\times d_{G_2}(v_2)}\big) \\
&\times \prod_{u_2\in V(G_2)} \prod_{u_1v_1\in E(G_1)} \big(2\sqrt{d_{G_1}(u_1)\times d_{G_2}(u_2)}\big)\big(2\sqrt{d_{G_1}(v_1)\times d_{G_2}(u_2)}\big) \\
=& 4^{n_1m_2+n_2m_1}\sqrt{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1}\Pi_2(G_1)^{n_2}\Pi_2(G_2)^{n_1}}.
\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$, $d_{G_1}(u_1)+d_{G_2}(u_2) = 2\sqrt{d_{G_1}(u_1)\times d_{G_2}(u_2)}$, $d_{G_1}(u_1)+d_{G_2}(v_2) = 2\sqrt{d_{G_1}(u_1)\times d_{G_2}(v_2)}$, and for every $u_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)$, $d_{G_1}(u_1)+d_{G_2}(u_2) = 2\sqrt{d_{G_1}(u_1)\times d_{G_2}(u_2)}$, $d_{G_1}(v_1)+d_{G_2}(u_2) = 2\sqrt{d_{G_1}(v_1)\times d_{G_2}(u_2)}$. By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$, $d_{G_1}(u_1) = d_{G_2}(u_2) = d_{G_2}(v_2)$, and for every $u_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)$, $d_{G_2}(u_2) = d_{G_1}(u_1) = d_{G_1}(v_1)$. This clearly implies that G_1 and G_2 must be regular graphs with the same regularities. ■

Theorem 2.20. *The multiplicative sum Zagreb index of $G_1 \square G_2$ satisfies the following inequality:*

$$\Pi_1^*(G_1\square G_2) \geq (2\sqrt{2})^{n_1m_2+n_2m_1}\sqrt[4]{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1}}\sqrt{\Pi_1^*(G_1)^{n_2}\Pi_1^*(G_2)^{n_1}},$$

with equality if and only if G_1 and G_2 are regular graphs with the same regularities.

Proof. Let $G = G_1 \square G_2$. By definition of the multiplicative sum Zagreb index, we have

$$\begin{aligned}
\Pi_1^*(G) =& \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} \big[d_G((u_1,u_2))+d_G((v_1,v_2))\big] \\
=& \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \big[\big(d_{G_1}(u_1)+d_{G_2}(u_2)\big)+\big(d_{G_1}(u_1)+d_{G_2}(v_2)\big)\big] \\
&\times \prod_{u_2\in V(G_2)} \prod_{u_1v_1\in E(G_1)} \big[\big(d_{G_1}(u_1)+d_{G_2}(u_2)\big)+\big(d_{G_1}(v_1)+d_{G_2}(u_2)\big)\big] \\
=& \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} \big[2d_{G_1}(u_1)+\big(d_{G_2}(u_2)+d_{G_2}(v_2)\big)\big] \\
&\times \prod_{u_2\in V(G_2)} \prod_{u_1v_1\in E(G_1)} \big[2d_{G_2}(u_2)+\big(d_{G_1}(u_1)+d_{G_1}(v_1)\big)\big].
\end{aligned}$$

Now by Lemmas 2.1 and 2.2, we have

$$\Pi_1^*(G) \geq \prod_{u_1\in V(G_1)} \prod_{u_2v_2\in E(G_2)} 2\sqrt{2d_{G_1}(u_1)\times\big(d_{G_2}(u_2)+d_{G_2}(v_2)\big)}$$

$$\times \prod_{u_2 \in V(G_2)} \prod_{u_1v_1 \in E(G_1)} 2\sqrt{2d_{G_2}(u_2) \times \big(d_{G_1}(u_1) + d_{G_1}(v_1)\big)}$$
$$= (2\sqrt{2})^{n_1m_2} \sqrt[4]{\Pi_1(G_1)^{m_2}} \sqrt{\Pi_1^*(G_2)^{n_1}} \times (2\sqrt{2})^{n_2m_1} \sqrt[4]{\Pi_1(G_2)^{m_1}} \sqrt{\Pi_1^*(G_1)^{n_2}}$$
$$= (2\sqrt{2})^{n_1m_2+n_2m_1} \sqrt[4]{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1}} \sqrt{\Pi_1^*(G_1)^{n_2}\Pi_1^*(G_2)^{n_1}}.$$

By Lemma 2.2, the above equality holds if and only if for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$,

$$2d_{G_1}(u_1) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) = 2\sqrt{2d_{G_1}(u_1) \times \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)},$$

and for every $u_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)$,

$$2d_{G_2}(u_2) + \big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) = 2\sqrt{2d_{G_2}(u_2) \times \big(d_{G_1}(u_1) + d_{G_1}(v_1)\big)}.$$

By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$, $2d_{G_1}(u_1) = d_{G_2}(u_2) + d_{G_2}(v_2)$, and for every $u_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)$, $2d_{G_2}(u_2) = d_{G_1}(u_1) + d_{G_1}(v_1)$. This clearly implies that G_1 and G_2 must be regular graphs with the same regularities. ■

2.7 Strong product

The *strong product* $G_1 \boxtimes G_2$ of graphs G_1 and G_2 has the vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if [$u_1 = v_1$ and $u_2v_2 \in E(G_2)$] or [$u_2 = v_2$ and $u_1v_1 \in E(G_1)$] or [$u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$]. The degree of a vertex $u = (u_1, u_2)$ of $G_1 \boxtimes G_2$ is given by

$$d_{G_1 \boxtimes G_2}(u) = d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2).$$

In the following theorems, lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the strong product $G_1 \boxtimes G_2$ are presented.

Theorem 2.21. *The first multiplicative Zagreb index of $G_1 \boxtimes G_2$ satisfies the following inequality:*

$$\Pi_1(G_1 \boxtimes G_2) \geq 9^{n_1n_2} \sqrt[3]{\Pi_1(G_1)^{n_2}\Pi_1(G_2)^{n_1}},$$

with equality if and only if G_1 and G_2 are $1-$regular graphs.

Proof. Let $G = G_1 \boxtimes G_2$. By definition of the first multiplicative Zagreb index and Lemmas 2.1 and 2.2, we have

$$\Pi_1(G) = \prod_{(u_1,\, u_2) \in V(G)} d_G((u_1, u_2))^2$$
$$= \prod_{u_1 \in V(G_1)} \prod_{u_2 \in V(G_2)} \big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2)\big)^2$$
$$\geq \prod_{u_1 \in V(G_1)} \prod_{u_2 \in V(G_2)} \big(3\sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(u_2) \times d_{G_1}(u_1)d_{G_2}(u_2)}\big)^2$$

$$
\begin{aligned}
&= \prod_{u_1 \in V(G_1)} \prod_{u_2 \in V(G_2)} 9 \sqrt[3]{d_{G_1}(u_1)^2 \times d_{G_2}(u_2)^2} \\
&= 9^{n_1 n_2} \sqrt[3]{\Pi_1(G_1)^{n_2} \Pi_1(G_2)^{n_1}}.
\end{aligned}
$$

By Lemma 2.2, the above equality holds if and only if for every $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$,

$$
d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1) d_{G_2}(u_2) = 3 \sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(u_2) \times d_{G_1}(u_1) d_{G_2}(u_2)}.
$$

By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2 \in V(G_2)$, $d_{G_1}(u_1) = d_{G_2}(u_2) = d_{G_1}(u_1) d_{G_2}(u_2)$. So, the equality holds if and only if G_1 and G_2 are $1-$regular graphs. ■

Theorem 2.22. *The second multiplicative Zagreb index of $G_1 \boxtimes G_2$ satisfies the following inequality:*

$$
\Pi_2(G_1 \boxtimes G_2) \geq 9^{n_1 m_2 + n_2 m_1 + 2 m_1 m_2} \sqrt[3]{\Pi_1(G_1)^{2m_2} \Pi_1(G_2)^{2m_1} \Pi_2(G_1)^{2n_2 + 4m_2} \Pi_2(G_2)^{2n_1 + 4m_1}},
$$

with equality if and only if G_1 and G_2 are $1-$regular graphs.

Proof. Let $G = G_1 \boxtimes G_2$. By definition of the second multiplicative Zagreb index, we have

$$
\Pi_2(G) = \prod_{(u_1,u_2)(v_1,v_2) \in E(G)} d_G((u_1, u_2)) d_G((v_1, v_2)).
$$

By definition of the strong product, we can partition the above product into three products as follows.

The first product P_1 is taken over all edges $(u_1, u_2)(v_1, v_2) \in E(G)$ such that $u_1 = v_1$ and $u_2 v_2 \in E(G_2)$. By Lemmas 2.1 and 2.2, we have

$$
\begin{aligned}
P_1 = &\prod_{u_1 \in V(G_1)} \prod_{u_2 v_2 \in E(G_2)} \big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1) d_{G_2}(u_2)\big) \\
&\times \big(d_{G_1}(u_1) + d_{G_2}(v_2) + d_{G_1}(u_1) d_{G_2}(v_2)\big) \\
\geq &\prod_{u_1 \in V(G_1)} \prod_{u_2 v_2 \in E(G_2)} \big[3 \sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(u_2) \times d_{G_1}(u_1) d_{G_2}(u_2)} \\
&\times 3 \sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(v_2) \times d_{G_1}(u_1) d_{G_2}(v_2)}\big] \\
= &\prod_{u_1 \in V(G_1)} \prod_{u_2 v_2 \in E(G_2)} 9 \sqrt[3]{d_{G_1}(u_1)^4 \times \big(d_{G_2}(u_2) d_{G_2}(v_2)\big)^2} \\
= &9^{n_1 m_2} \sqrt[3]{\Pi_1(G_1)^{2m_2} \Pi_2(G_2)^{2n_1}}.
\end{aligned}
$$

By Lemma 2.2, the above equality holds if and only if for every $u_1 \in V(G_1)$ and $u_2 v_2 \in E(G_2)$,

$$
d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1) d_{G_2}(u_2) = 3 \sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(u_2) \times d_{G_1}(u_1) d_{G_2}(u_2)}
$$

and

$$
d_{G_1}(u_1) + d_{G_2}(v_2) + d_{G_1}(u_1) d_{G_2}(v_2) = 3 \sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(v_2) \times d_{G_1}(u_1) d_{G_2}(v_2)}.
$$

By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2 v_2 \in E(G_2)$,

$$
d_{G_1}(u_1) = d_{G_2}(u_2) = d_{G_2}(v_2) = d_{G_1}(u_1) d_{G_2}(u_2) = d_{G_1}(u_1) d_{G_2}(v_2).
$$

So, the equality holds if and only if G_1 and G_2 are $1-$regular graphs.

The second product P_2 is taken over all edges $(u_1, u_2)(v_1, v_2) \in E(G)$ such that $u_1v_1 \in E(G_1)$ and $u_2 = v_2$. So,

$$P_2 = \prod_{u_1v_1 \in E(G_1)} \prod_{u_2 \in V(G_2)} \big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2)\big) \times \big(d_{G_1}(v_1) + d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(u_2)\big).$$

By symmetry,

$$P_2 \geq 9^{n_2m_1}\sqrt[3]{\Pi_1(G_2)^{2m_1}\Pi_2(G_1)^{2n_2}},$$

with equality if and only if G_1 and G_2 are $1-$regular graphs.

The third product P_3 is taken over all edges $(u_1, u_2)(v_1, v_2) \in E(G)$ such that $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$. By Lemmas 2.1 and 2.2, we have

$$\begin{aligned}
P_3 = & \prod_{u_1v_1 \in E(G_1)} \prod_{u_2v_2 \in E(G_2)} \Big[\big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2)\big) \\
& \times \big(d_{G_1}(v_1) + d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(v_2)\big)\Big] \\
& \times \Big[\big(d_{G_1}(u_1) + d_{G_2}(v_2) + d_{G_1}(u_1)d_{G_2}(v_2)\big) \\
& \times \big(d_{G_1}(v_1) + d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(u_2)\big)\Big] \\
\geq & \prod_{u_1v_1 \in E(G_1)} \prod_{u_2v_2 \in E(G_2)} \Big[3\sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(u_2) \times d_{G_1}(u_1)d_{G_2}(u_2)} \\
& \times 3\sqrt[3]{d_{G_1}(v_1) \times d_{G_2}(v_2) \times d_{G_1}(v_1)d_{G_2}(v_2)}\Big] \\
& \times \Big[3\sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(v_2) \times d_{G_1}(u_1)d_{G_2}(v_2)} \\
& \times 3\sqrt[3]{d_{G_1}(v_1) \times d_{G_2}(u_2) \times d_{G_1}(v_1)d_{G_2}(u_2)}\Big] \\
= & \prod_{u_1v_1 \in E(G_1)} \prod_{u_2v_2 \in E(G_2)} 81\sqrt[3]{\big(d_{G_1}(u_1)d_{G_1}(v_1)\big)^4 \times \big(d_{G_2}(u_2)d_{G_2}(v_2)\big)^4} \\
= & 81^{m_1m_2}\sqrt[3]{\Pi_2(G_1)^{4m_2}\Pi_2(G_2)^{4m_1}}.
\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$,

$$d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2) = 3\sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(u_2) \times d_{G_1}(u_1)d_{G_2}(u_2)},$$

$$d_{G_1}(v_1) + d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(v_2) = 3\sqrt[3]{d_{G_1}(v_1) \times d_{G_2}(v_2) \times d_{G_1}(v_1)d_{G_2}(v_2)},$$

$$d_{G_1}(u_1) + d_{G_2}(v_2) + d_{G_1}(u_1)d_{G_2}(v_2) = 3\sqrt[3]{d_{G_1}(u_1) \times d_{G_2}(v_2) \times d_{G_1}(u_1)d_{G_2}(v_2)},$$

and

$$d_{G_1}(v_1) + d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(u_2) = 3\sqrt[3]{d_{G_1}(v_1) \times d_{G_2}(u_2) \times d_{G_1}(v_1)d_{G_2}(u_2)}.$$

By Lemma 2.1, this implies that for every $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$,

$$d_{G_1}(u_1) = d_{G_2}(u_2) = d_{G_1}(u_1)d_{G_2}(u_2),$$

$$d_{G_1}(v_1) = d_{G_1}(v_2) = d_{G_1}(v_1)d_{G_2}(v_2),$$

$$d_{G_1}(u_1) = d_{G_1}(v_2) = d_{G_1}(u_1)d_{G_2}(v_2),$$

and

$$d_{G_1}(v_1) = d_{G_1}(u_2) = d_{G_1}(v_1)d_{G_2}(u_2).$$

So, the equality holds if and only if G_1 and G_2 are $1-$regular graphs.

Hence,

$$\begin{aligned}\Pi_2(G) =&P_1P_2P_3\\ \geq&9^{n_1m_2+n_2m_1+2m_1m_2}\sqrt[3]{\Pi_1(G_1)^{2m_2}\Pi_1(G_2)^{2m_1}\Pi_2(G_1)^{2n_2+4m_2}\Pi_2(G_2)^{2n_1+4m_1}},\end{aligned}$$

with equality if and only if G_1 and G_2 are $1-$regular graphs. ■

Theorem 2.23. *The multiplicative sum Zagreb index of $G_1 \boxtimes G_2$ satisfies the following inequality:*

$$\begin{aligned}\Pi_1^*(G_1 \boxtimes G_2) >&16^{m_1m_2}\ (3\sqrt[3]{2})^{n_1m_2+n_2m_1}\sqrt[3]{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1}}\sqrt{\Pi_2(G_1)^{m_2}\Pi_2(G_2)^{m_1}}\\ &\times\sqrt[6]{\Pi_1^*(G_1)^{4n_2+3m_2}\Pi_1^*(G_2)^{4n_1+3m_1}}.\end{aligned}$$

Proof. Let $G = G_1 \boxtimes G_2$. By definition of the multiplicative sum Zagreb index, we have

$$\Pi_1^*(G) = \prod_{(u_1,u_2)(v_1,v_2)\in E(G)} \big[d_G((u_1,u_2)) + d_G((v_1,v_2))\big].$$

By definition of the strong product, we can partition the above product into three products as follows.

The first product P_1 is taken over all edges $(u_1,u_2)(v_1,v_2) \in E(G)$ such that $u_1 = v_1$ and $u_2v_2 \in E(G_2)$. By Lemmas 2.1 and 2.2, we have

$$\begin{aligned}P_1 =& \prod_{u_1\in V(G_1)}\prod_{u_2v_2\in E(G_2)} \big[\big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2)\big)\\ &+\big(d_{G_1}(u_1) + d_{G_2}(v_2) + d_{G_1}(u_1)d_{G_2}(v_2)\big)\big]\\ =& \prod_{u_1\in V(G_1)}\prod_{u_2v_2\in E(G_2)} \big[2d_{G_1}(u_1) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) + d_{G_1}(u_1)\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)\big]\\ \geq& \prod_{u_1\in V(G_1)}\prod_{u_2v_2\in E(G_2)} 3\sqrt[3]{2d_{G_1}(u_1) \times \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) \times d_{G_1}(u_1)\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)}\\ =&(3\sqrt[3]{2})^{n_1m_2}\sqrt[3]{\Pi_1(G_1)^{m_2}\Pi_1^*(G_2)^{2n_1}}.\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$,

$$\begin{aligned}&2d_{G_1}(u_1) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) + d_{G_1}(u_1)\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)\\ =&3\sqrt[3]{2d_{G_1}(u_1) \times \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) \times d_{G_1}(u_1)\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)}.\end{aligned}$$

By Lemma 2.1, this implies that for every $u_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)$,

$$2d_{G_1}(u_1) = d_{G_2}(u_2) + d_{G_2}(v_2) = d_{G_1}(u_1)\big(d_{G_2}(u_2) + d_{G_2}(v_2)\big).$$

So, the equality holds if and only if for every $u_1 \in V(G_1)$, $d_{G_1}(u_1) = 1$ and for every $u_2v_2 \in E(G_2)$, $d_{G_2}(u_2) + d_{G_2}(v_2) = 2$. That is G_1 and G_2 are $1-$regular graphs.

The second product P_2 is taken over all edges $(u_1, u_2)(v_1, v_2) \in E(G)$ such that $u_1v_1 \in E(G_1)$ and $u_2 = v_2$. So,

$$\begin{aligned}P_2 = &\prod_{u_1v_1 \in E(G_1)} \prod_{u_2 \in V(G_2)} \big[\big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2)\big)\\ &+ \big(d_{G_1}(v_1) + d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(u_2)\big)\big].\end{aligned}$$

By symmetry,

$$P_2 \geq (3\sqrt[3]{2})^{n_2m_1} \sqrt[3]{\Pi_1(G_2)^{m_1} \Pi_1^*(G_1)^{2n_2}},$$

with equality if and only if G_1 and G_2 are $1-$regular graphs.

The third product P_3 is taken over all edges $(u_1, u_2)(v_1, v_2) \in E(G)$ such that $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$. By Lemmas 2.1 and 2.2, we have

$$\begin{aligned}P_3 = &\prod_{u_1v_1 \in E(G_1)} \prod_{u_2v_2 \in E(G_2)} \big[\big(d_{G_1}(u_1) + d_{G_2}(u_2) + d_{G_1}(u_1)d_{G_2}(u_2)\big)\\ &+ \big(d_{G_1}(v_1) + d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(v_2)\big)\big]\\ &\times \big[\big(d_{G_1}(u_1) + d_{G_2}(v_2) + d_{G_1}(u_1)d_{G_2}(v_2)\big)\\ &+ \big(d_{G_1}(v_1) + d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(u_2)\big)\big]\\ = &\prod_{u_1v_1 \in E(G_1)} \prod_{u_2v_2 \in E(G_2)} \big[\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)\\ &+ d_{G_1}(u_1)d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(v_2)\big]\\ &\times \big[\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)\\ &+ d_{G_1}(u_1)d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(u_2)\big]\\ \geq &\prod_{u_1v_1 \in E(G_1)} \prod_{u_2v_2 \in E(G_2)} 16\sqrt{\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) \times \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big)}\\ &\times \sqrt{d_{G_1}(u_1)d_{G_1}(v_1) \times d_{G_2}(u_2)d_{G_2}(v_2)}\\ =&16^{m_1m_2}\sqrt{\big(\Pi_1^*(G_1)\Pi_2(G_1)\big)^{m_2}\big(\Pi_1^*(G_2)\Pi_2(G_2)\big)^{m_1}}\ .\end{aligned}$$

By Lemma 2.2, the above equality holds if and only if for every $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$,

$$\begin{aligned}&\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) + d_{G_1}(u_1)d_{G_2}(u_2) + d_{G_1}(v_1)d_{G_2}(v_2)\\ =&4\sqrt[4]{\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) \times \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) \times d_{G_1}(u_1)d_{G_2}(u_2) \times d_{G_1}(v_1)d_{G_2}(v_2)},\end{aligned}$$

and

$$\begin{aligned}&\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) + \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) + d_{G_1}(u_1)d_{G_2}(v_2) + d_{G_1}(v_1)d_{G_2}(u_2)\\ =&4\sqrt[4]{\big(d_{G_1}(u_1) + d_{G_1}(v_1)\big) \times \big(d_{G_2}(u_2) + d_{G_2}(v_2)\big) \times d_{G_1}(u_1)d_{G_2}(v_2) \times d_{G_1}(v_1)d_{G_2}(u_2)}.\end{aligned}$$

By Lemma 2.1, this implies that for every $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$,

$$d_{G_1}(u_1) + d_{G_1}(v_1) = d_{G_2}(u_2) + d_{G_2}(v_2) = d_{G_1}(u_1)d_{G_2}(u_2) = d_{G_1}(v_1)d_{G_2}(v_2)$$
$$= d_{G_1}(u_1)d_{G_2}(v_2) = d_{G_1}(v_1)d_{G_2}(u_2).$$

So, G_1 and G_2 must be 2-regular graphs.

Hence,

$$\Pi_1^*(G) = P_1P_2P_3 > 16^{m_1m_2}\,(3\sqrt[3]{2})^{n_1m_2+n_2m_1}\sqrt[3]{\Pi_1(G_1)^{m_2}\Pi_1(G_2)^{m_1}}\sqrt{\Pi_2(G_1)^{m_2}\Pi_2(G_2)^{m_1}}$$
$$\times \sqrt[6]{\Pi_1^*(G_1)^{4n_2+3m_2}\Pi_1^*(G_2)^{4n_1+3m_1}}.$$

■

3. Bounds on multiplicative versions of Zagreb indices of subdivision operators

In this section, we compare the multiplicative versions of Zagreb indices under the subdivision operators L, S, R, Q, and T. Results are applied to obtain some upper and/or lower bounds for the first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of these operators in terms of the order, size, first Zagreb index, first and second multiplicative Zagreb indices and multiplicative sum Zagreb index of the primary graph. The results of this section have been taken from [5].

At first, we recall the definitions of subdivision-related graphs and state some preliminary results about them.

Let $G = (V(G), E(G))$ be a nontrivial simple connected graph with vertex set $V(G)$ and edge set $E(G)$ and let $|V(G)| = n$ and $|E(G)| = m$. Related to the graph G, the *line graph* $L(G)$, the *subdivision graph* $S(G)$, and the *total graph* $T(G)$ are defined as follows.

The line graph $L(G)$ is the graph whose vertices correspond to the edges of G with two vertices being adjacent if and only if the corresponding edges in G have a vertex in common.

The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edges by a path of length two, or equivalently, by inserting an additional vertex into each edge of G.

The total graph $T(G)$ is the graph whose vertex set is $V(G) \cup E(G)$, with two vertices of $T(G)$ being adjacent if and only if the corresponding elements of G are adjacent or incident.

Two extra subdivision operators named $R(G)$ and $Q(G)$ are defined as follows.

$R(G)$ is the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.

$Q(G)$ is the graph obtained from G by inserting a new vertex into each edge of G and by joining with edges those pairs of these new vertices which lie on adjacent edges of G.

Now consider the sets $EE(G)$ and $EV(G)$ for the graph $G = (V(G), E(G))$ as follows.

$$EE(G) = \{ee' | e, e' \in E(G), |V(e) \cap V(e')| = 1\}, \quad EV(G) = \{ev | e \in E(G), v \in V(e)\}.$$

It is easy to see that,

$$|EE(G)| = \sum_{u\in V(G)} \binom{d(u)}{2} = \frac{1}{2}M_1(G) - m, \ \ |EV(G)| = 2m.$$

Based on the definitions of these sets, we may write the subdivision-related graphs as follows.

$$\begin{aligned} L(G) &= (E(G), EE(G)),\\ S(G) &= (V(G) \cup E(G), EV(G)),\\ R(G) &= (V(G) \cup E(G), E(G) \cup EV(G)),\\ Q(G) &= (V(G) \cup E(G), EE(G) \cup EV(G)),\\ T(G) &= (V(G) \cup E(G), E(G) \cup EE(G) \cup EV(G)). \end{aligned}$$

Obviously,

$$|V(L(G))| = m, \ |V(S(G))| = |V(R(G))| = |V(Q(G))| = |V(T(G))| = n + m,$$

and

$$\begin{aligned} |E(S(G))| =& 2m, \ |E(R(G))| = 3m,\\ |E(L(G))| =& \frac{1}{2}M_1(G) - m, \ |E(Q(G))| = \frac{1}{2}M_1(G) + m, \ |E(T(G))| = \frac{1}{2}M_1(G) + 2m. \end{aligned}$$

In the following lemma, we find the relationship among the degree of vertices in subdivision-related graphs.

Lemma 3.1. *For any vertex $v \in V(G)$,*

$$d_{R(G)}(v) = d_{T(G)}(v) = 2d_{S(G)}(v) = 2d_{Q(G)}(v) = 2d_G(v),$$

and for any edge $e = uv \in E(G)$,

$$d_{S(G)}(e) = d_{R(G)}(e) = 2, \ \ d_{Q(G)}(e) = d_{T(G)}(e) = d_{L(G)}(e) + 2 = d_G(u) + d_G(v).$$

Proof. By definition of the subdivision-related graphs, the proof is obvious. ■

In the following theorem, the first multiplicative Zagreb index of the subdivision operators S, R, Q and T are computed.

Theorem 3.2. *Let G be a graph of order n and size m. Then*

$$\begin{aligned} &(i)\ \Pi_1(S(G)) = 4^m \Pi_1(G),\\ &(ii)\ \Pi_1(R(G)) = 4^{n+m} \Pi_1(G),\\ &(iii)\ \Pi_1(Q(G)) = \Pi_1(G)\Pi_1^*(G)^2,\\ &(iv)\ \Pi_1(T(G)) = 4^n \Pi_1(G)\Pi_1^*(G)^2. \end{aligned}$$

Proof. *(i)* By definition of $S(G)$ and Lemma 3.1,

$$\Pi_1(S(G)) = \prod_{u\in V(G)} d_G(u)^2 \times \prod_{e\in E(G)} 2^2 = 4^m \Pi_1(G).$$

(ii) By definition of $R(G)$ and Lemma 3.1,

$$\Pi_1(R(G)) = \prod_{u\in V(G)} (2d_G(u))^2 \times \prod_{e\in E(G)} 2^2 = 4^n \Pi_1(G) \times 4^m = 4^{n+m}\Pi_1(G).$$

(iii) By definition of $Q(G)$ and Lemma 3.1,

$$\Pi_1(Q(G)) = \prod_{u\in V(G)} d_G(u)^2 \times \prod_{uv\in E(G)} [d_G(u) + d_G(v)]^2 = \Pi_1(G)\Pi_1^*(G)^2.$$

(iv) By definition of $T(G)$ and Lemma 3.1,

$$\Pi_1(T(G)) = \prod_{u\in V(G)} (2d_G(u))^2 \times \prod_{uv\in E(G)} [d_G(u) + d_G(v)]^2 = 4^n \Pi_1(G)\Pi_1^*(G)^2.$$

■

As a direct consequence of Theorem 3.2, we get the following corollary.

Corollary 3.3. *Let G be a graph of order n. Then*

$$\frac{\Pi_1(R(G))}{\Pi_1(S(G))} = \frac{\Pi_1(T(G))}{\Pi_1(Q(G))} = 4^n.$$

Using Lemmas 2.1 and 3.1, we obtain a sharp upper bound for the first multiplicative Zagreb index of the line graph $L(G)$ in terms of the multiplicative sum Zagreb index and the size of the graph G.

Theorem 3.4. *Let G be a graph of size m. Then*

$$\Pi_1(L(G)) \le \frac{\Pi_1^*(G)^4}{64^m},$$

with equality if and only if G is a cycle or the star graph on 4 vertices.

Proof. By definition of the multiplicative sum Zagreb index and Lemma 3.1,

$$\Pi_1^*(G)^4 = \prod_{uv\in E(G)} [d_G(u) + d_G(v)]^4 = \prod_{uv\in V(L(G))} [d_{L(G)}(uv) + 2]^4.$$

Now by Lemma 2.1,

$$\Pi_1^*(G)^4 \ge \prod_{uv\in V(L(G))} \left[2\sqrt{d_{L(G)}(uv) \times 2}\right]^4 = \prod_{uv\in V(L(G))} 64\, d_{L(G)}(uv)^2 = 64^m \Pi_1(L(G)).$$

So,

$$\Pi_1(L(G)) \le \frac{\Pi_1^*(G)^4}{64^m}.$$

By Lemma 2.1, the above equality holds if and only if for every $uv \in E(G)$, $d_{L(G)}(uv) = 2$. This by Lemma 3.1 implies that, for every $uv \in E(G)$, $d_G(u) + d_G(v) = 4$. So, G is a cycle or the star graph on 4 vertices. ■

Now, we introduce the quantity $\Gamma(G)$ related to a simple connected graph G as follows.

$$\Gamma(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(v)]^{d_G(u)+d_G(v)}.$$

In the following theorem, we determine the second multiplicative Zagreb index of subdivision operators.

Theorem 3.5. *Let G be a graph of size m. Then*

$$\begin{aligned}
&(i)\ \Pi_2(S(G)) = 4^m \Pi_2(G),\\
&(ii)\ \Pi_2(R(G)) = 64^m \Pi_2(G)^2,\\
&(iii)\ \Pi_2(Q(G)) = \Pi_2(G)\Gamma(G),\\
&(iv)\ \Pi_2(T(G)) = 16^m \Pi_2(G)^2 \Gamma(G).
\end{aligned}$$

Proof. *(i)* By definition of $S(G)$ and Lemma 3.1,

$$\Pi_2(S(G)) = \prod_{u \in V(G)} d_G(u)^{d_G(u)} \times \prod_{e \in E(G)} 2^2 = 4^m \Pi_2(G).$$

(ii) By definition of $R(G)$ and Lemma 3.1,

$$\begin{aligned}
\Pi_2(R(G)) &= \prod_{u \in V(G)} (2d_G(u))^{2d_G(u)} \times \prod_{e \in E(G)} 2^2\\
&= \prod_{u \in V(G)} 4^{d_G(u)} \times \prod_{u \in V(G)} \left(d_G(u)^{d_G(u)}\right)^2 \times 4^m\\
&=4^{2m} \times \Pi_2(G)^2 \times 4^m = 64^m \Pi_2(G)^2.
\end{aligned}$$

(iii) By definition of $Q(G)$ and Lemma 3.1,

$$\Pi_2(Q(G)) = \prod_{u \in V(G)} d_G(u)^{d_G(u)} \times \prod_{uv \in E(G)} [d_G(u) + d_G(v)]^{d_G(u)+d_G(v)} = \Pi_2(G)\Gamma(G).$$

(iv) By definition of $T(G)$ and Lemma 3.1,

$$\begin{aligned}
\Pi_2(T(G)) = &\prod_{u \in V(G)} (2d_G(u))^{2d_G(u)} \times \prod_{uv \in E(G)} [d_G(u) + d_G(v)]^{d_G(u)+d_G(v)}\\
=&16^m \Pi_2(G)^2 \Gamma(G).
\end{aligned}$$

■

As a direct consequence of Theorem 3.5, we get the following corollary.

Corollary 3.6. *Let G be a graph of size m. Then*

$$\frac{\Pi_2(R(G))}{\Pi_2(S(G))} = \frac{\Pi_2(T(G))}{\Pi_2(Q(G))} = 16^m \Pi_2(G).$$

In the following theorem, we obtain a sharp upper bound for the second multiplicative Zagreb index of $L(G)$ in terms of the quantity $\Gamma(G)$, the first Zagreb index, the multiplicative sum Zagreb index and size of the graph G.

Theorem 3.7. *Let G be a graph of size m. Then*

$$\Pi_2(L(G)) \leq \frac{\Gamma(G)^2}{8^{M_1(G)-2m}\,\Pi_1^*(G)^4},$$

with equality if and only if G is a cycle or the star graph on 4 vertices.

Proof. By definition of $\Gamma(G)$, we have

$$\begin{aligned}\Gamma(G)^2 = &\prod_{uv\in E(G)} [d_G(u)+d_G(v)]^{2(d_{L(G)}(uv)+2)}\\ =&\Pi_1^*(G)^4 \times \prod_{uv\in V(L(G))} [d_{L(G)}(uv)+2]^{2d_{L(G)}(uv)}.\end{aligned}$$

Now by Lemma 2.1,

$$\begin{aligned}\Gamma(G)^2 \geq &\Pi_1^*(G)^4 \times \prod_{uv\in V(L(G))} \left[2\sqrt{d_{L(G)}(uv)\times 2}\,\right]^{2d_{L(G)}(uv)}\\ =&\Pi_1^*(G)^4 \times \prod_{uv\in V(L(G))} 8^{d_{L(G)}(uv)} \times \prod_{uv\in V(L(G))} d_{L(G)}(uv)^{d_{L(G)}(uv)}\\ =&\Pi_1^*(G)^4 \times 8^{\sum_{uv\in V(L(G))} d_{L(G)}(uv)} \times \Pi_2(L(G))\\ =&8^{M_1(G)-2m}\,\Pi_1^*(G)^4\,\Pi_2(L(G)).\end{aligned}$$

So,

$$\Pi_2(L(G)) \leq \frac{\Gamma(G)^2}{8^{M_1(G)-2m}\,\Pi_1^*(G)^4}.$$

By Lemma 2.1, the above equality holds if and only if for every $uv \in E(G)$, $d_{L(G)}(uv) = 2$, that is, $d_G(u) + d_G(v) = 4$. So, G is a cycle or the star graph on 4 vertices. ∎

Using parts *(iii)* and *(iv)* of Theorem 3.5 and then Theorem 3.7, we can obtain sharp inequalities for the second multiplicative Zagreb index of $Q(G)$ and $T(G)$.

Corollary 3.8. *Let G be a graph of size m. Then*

$$\Pi_2(Q(G)) \geq (2\sqrt{2})^{M_1(G)-2m}\,\Pi_1^*(G)^2\,\Pi_2(G)\sqrt{\Pi_2(L(G))},$$

with equality if and only if G is a cycle or the star graph on 4 vertices.

Corollary 3.9. *Let G be a graph of size m. Then*

$$\Pi_2(T(G)) \geq 2^m(2\sqrt{2})^{M_1(G)}\,(\Pi_1^*(G)\Pi_2(G))^2\,\sqrt{\Pi_2(L(G))},$$

with equality if and only if G is a cycle or the star graph on 4 vertices.

Now, we turn our attention toward multiplicative sum Zagreb index of subdivision operators. In the following theorem, we find a formula for the multiplicative sum Zagreb index of the subdivision graph $S(G)$.

Theorem 3.10. *Let G be a graph. Then*

$$\Pi_1^*(S(G)) = \prod_{u\in V(G)} (d_G(u)+2)^{d_G(u)}.$$

Proof. By definition of $S(G)$ and Lemma 3.1,

$$\Pi_1^*(S(G)) = \prod_{ev\in EV(G)} [d_{S(G)}(e) + d_{S(G)}(v)] = \prod_{uv\in E(G)} (d_G(u)+2)(d_G(v)+2).$$

The vertex $u \in V(G)$ is the endpoint of $d_G(u)$ edges of G. Therefore in the above product, the factor $d_G(u) + 2$ occurs $d_G(u)$ times. So,

$$\Pi_1^*(S(G)) = \prod_{u\in V(G)} (d_G(u)+2)^{d_G(u)}.$$

■

Using Theorem 3.10 and Lemma 2.1, we can obtain a sharp lower bound for the multiplicative sum Zagreb index of $S(G)$ in terms of the second multiplicative Zagreb index and the size of the graph G.

Corollary 3.11. *Let G be a graph of size m. Then*

$$\Pi_1^*(S(G)) \geq 8^m \sqrt{\Pi_2(G)},$$

with equality if and only if G is a cycle.

Proof. Using Theorem 3.10 and then Lemma 2.1, we have

$$\begin{aligned}\Pi_1^*(S(G)) &= \prod_{u\in V(G)} (d_G(u)+2)^{d_G(u)} \\ &\geq \prod_{u\in V(G)} (2\sqrt{d_G(u)\times 2})^{d_G(u)} \\ &=(2\sqrt{2})^{\sum_{u\in V(G)} d_G(u)} \times \sqrt{\prod_{u\in V(G)} d_G(u)^{d_G(u)}} = 8^m \sqrt{\Pi_2(G)}.\end{aligned}$$

By Lemma 2.1, the above equality holds if and only if for every $u \in V(G)$, $d_G(u) = 2$. This implies that G is a cycle. ■

In the following theorem, we find a formula for the multiplicative sum Zagreb index of $R(G)$.

Theorem 3.12. *Let G be a graph of size m. Then*

$$\Pi_1^*(R(G)) = 8^m\, \Pi_1^*(G) \prod_{u\in V(G)} (d_G(u)+1)^{d_G(u)}.$$

Proof. By definition of $R(G)$ and Lemma 3.1,

$$\begin{aligned}
\Pi_1^*(R(G)) = &\prod_{uv\in E(G)} [d_{R(G)}(u) + d_{R(G)}(v)] \times \prod_{ev\in EV(G)} [d_{R(G)}(e) + d_{R(G)}(v)] \\
= &\prod_{uv\in E(G)} [2d_G(u) + 2d_G(v)] \times \prod_{uv\in E(G)} (2d_G(u) + 2)(2d_G(v) + 2) \\
=&2^m \prod_{uv\in E(G)} [d_G(u) + d_G(v)] \times 4^m \prod_{uv\in E(G)} (d_G(u) + 1)(d_G(v) + 1) \\
=&8^m \Pi_1^*(G) \prod_{u\in V(G)} (d_G(u) + 1)^{d_G(u)}.
\end{aligned}$$

■

Using Theorem 3.12 and Lemma 2.1, we can obtain a sharp lower bound for the multiplicative sum Zagreb index of $R(G)$ in terms of the multiplicative sum Zagreb index, second multiplicative Zagreb index and size of the graph G.

Corollary 3.13. *Let G be a graph of size m. Then*

$$\Pi_1^*(R(G)) \geq 32^m\, \Pi_1^*(G)\sqrt{\Pi_2(G)},$$

with equality if and only if G is the $2-$vertex path P_2.

Proof. Using Theorem 3.12 and Lemma 2.1, we have

$$\begin{aligned}
\Pi_1^*(R(G)) =&8^m\, \Pi_1^*(G) \prod_{u\in V(G)} (d_G(u) + 1)^{d_G(u)} \\
\geq&8^m\, \Pi_1^*(G) \prod_{u\in V(G)} (2\sqrt{d_G(u) \times 1})^{d_G(u)} \\
=&8^m\, \Pi_1^*(G) \times 2^{\sum_{u\in V(G)} d_G(u)} \times \sqrt{\prod_{u\in V(G)} d_G(u)^{d_G(u)}} \\
=&32^m\, \Pi_1^*(G)\sqrt{\Pi_2(G)}.
\end{aligned}$$

By Lemma 2.1, the above equality holds if and only if for every $u \in V(G)$, $d_G(u) = 1$. So, G is the $2-$vertex path P_2. ■

In order to obtain some lower bounds on the multiplicative sum Zagreb index of $Q(G)$ and $T(G)$, we need to prove two following lemmas.

Lemma 3.14. *Let G be a graph of size m. Then*

$$\begin{aligned}
\prod_{ee'\in EE(G)} [d_{Q(G)}(e) + d_{Q(G)}(e')] = &\prod_{ee'\in EE(G)} [d_{T(G)}(e) + d_{T(G)}(e')] \\
&\geq 2^{M_1(G)-2m}\sqrt{\Pi_1^*(L(G))},
\end{aligned}$$

with equality if and only if G is a cycle or the star graph on 4 vertices.

Proof. Using Lemma 3.1, we have

$$\begin{aligned}\prod_{ee'\in EE(G)}[d_{Q(G)}(e)+d_{Q(G)}(e')] &= \prod_{ee'\in EE(G)}[d_{T(G)}(e)+d_{T(G)}(e')]\\ &= \prod_{ee'\in E(L(G))}[d_{L(G)}(e)+d_{L(G)}(e')+4].\end{aligned}$$

Now by Lemma 2.1,

$$\begin{aligned}\prod_{ee'\in E(L(G))}[d_{L(G)}(e)+d_{L(G)}(e')+4] &\geq \prod_{ee'\in E(L(G))}2\sqrt{\big(d_{L(G)}(e)+d_{L(G)}(e')\big)\times 4}\\ &=4^{|E(L(G))|}\sqrt{\prod_{ee'\in E(L(G))}\big(d_{L(G)}(e)+d_{L(G)}(e')\big)}\\ &=2^{M_1(G)-2m}\sqrt{\Pi_1^*(L(G))}.\end{aligned}$$

By Lemma 2.1, the above equality holds if and only if for every $ee'\in E(L(G))$, $d_{L(G)}(e)+d_{L(G)}(e')=4$. So, for every $uv, zv\in E(G)$,

$$(d_G(u)+d_G(v)-2)+(d_G(z)+d_G(v)-2)=4,$$

that is $2d_G(v)+d_G(u)+d_G(z)=8$. This implies that, for every $uv, zv\in E(G)$, $d_G(u)=d_G(v)=d_G(z)=2$ or $d_G(v)=3, d_G(u)=d_G(z)=1$. So, G is a cycle or the star graph on 4 vertices. ■

Lemma 3.15. *Let G be a graph of size m. Then*

$$(i)\quad \prod_{ev\in EV(G)}[d_{Q(G)}(e)+d_{Q(G)}(v)] > (2\sqrt{2})^m\,\Pi_1^*(G)\sqrt{\Pi_2(G)},$$

$$(ii)\quad \prod_{ev\in EV(G)}[d_{T(G)}(e)+d_{T(G)}(v)] > (4\sqrt{3})^m\,\Pi_1^*(G)\sqrt{\Pi_2(G)}.$$

Proof. (i) Using Lemma 3.1, we have

$$\begin{aligned}&\prod_{ev\in EV(G)}[d_{Q(G)}(e)+d_{Q(G)}(v)]\\ &=\prod_{uv\in E(G)}\big[d_G(u)+\big(d_G(u)+d_G(v)\big)\big]\big[d_G(v)+\big(d_G(u)+d_G(v)\big)\big]\\ &=\prod_{uv\in E(G)}\big(2d_G(u)+d_G(v)\big)\big(2d_G(v)+d_G(u)\big)\\ &=\prod_{uv\in E(G)}\big[2\big(d_G(u)+d_G(v)\big)^2+d_G(u)d_G(v)\big].\end{aligned}$$

Now by Lemma 2.1,

$$\begin{aligned}\prod_{ev\in EV(G)}[d_{Q(G)}(e)+d_{Q(G)}(v)] &> \prod_{uv\in E(G)}2\sqrt{2\big(d_G(u)+d_G(v)\big)^2\times d_G(u)d_G(v)}\\ &=(2\sqrt{2})^m\,\Pi_1^*(G)\sqrt{\Pi_2(G)}.\end{aligned}$$

The above inequality is strict. Since by Lemma 2.1, the equality holds if and only if for every $uv \in E(G)$, $2\big(d_G(u) + d_G(v)\big)^2 = d_G(u)d_G(v)$, which is a contradiction.
(ii) Using the same argument as in the proof of part *(i)*, we can get the desired result. ■

Now, we apply Lemmas 3.14 and 3.15 to obtain lower bounds on the multiplicative sum Zagreb index of $Q(G)$ and $T(G)$.

Lemma 3.16. *Let G be a graph of size m. Then*

$$\textbf{(i)}\ \Pi_1^*(Q(G)) > (\sqrt{2})^{2M_1(G)-m}\ \Pi_1^*(G)\sqrt{\Pi_2(G)\,\Pi_1^*(L(G))}\,,$$
$$\textbf{(ii)}\ \Pi_1^*(T(G)) > 2^{M_1(G)+m}(\sqrt{3})^m\ \Pi_1^*(G)^2\sqrt{\Pi_2(G)\,\Pi_1^*(L(G))}\,.$$

Proof. *(i)* By definition of the multiplicative sum Zagreb index, we have

$$\Pi_1^*(Q(G)) = \prod_{ee'\in EE(G)} [d_{Q(G)}(e) + d_{Q(G)}(e')] \times \prod_{ev\in EV(G)} [d_{Q(G)}(e) + d_{Q(G)}(v)].$$

Now using Lemmas 3.14 and 3.15, we have

$$\begin{aligned}\Pi_1^*(Q(G)) >& 2^{M_1(G)-2m}\sqrt{\Pi_1^*(L(G))} \times (2\sqrt{2})^m\ \Pi_1^*(G)\sqrt{\Pi_2(G)}\\ =&(\sqrt{2})^{2M_1(G)-m}\ \Pi_1^*(G)\ \sqrt{\Pi_2(G)\,\Pi_1^*(L(G))}.\end{aligned}$$

(ii) By definition of the multiplicative sum Zagreb index, we have

$$\begin{aligned}\Pi_1^*(T(G)) = \prod_{uv\in E(G)} [d_{T(G)}(u) + d_{T(G)}(v)] \times \prod_{ee'\in EE(G)} [d_{T(G)}(e) + d_{T(G)}(e')]\\ \times \prod_{ev\in EV(G)} [d_{T(G)}(e) + d_{T(G)}(v)].\end{aligned}$$

By Lemma 3.1,

$$\prod_{uv\in E(G)} [d_{T(G)}(u) + d_{T(G)}(v)] = \prod_{uv\in E(G)} [2d_G(u) + 2d_G(v)] = 2^m\Pi_1^*(G).$$

Now using Lemmas 3.14 and 3.15, we have

$$\begin{aligned}\Pi_1^*(T(G)) >& 2^m\Pi_1^*(G) \times\ 2^{M_1(G)-2m}\sqrt{\Pi_1^*(L(G))} \times (4\sqrt{3})^m\ \Pi_1^*(G)\sqrt{\Pi_2(G)}\\ =&2^{M_1(G)+m}(\sqrt{3})^m\Pi_1^*(G)^2\sqrt{\Pi_2(G)\,\Pi_1^*(L(G))}.\end{aligned}$$

■

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Saturation Number of a Graph

M. B. Ahmadi, V. Amiri Khorasani

Department of Mathematics, College of Sciences, Shiraz University 71454, Shiraz, I. R. Iran
mbahmadi@shirazu.ac.ir

Contents

1. Introduction

Many problems in natural, technical and social sciences can be successfully formulated in terms of matchings in graphs. Today the matching theory is a well-developed branch of graph theory, studying both structural and enumerative aspects of matchings. Its development has been strongly stimulated by chemical applications, in particular by the study of perfect matchings in benzenoid graphs [15]. Additional impetus came with the discovery of fullerenes, again mostly dealing with perfect matchings [9, 10, 24, 39], but including also some structural results [3, 11].

For a general background on matching theory and terminology, we refer the reader to the classical monograph by Lovasz and Plummer [31]. For graph theory terms not defined here, we also recommend [37].

Let $G = (V, E)$ be a simple graph. A subset M of E is called a **matching** if no two edges in M are adjacent. The cardinality of M is called the size of the matching. As the matchings of small size are not interesting (each edge is a matching of size one, and the empty set is the unique matching of size 0), we will be mostly interested in matchings that are, in a sense, large. Most often, we are interested in matchings that are as large as possible. A matching *M* is **maximum** if there is no matching in G with more edges than M. The cardinality of any maximum matching in G is called the matching number of G and denoted by $\nu(G)$. Since each vertex can be incident to at most one edge of a matching, it follows that the matching number of a graph on n vertices cannot exceed $\lfloor n/2 \rfloor$. A vertex $v \in V$ is said to be **saturated** by the matching M if some edge of M is incident with v. A vertex which is not saturated by a matching is called **exposed**. A matching M is said to be **perfect** if all the vertices of G are saturated by M. Perfect matchings are obviously also maximum matchings. The perfect matchings, also known as **Kekulé structures** in the chemical literature, have played a central role in the study of matchings for several decades. There is, however, an alternative way to quantify the idea of large matchings. A matching M is said to be **maximal** if for any $e \in E/M$, $M \cup \{e\}$ is not a matching.

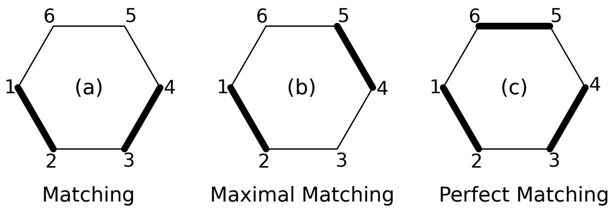


Figure 1. Matching examples.

In Figure 1, the thick edges of the graph in (a) form a matching that is neither perfect nor maximal. The thick edges in (b) form a maximal matching that is not perfect. The thick edges in (c) on the other hand form a maximal matching that is also perfect. Obviously, every maximum matching is also maximal, but the opposite is generally not true.

Maximal matchings are much less researched that their maximum counterparts. That goes both for their structural and their enumerative aspects. While there is vast literature on perfect and maximum matchings (see, for example, monographs [31] and [6]), the results about maximal matchings are few and scattered through the literature. We mention here two papers that treat, among other topics, maximal matchings in trees [27, 36], one concerned with the structure of equimatchable graphs [20], and recent two paper by the present authors about saturation numbers of benzenoid graphs [1, 8].

Maximal matchings can serve as models of several physical and technical problems such as the block allocation of a sequential resource or adsorption of dimers on a structured substrate or a molecule.

In a chemical context, maximal matchings appear, for example, when one considers adsorption of dimers (diatomic molecules) on a larger molecule, where each dimer binds to a pair of adjacent atoms in the large molecule. Obviously, any adsorption pattern corresponds to a matching in the graph representing the large molecule, and the situation when no further adsorption is possible since there are no free pairs of adjacent atoms in the large molecule is represented by a maximal matching in the corresponding graph. When that process is random, it is clear that the substrate can become saturated by a number of dimers much smaller than the theoretical maximum. The cardinality of any smallest maximal matching in G is called the **saturation number** of G. We denote by $S(G)$, the saturation number of a graph G. (The same term, saturation number, is also used in the literature with a different meaning; we refer the reader to [18] for more information.)

It is easy to see that the saturation number of a graph G is at least one-half of the matching number of G, i.e., $S(G) \geq \nu(G)/2$. Hence, the saturation number provides information on the worst possible case of clogging; it is a measure of how inefficient the adsorption process can be. However, to fully assess its efficiency, we also need to know how likely it is that the substrate gets saturated by a given number of dimers.

Finding the saturation number of a graph is an NP-hard problem in general. In [38], Yannakakis and Gavril show that saturation number problem is NP-hard in several classes of graphs including bipartite (or planar) graphs with maximum degree 3. In [22], Horton and Kilakos extended these results by showing the NP-hardness of the saturation number problem in planar bipartite graphs and planar cubic graphs. In [40], Zito shows that the problem remains NP-hard in the so-called almost regular bipartite graphs, that are bipartite graphs for which the ratio between the maximum degree Δ and the minimum degree δ is bounded. Another strengthening of the result of Yannakakis and Gavril in [38] is given in [7] by showing that saturation number problem is NP-hard in k-regular bipartite graphs for any fixed $k \geq 3$. On the other hand, polynomial time algorithms for the saturation number problem are designed for trees [32], for block graphs [23], for series-parallel graphs [34], for bipartite permutation graphs and cotrianglated graphs [35], and for clique-width bounded graphs [16].

The saturation number and its associated structure of a fullerene and benzenoid play a key role in molecular energy and stability. In the following, we express improved lower and upper bounds on this quantity in the class of fullerene and benzenoid graphs.

In section 2, we review the literature dealing with the fullerene and its saturation number.

2. Fullerene graph

The first fullerene molecule, with a structure like a football, was discovered experimentally in 1985 by Kroto et al. [30]. The discovered molecule C_{60}, is comprised only of 60 carbon atoms, and it resembles the Richard Buckminster Fullers geodetic dome, therefore it was named buckminsterfullerene. Until that moment the only all-carbon structures, the modern science was aware of were graphite and diamond. In 1991, the Science magazine pronounced the buckminsterfullerene for the Molecule of the year, and later in 1996 the discovery of C_{60} was rewarded with the Nobel price for chemistry. Soon after the experimental discovery of the buckminsterfullerene, its existence in nature was confirmed along with similar structures having 70, 76, 78, 82, 84, 90, 94, or 96 carbon atoms. Each of these all-carbon molecules has polyhedral structure, and all faces of the polyhedron are either pentagons or hexagons. All polyhedral molecules made entirely of carbon atoms are called fullerenes. The discovery of the Buckminsterfullerene marked the birth of fullerene chemistry and nanotechnology, but at the same time, the fullerenes were studied from different perspectives. The experimental work was paralleled by theoretical investigations, applying the methods of graph theory to the mathematical models of fullerene molecules called fullerene graphs.

The study from graph-theoretical point of view has been motivated by a search for invariants that will correlate with their stability as a chemical compound. Later graph invariant was used in order to predict the physical and chemical properties of a fullerene compound. A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success [13, 17]. Graph theory invariants that have been considered as possible stability predictors are the bipartite edge frustration, the independence number, the saturation number, the number of perfect matchings, etc.

Fullerenes can also be seen as graphs, vertices represent atoms, and edges represent bonds between atoms. A fullerene graph is a 3-connected 3-regular planar graph with only pentagonal and hexagonal faces. In what follows fullerene graphs will be also called fullerenes. Due to Whitneys Theorem (1933), simple planar 3-connected graphs have a unique planar embedding, and therefore the same holds for fullerene graphs. By Eulers formula follows the next property of fullerene graphs.

Proposition 2.1. The number of pentagonal faces in a fullerene graph is 12 [4].

The previous result gives no restriction on the number of hexagons. Grunbaum and Motzkin [21] showed that fullerene graphs exist for any number of hexagonal faces except for 1, i.e., they proved the following.

Theorem 2.2. Fullerene graphs with n vertices exist for all even $n \geq 24$ and for $n = 20$.

Usually, in chemistry, the fullerene molecule on n vertices is denoted by C_n. Although the number of pentagonal faces is negligible compared to the number of hexagonal faces, their layout is crucial for the shape of the corresponding fullerene molecule. Notice that as the number of vertices (hexagons) grows, the number of fullerenes increases as well. For example, the fullerenes on 20, 24 and 26 vertices have the unique layout, but the fullerene C_{40} has 40 isomers, while the buckminsterfullerene has 1812 different isomers. There is a believe that a number of fullerenes on *n* vertices is of order $\Theta(n^9)$, see Fowler and Manolopoulos in [19] and Cioslowski [5] for more details.

Carbon atoms form four chemical bonds. Three of these are strong bonds, and one is weak. In the graphical representation of a fullerene, we represent the three strong bonds by the edges in the graph. The fourth bond is represented chemically as a double bond. A perfect matching of a graph is a set of edges of G such that each vertex is incident with exactly one edge. Over a fullerene, the edges of a perfect matching correspond to double bonds, and chemists call this matching a Kekulé structure. We refer to edges in a given Kekulé structure as Kekulé edges. Petersens Theorem states that in a bridgeless 3-regular graph, there is always a perfect matching [33]. We, therefore, know that a fullerene always has at least one Kekulé structure.

Proposition 2.3. Let K be a Kekulé structure on a fullerene G. Let P be the set of pentagons and H be the set of hexagons in G. Then

1. $|K| = \frac{|V|}{2}$
2. $|E| = \frac{3|V|}{2}$
3. $|P| = 12$
4. $|H| = \frac{|V|}{2} - 10$

Regarding the position of the pentagons, we distinguish several types of fullerene graphs. The fullerene graphs where no two pentagons are adjacent, i.e., each pentagon is surrounded by five hexagons, satisfy the isolated pentagon rule or shortly IPR, and they are considered as stable fullerene compounds [29]. Cioslowski [5] stated the following conjecture concerning the number of IPR fullerenes on n vertices.

Conjecture 2.4. For all $n > 106$, the number of the IPR fullerene isomers with n carbon atoms is bracketed by the total numbers of isomers of the C_{n-50} and C_{n-48} fullerenes.

If all pentagonal faces are equally distributed, we obtain fullerene graphs of icosahedral symmetry, whose smallest representative is the dodecahedron. The dodecahedron is the only icosahedral fullerene that does not satisfy the IPR. On the other hand, if the pentagonal faces are grouped in two clusters by six, we obtain nanotubical fullerene graphs.

The common feature of all icosahedral fullerenes is their geometrical shape. The simplest icosahedral fullerene graph is the dodecahedron, C_{20}; the next one is the famous buckminsterfullerene C_{60}.

It is well known (see, e.g. [19], pp. 1021) that an icosahedral fullerene on p vertices can be constructed using the **Coxeter construction** for each p satisfying $p = 20(i^2 + ij + j^2)$, where i and j are integers, $i \geq j \geq 0$ and $i > 0$. Here each distinct pair of Coxeter parameters (i, j) gives rise to a distinct isomer, and the geometric meaning of the parameters i and j is given by the distances between the pentagons in two directions on a hexagonal lattice. When $i = j$ or $j = 0$, the fullerene has the full icosahedral symmetry group I_h, while for $0 < j < i$ its symmetry group is the rotational subgroup I. All icosahedral fullerenes except the smallest one (C_{20}, generated by $i = 1, j = 0$) have isolated pentagons.

While the icosahedral fullerenes have spherical shape, there is a class of fullerene graphs of tubular shapes, called nanotubical graphs or simply nanotubes. From the aspect of mathematics, they are not well defined. However, they are cylindrical in shape, with the two ends capped with a subgraph containing six pentagons and possibly some hexagons. The cylindrical part of a nanotube can be obtained by rolling a planar hexagonal grid. The way the grid is wrapped is represented by a Coxeter vector (i,j), called also the type of the nanotube.

The distance between two vertices $u, v \in V(G)$ in a connected graph G is the length of any shortest path between these vertices, and it is denoted by $d(u, v)$. A diameter of connected graph G, diam (G), is the maximum distance between two vertices of G, i.e., diam $(G) = max\{d(u, v) \vee u, v \in V(G)\}$. While the diameter of fullerene graphs having icosahedral symmetry is small, the diameter of nanotubes is linear in the number of vertices.

2.1 Saturation number of fullerene graphs

Every fullerene graph admits a perfect matching [28], and the lower bounds on the number of perfect matchings have been presented in a number of recent papers [9, 14, 39].

Maximal matchings in fullerenes have been for the first in [12], where the following bounds were established.

Proposition 2.5. [12]. Let G be a fullerene graph on p vertices. Then

$$\left\lceil \frac{p}{4}+1\right\rceil \leq S\left(G\right)\leq \frac{p}{2}-2$$

The only property of fullerene graphs used to establish the bounds of proposition 2.5 was their 2-extendibility. (A graph *G* on $p\geq 2(n+1)$ vertices is n-extendable if it contains a set of n-independent edges and if any such set can be extended to a perfect matching in G.)

Došlić in [11] by using another property of fullerene graphs, their 3-regularity and the following result, yields a better lower bound on $S(G)$.

Proposition 2.6. [40]. Let G be a d-regular graph. Then the size of any maximal matching in G is at most

$$\left(2-\frac{1}{d}\right)S\left(G\right).$$

Theorem 2.7. [11] Let G be a fullerene graph on p vertices. Then $S(G)\geq 0.3p$.

Proof. Every fullerene graph contains a perfect matching, i.e., a matching of size $p/2$. As any perfect matching is also maximal, from proposition 2.6 one has $\frac{p}{2}\leq\frac{5}{3}S(G)$, and the claim follows.

Došlić in [11] proved that the lower bound of proposition 2.5 is sharp for only two icosahedral fullerenes and stated and proved an upper bound on the saturation number valid for all fullerene graphs.

Theorem 2.8. [11] Let G be an icosahedral fullerene on p vertices such that $S(G)=0.3p$. Then *G* is either the dodecahedron C_{20} or buckminsterfullerene C_{60}.

Theorem 2.9. [11] There exists an absolute constant $c>0$ such that $S\left(G\right)\leq\frac{p}{2}-c\log_2 p$, for any fullerene graph G on p vertices.

Proof. Let G be a fullerene graph on p vertices. Then for its diameter D we have the following lower bound:

$$D\geq D_0=\lceil\log_2(p+1)-1\rceil=\lfloor\log_2 p\rfloor.$$

Let us take two vertices, u and v, such that the distance between them is equal to D_0. On a path P of length D_0 connecting u and v we can take an independent set I_0 of cardinality $(D_0+2)/2$ in the manner shown in figure 2. Let M_0 be a maximal matching in $G-I_0$ that covers all vertices adjacent to the vertices of I_0 . It is obvious that such a maximal matching always exists, due to the defining properties of fullerene graphs. The cardinality of such a matching cannot exceed $(p-\vee I_0\vee?/2$. This quantity is roughly of the order of $\frac{p}{4}-\frac{1}{4}\log_2 p$. Since M_0 is also a maximal matching in G, the claim of the theorem follows.

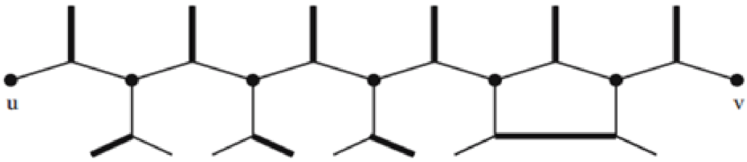


Figure 2. An independent set with $c\log_2 p$ vertices.

Theorem 2.10. Let G be an icosahedral fullerene on p vertices with Coxeter parameters $(3m, 0)$ for some $m\geq 1$. Then

$$S\left(G\right)\leq\frac{p}{3}+\frac{\sqrt{5}}{10}\sqrt{p}-36=\frac{p}{3}+O\left(\sqrt{p}\right).$$

Using the lower bound on the diameter the bounds on the saturation number were improved in [2]:

Theorem 2.11. Let G be a fullerene graph with p vertices. Then,

$$S\left(G\right)\leq\frac{p}{2}-\frac{1}{4}\left(diam\left(G\right)-2\right).$$

In particular,

$$S\left(G\right)\leq\frac{p}{2}-\frac{\sqrt{24n-15}-15}{24}.$$

In [3], V. Andova et al. proved that the saturation number for fullerenes on p vertices is essentially $n/3$.

Theorem 2.12. Let G be a fullerene graph on p vertices. Then

$$\frac{p}{3}-2\leq S\left(G\right)\leq\frac{p}{3}+O\left(\sqrt{p}\right).$$

In order to prove the lower bound of this theorem, they used the discharging method. For the upper bound, they first used Theorem following and obtained a bipartite graph F_0. Later, they established that F_0 is an induced subgraph of a hexagonal lattice or an induced subgraph of a hexagonal tube (defined as on Figure 3). Then they defined a maximal matching on F_0 such that from each hexagon precisely four vertices are covered by the matching.

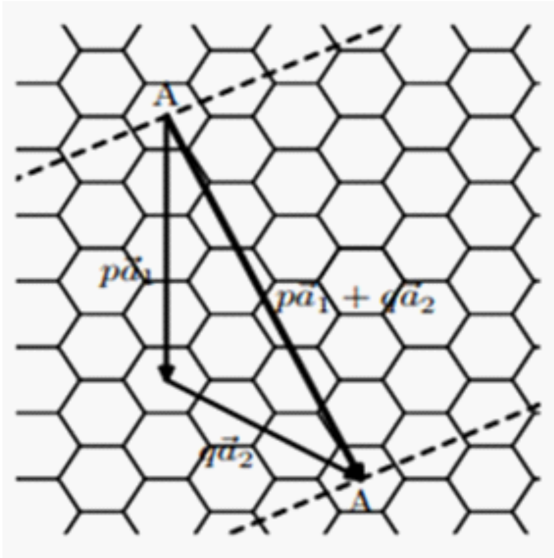


Figure 3. Example of a (2,4) nanotube. The hexagons denoted equally overlap.

The question to determine the exact value of the saturation number remains still open. In [3] V. Andova et al. posed a conjecture concerning the problem.

Conjecture 2.13. There is a constant c such that

$$S\left(G\right) \leq \frac{p}{3} + c$$

for any fullerene graph G on p vertices.

The problem of finding of minimal independent dominating set is NP-complete [41]. This problem is NP-complete even when restricted to planar or bipartite graphs of maximal degree three [41], and remains NP-complete for planar cubic graphs [22]. These results imply the next question.

Problem 2.14. Is the problem to determine the saturation number for the class of fullerene graphs NP-complete?

In the next section, we review the literature dealing with the benzenoid and its saturation number.

3. Benzenoid graphs

Matchings in graphs serve as successful models of many phenomena in engineering, natural and social sciences. A strong initial impetus to their study came from the chemistry of benzenoid compounds after it was observed that the stability of benzenoid compounds is related to the existence and the number of perfect matchings in the corresponding graphs. That observation gave rise to a number of enumerative results that were accumulated over the course of several decades; we refer the reader to monograph [6] for a survey. Further motivation came from the statistical mechanics via the Kasteleyns solution of the dimer problem [25, 26] and its applications to evaluations of partition functions for a given value of temperature. In both cases, the matchings under consideration are perfect.

3.1 Benzenoid hydrocarbons

Chemists have been faced with benzenoid hydrocarbons and their derivatives from the earliest days of organic chemistry. These chemical compounds are usually insensitive, stable over long periods of time, available in large amounts and cheap. They can be easily purified and characterized and undergo well understood chemical reactions.

Benzenoid hydrocarbons are ubiquitous substances, produced by incomplete oxidation of wood, coal or petroleum, by frying food etc. They are contained in soot and smoke. There are strong indications for their existence even in the interstellar clouds.

Kekulé structures play (more or less) significant roles in numerous chemical theories, of which resonance theory and valence bond theory are the best-known examples (see, e.g. Pauling 1939).

A **benzenoid system** is a combinatorial (or if one prefers: geometrical) object obtained by arranging congruent regular hexagons in a plane so that two hexagons are either disjoint or have a common edge. What is meant under this awkward definition should be immediately clear after a glance at Figure 4 (and subsequent figures).

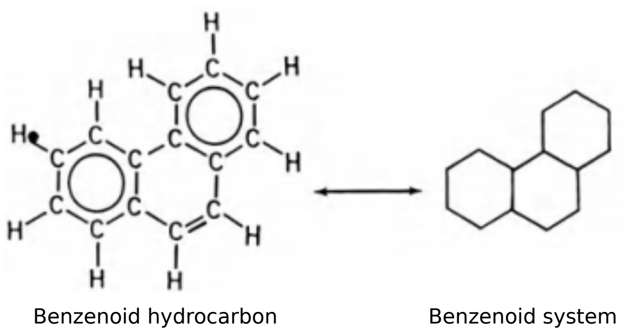


Figure 4. Benzenoid system examples.

A more precise definition of benzenoid systems is a subset (with 1-connected interior) of a regular tiling of the plane by hexagonal tiles. To each benzenoid system, we can assign a graph, taking the vertices of hexagons as the vertices, and the sides of hexagons as the edges of the graph. The resulting simple, plane and bipartite graph is called a **benzenoid graph**.

Let B be a benzenoid systems with n vertices; m edges and h hexagons. These three quantities are mutually related as $h + n = m + 1$.

A perfect matching of a benzenoid system is a selection of mutually independent edges of a benzenoid system which cover all vertices of a benzenoid system. Hence if a benzenoid system has n vertices, then its perfect matching contains $n/2$ vertices and n must be even.

The general one-to-one correspondence between the (mathematical) notion of a perfect matching of a benzenoid system and the (chemical) notion of a Kekulé structural formula of a benzenoid hydrocarbon becomes evident. It is clear in particular that the number of perfect matchings of a benzenoid system is equal to the number of Kekulé structures of the corresponding benzenoid hydrocarbon.

3.2 Benzenoid chains

All faces of a benzenoid graph except the unbounded one are hexagons. The vertices which lie on the perimeter of benzenoid system are called **external**. Those vertices (if any) which lie in the interior of the perimeter are **internal**. Their number is denoted by n_e and n_i , respectively. Then $n_e + n_i = n$. The following relations hold:

$$n + n_i = 4h + 2$$

$$m + n_i = 5h + 1$$

A benzenoid system without internal vertices is said to be **catacondensed**. Otherwise, it is **pericondensed**. Hence, for catacondensed benzenoids n_i= 0 whereas for pericondensed $n_i > O$. A benzenoid is pericondensed if and only if it contains a vertex which simultaneously belongs to three hexagons. If no hexagon in a catacondensed benzenoid is adjacent to three other hexagons, we say that the benzenoid is a **chain**. In each benzenoid chain, there are exactly two hexagons adjacent to one other hexagon; those two hexagons are called **terminal**, while any other hexagons are called **interior**. The number of hexagons in a benzenoid chain is called its **length**. An interior hexagon is called **straight** if the two edges it shares with other hexagons are parallel, i.e., opposite to each other. If the shared edges are not parallel, the hexagon is called **kinky**. (Note that the shared edges cannot be adjacent, since this would result in an internal vertex. Hence the above definitions cover all possible cases.)

If all $h - 2$ interior hexagons of a benzenoid chain with h hexagons are straight, we call the chain a **polyacene** and denote it by A_h. If all interior hexagons are kinky, the chain is called a **polyphenacene** and denoted by Z_h. Since the number of perfect matchings in Z_h is equal to the ($h + 2$)-nd Fibonacci number F_{h+2}, polyphenacenes are also known as **fibonacenes** [6].

A benzenoid in a parallelogram-like shape called the **benzenoid parallelogram** and denoted by $P_{p,q}$, consists of $p \times q$ benzene rings, arranged in p rows, each row containing q benzene rings, shifted by a half benzene ring to the right from the row immediately below. Clearly, $P_{p,q}$ is the same as $P_{q,p}$.

3.3 Saturation number of benzenoid graphs

The saturation number of the benzenoid graph was studied by Došlić and Zubac [8], and Ahmadi et al. in [1], where the following bounds were established.

Proposition 3.1. [8] Let B_h be a benzenoid chain with h hexagons. Then $S(B_h) \geq h + 1$.

Proof. The chain B_h has $4h + 2$ vertices. Since B_h has a perfect matching, its matching number is equal to $2h + 1$. Hence, $S(G) \geq (2h + 1)/2$, and since it must be an integer, $S(G) \geq h + 1$.

Proposition 3.2. [8] $S(B_h)+1 \leq S(B_{h+1}) \leq S(B_h)+2$.

Proposition 3.3. [8] $S(B_h)=h+1$ if and only if $B_h=A_h$.

Proof. All vertical edges of A_h make a maximal matching; hence, $S(A_h) \leq h+1$. Together with Proposition 3.1, this yields $S(A_h)=h+1$.

Let $S(B_h)=h+1$. There are $4h+2$ vertices in B_h and $2h+2$ are saturated by a maximal matching M of cardinality $h+1$. Then the remaining $2h$ vertices must be incident by $4h$ edges not in M. Since there are no vertices of degree one, each unsaturated vertex must be incident with exactly two edges not in M. Further, no hexagon can contain three unsaturated vertices. Hence each hexagon contains two unsaturated vertices of degree 2 which are not adjacent. That is possible only in A_h.

Proposition 3.4. [8] Let $B_{k,m}$ be a benzenoid chain of length h with k kinky hexagons such that no two kinky hexagons are adjacent. Then $S(B_{k,m})=k+m+1$.

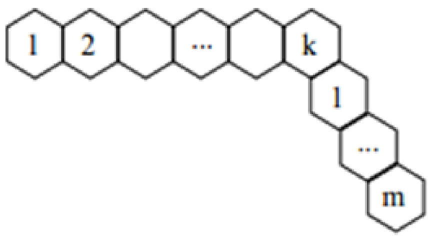


Figure 5. A chain with one kinky hexagon.

Proposition 3.5. [8] Let $S_{k,m}$ be a benzenoid chain shown in Figure 5. Then $S(S_{k,m})=k+m+2$.

Proof. Matching M shown by bold lines in Figure 6 is obviously maximal, hence $S(S_{k,m}) \leq k+m+2$. On the other hand, by Proposition 3.3, we have $S(S_{k,m})>k+m+1$, and the claim follows.

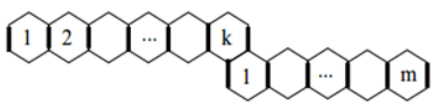


Figure 6. A chain with adjacent kinky hexagons.

Proposition 3.6. [8] Let Z_h be a fibonacene of length h. Then $S(Z_h)=\lfloor \frac{4h}{3} \rfloor+1$.

Theorem 3.7. [8] Let CB_h be a catacondensed benzenoid with h hexagons. Then

$$S\left(CB_h\right) \geq h+2\ .$$

Theorem 3.8. [8] Let $P_{p,q}$ be a benzenoid parallelogram. Then

$$S\left(P_{p,q}\right) \leq \left\lceil \frac{2p+1}{3} \right\rceil q+p\ .$$

In what follows Ahmadi et al. in [1] proved an upper bound of Theorem 3.8 is sharp for benzenoid parallelograms.

Theorem 3.9. Let $P_{p,q}$ be a benzenoid parallelogram and $k, k' \in N$. Then

$$S\left(P_{p,q}\right) \leq \begin{cases} (2k-1)(q+1) & p = 3k-2,\ q = 3k'-2,\ p \geq q; \\ (2k-1)(q+1) & p = 3k-2,\ q \neq 3k'-2; \\ 2k(q+1) & p = 3k-1,\ q \neq 3k'-2; \\ 2k(q+1)+q & p = 3k,\ q = 3k',\ p \geq q\ . \end{cases}$$

Proof. If $(p = 3k-2, q = 3k'-2, p \geq q)$ or $(p = 3k-2, q \neq 3k'-2)$, Since the matching *M* shown in bold in Figure 7.a is maximal, then $S\left(P_{p,q}\right) \leq (2k-1)(q+1)$. If $(p = 3k-1, q \neq 3k'-2)$, then $S\left(P_{p,q}\right) \leq 2k(q+1)$ (Figure 7.b). Similarly, if $(p = 3k, q = 3k')$, then $S\left(P_{p,q}\right) \leq 2k(q+1) + q$ (Figure 7.c).

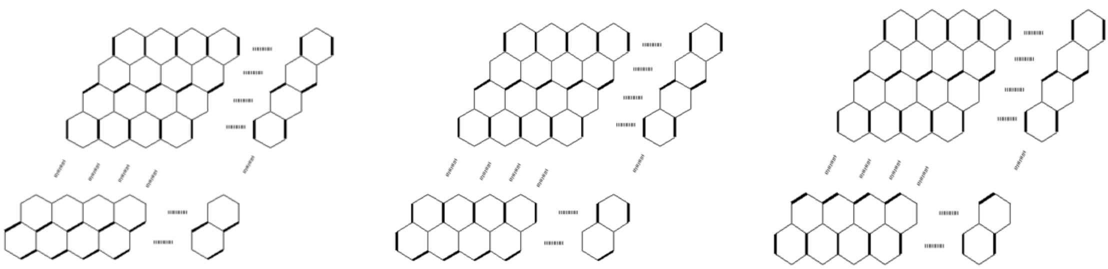

a. (p=3k-2, q=3k'-2, $p \geq q$) or (p=3k-2, $q \neq 3k'$-2)   b. (p=3k-1, q=3k'-2)   c. (p=3k, q=3k', $p \geq q$)

Figure 7. The upper bound on the saturation number and corresponding structure of Pp, q.

Conjecture 3.10. The upper bound presented in theorem 3.9, for $P_{p,q}$ with $(p = 3k-2, q = 3k'-2, p \geq q)$ or $(p = 3k-2, q \neq 3k'-2)$ that $k, k' \in N$, is the saturation number of $P_{p,q}$, i.e.,

$$S\left(P_{p,q}\right) = (2k-1)(q+1)\ .$$

4. Mathematical programming formulation for finding the saturation number

Due to the hardness of solving the saturation number problem even in very restricted classes of graphs, many recent works on the saturation number problem concentrate on two aspects: the approximation point of view and the exact resolution of the saturation number problem in general graphs via mathematical programming techniques [1].

In [1] Ahmadi et al. introduced an integer programming model for saturation number of a graph and later they apply it on fullerene and benzenoid graphs.

Let $A_{n\times n}$ be the adjacency matrix describing graph G. Let d_i degree of vertex i and for each edge (i,j), joining the vertices i and j, a binary variable x_{ij} is associated. Given a maximal matching as a set of edges, the x_{ij} in which participated take the value 1 and otherwise 0.

With respect to the above parameters and variables definition, the mathematical binary integer linear programming problem (BILP) for finding the saturation number of a graph would be as follows:

$$\text{Minimize} \sum_{(i,j)\in E} x_{ij} \tag{1}$$

$$\text{Subject to}$$

$$\sum_{(i,j)\in E} x_{ij} \leq 1 \qquad \forall i \in V \tag{2}$$

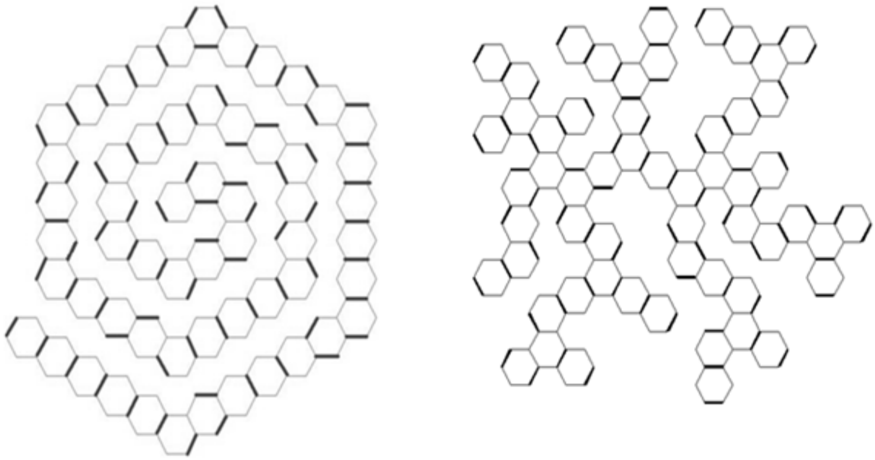
$$d_i \sum_{(i,j)\in E} x_{ij} + \sum_{(i,j)\in E,(k,j)\in E} x_{jk} \geq d_i \qquad \forall i \in V \tag{3}$$

$$x_{ij} \in \{0,1\} \qquad \forall (i,j) \in E \tag{4}$$

Having in mind the definition of x_{ij}, constraints (2) ensures that no two edges of M have a vertex in common. Therefore, it is easy to see that edges of G satisfying the first group of constraints forms a matching of G. Constraints (3) guarantees that node i will not be covered by matching obtained by the constraints (2) if and only if each vertex adjacent to node i are covered by matching M. It is clear that constraints (2), (3) ensure that matching obtained by the constraints (2) is a maximal matching. The feasible solution space of the above mathematical programming problem, determined by inequality constraints (2) and (3), is a set of all possible maximal matching of graph G.

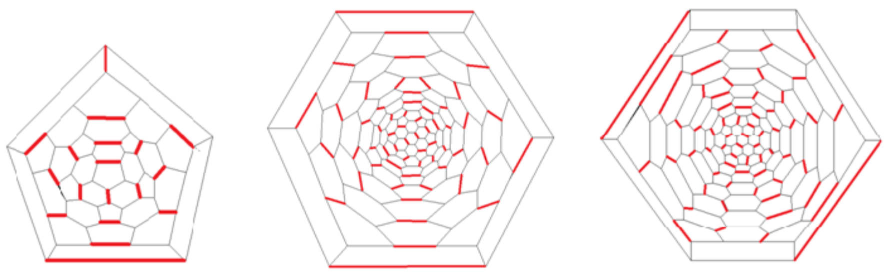
The saturation number and their corresponding structure for two classes of benzenoid graphs and some isomers of fullerenes computed by solving model are illustrated in Figure 8 and 9.

By relaxation the mathematical model, we obtain a linear programming model, that is a polynomial problem to find an upper bound for the saturation number of general graphs.



a. $S(B_{57}) = 70$ b. $S(CB_{56}) = 71$

Figure 8. The saturation number and corresponding structures of B_{57}, CB_{56} .



a. $S(C_{60}) = 18$ b. $S(C_{180}) = 58$ c. $S(C_{192}) = 62$

Figure 9. The saturation number and corresponding structures of C_{60}, C_{180} and C_{192}.

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Bounds on Subdivision and r-Subdivision Graphs and Degree Based Graph Indices

Ismail Naci Cangul[a,*], **Aysun Yurttas**[a], **Muge Togan**[a], **Ahmet Sinan Cevik**[b]

[a]*Department of Mathematics, Faculty of Arts and Science, Uludag University, Bursa, Turkey*
[b]*Department of Mathematics, Faculty of Science, Selcuk University, Konya, Turkey*
ncangul@gmail.com

Abstract

In this chapter, we consider a generalisation of the subdivision graphs which is called as r-subdivision graphs in connection with double graphs and some topological indices. We mainly concentrate on the first and second Zagreb indices together with multiplicative versions of them and obtain relations between several types of Zagreb indices of r-subdivision graphs and subdivision graphs.

Contents

1. Introduction

Let $G = (V, E)$ be a simple graph with $V(G) = n$ vertices and $E(G) = m$ edges. That is, we do not allow loops or multiple edges. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$. A vertex with degree one is called a pendant vertex. Similarly, we shall use the term "pendant edge" for an edge having a pendant vertex. As usual, we denote by $P_n,\ C_n,\ S_n,\ K_n,\ K_{r,s}$ and $T_{r,s}$ the path, cycle, star, complete, complete bipartite and tadpole graphs, respectively.

A molecular graph is a graph showing critical points and bonds of some function related to the required properties of the molecule. In such a molecular graph, atoms are represented by the vertices, and bonds are represented by the edges of the corresponding graph. In that way, it is possible to model a purely chemical molecule or compound mathematically, and by studying this mathematical model, we can determine chemical properties of the given molecule or compound. In Figure 2, the molecular graph corresponding to the ethane molecule given in Figure 1 is shown.

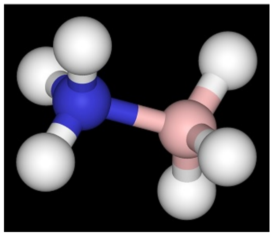

Figure 1. The ethane molecule

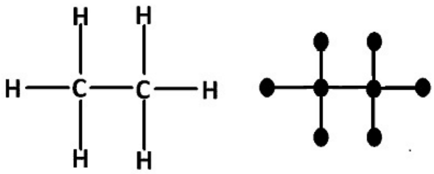

Figure 2. Molecular graph corresponding to the ethane molecule

In this chapter, we shall be concentrating on some vertex degree based topological indices with a special emphasis on Zagreb indices. In recent years, there is quite a long list of papers on these indices, see references. Subdivision graphs will be recalled and as a generalisation of a subdivision graph, the r-subdivision graph will be defined and some formulae and inequalities will be given for the topological indices of subdivision and r-subdivision graphs. In the final part, the double graphs will be recalled and Zagreb indices of double graphs, subdivision and r-subdivision graphs of them will be calculated.

To make the topic more visualised, we shall often make use of the path, cycle, star, complete, complete bipartite and tadpole graphs.

2. Subdivision and r-subdivision

The subdivision graph (or sometimes called as subgraph) $S(G)$ of a simple graph G is defined as the new graph obtained by adding an extra vertex into each edge of G. Equivalently, $S(G)$ is obtained by replacing each edge of the graph by a path of length 2. See e.g. Figure 3. The subdivision graphs have been studied in literature, see e.g. [13, 14, 21, 22, 26, 28].

The main reason to study the subdivision graphs is that, by means of topological indices, this makes combinatorically possible to calculate several properties of large graphs having some symmetry as r-subdivision graphs certainly have symmetrical shapes, in terms of smaller graphs G. Another reason is that we can obtain classified information about a series of graphs from a parent graph and calculate several properties which are usually in terms of topological indices.

In Molecular Chemistry, several chemical operations result in molecular graphs which are subdivision graphs of some other molecular graphs of some chemical compounds. In Figures 4 and 5, two examples to this situation are given:

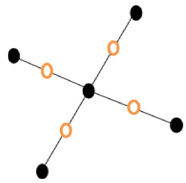

Figure 3. The subdivision graph $S(S_4)$

Figure 4 shows the molecular graph of the transition state of the first step of the nucleophilically unassisted solvolysis of protonated 2-endo- and 2-exo-norbornanol. There are three critical points: nuclear attractor critical point, bond critical point and ring critical point.

Similarly, Figure 5 shows the molecular graphs of the 2-norbornyl and oxabicycloheptanyl cations. It also shows atomic charges.

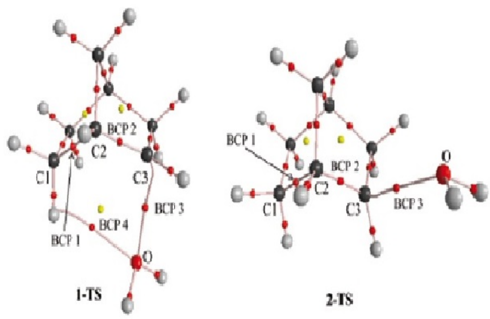

Figure 4. Molecular graphs of the transition state of solvolysis of 2-endo- and 2-exo-norbornanols

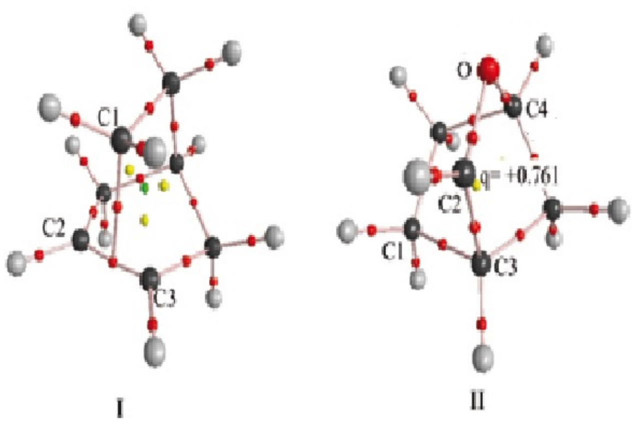

Figure 5. Molecular graphs of the 2-norbornyl and oxabicycloheptanyl cations

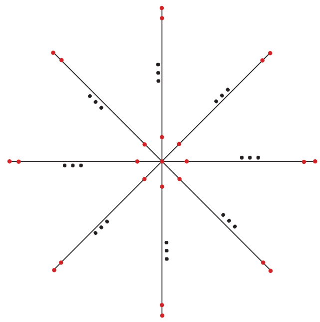

Figure 6. The r-subdivision graph $S^r(S_8)$

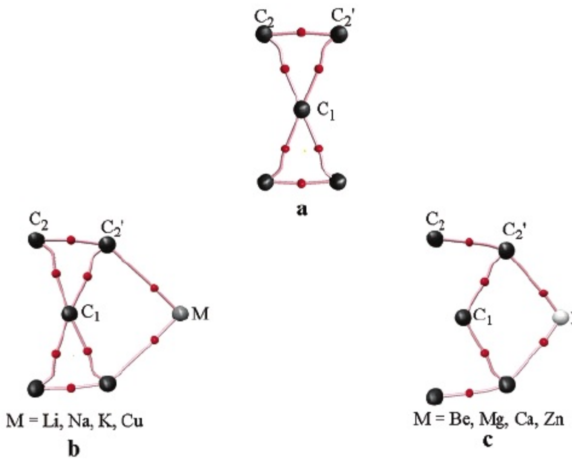

Figure 7. Molecular graphs of (a) C_5^{2-}, (b) C_5^{M-}, and (c) C_5^{M}

In [27], the r-subdivision graph of a graph G, which is denoted with $S^r(G)$ was defined as the new graph obtained from G by replacing each of its edges by a path of length $r+1$; or equivalently by inserting r additional vertices into each edge of G. Clearly, in the case of $r = 1$, the obtained 1-subdivision graph is the subgraph. For example, r-subgraph of the star graph is shown in Figure 6.

Again, the molecular graphs of (a) C_5^{2-}, (b) C_5^{M-}, and (c) C_5^{M}, where M is the metal cation indicated at the bottom of the corresponding graph are shown in Figure 7. The smaller red vertices correspond to bond critical points.

3. Topological indices

Measuring complexity in chemical systems or biological organisms requires the counting of things. Topological indices are widely used in Mathematics and Chemistry in calculating complexity by means of bonds of atoms and molecules. Most of the topological indices are used to study molecules and complexity of selected classes of molecules.

Several topological graph indices have been defined and studied by many mathematicians and chemists as most graphs are generated from molecules by replacing atoms with vertices and bonds with edges. Two of the most important topological graph indices are called first and second Zagreb indices denoted by $M_1(G)$ and $M_2(G)$, respectively:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{(u,v) \in E(G)} d_G(u) d_G(v).$$

They were first defined 41 years ago by Gutman and Trinajstic [10], and are referred to due to their uses in QSAR and QSPR. Ten types of Zagreb indices including the first and second Zagreb indices and the first and second multiplicative Zagreb indices of the subdivision and r-subdivision graphs were recently studied by Togan, Yurttas and Cangul, [26]. Li and Zhao introduced the first general Zagreb index in [17]:

$$M_\alpha(G) = \sum_{u \in V(G)} [d_G(u)]^\alpha.$$

If $\alpha = 2$, we get the first Zagreb index M_1.

Similarly to Zagreb indices, the first and second Zagreb co-indices are defined in [6] in 2008:

$$\overline{M_1}(G) = \sum_{(u,v) \notin E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad \overline{M_2}(G) = \sum_{(u,v) \notin E(G)} d_G(u) d_G(v)$$

which are useful in stating existing results in a more compact form.

Recently, Todeschini and Consonni, [25], have introduced the multiplicative variants of these additive graph invariants by

$$\Pi_1(G) = \prod_{u \in V(G)} d_G^2(u) \quad \text{and} \quad \Pi_2(G) = \prod_{(u,v) \in E(G)} d_G(u) d_G(v)$$

and called them multiplicative Zagreb indices.

The first and second Zagreb indices of some graph operations are found in [16]. In [5], the multiplicative Zagreb indices of these graph operations are calculated. In [12] and [14], the two Zagreb indices were compared for connected graphs.

Very recently, Xu, Das and Tang, [30], have defined two more graph invariants, called multiplicative Zagreb coindices, by

$$\overline{\Pi_1}(G) = \prod_{(u,v) \notin E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad \overline{\Pi_2}(G) = \prod_{(u,v) \notin E(G)} [d_G(u) d_G(v)]$$

and obtained upper and lower bounds for these two invariants of connected (molecular) graphs.

In the same paper, another graph invariant which is called the total multiplicative sum Zagreb index was defined by

$$\overset{T}{\Pi}(G) = \prod_{(u,v)\in V(G)} [d_G(u) + d_G(v)]$$

and as a variant of the multiplicative sum Zagreb index,

$$\Pi_1^*(G) = \prod_{(u,v)\in E(G)} [d_G(u) + d_G(v)]$$

was defined in [7] and some properties were studied in [29].

We must note that the sums and products in all definitions are taken for non-ordered pairs (u, v). That is, for example if $d_G(u) + d_G(v)$ is contained in a sum or product, then $d_G(v) + d_G(u)$ must not be contained.

In this section, relations between the first and second Zagreb indices and the first and second multiplicative Zagreb indices of a simple graph G, of the subdivision graph $S(G)$ and of the r-subdivision graph $S^r(G)$ will be given. The first and second Zagreb indices of the subdivision graph $S(G)$ for some well-known graph types were given in [26]:

Theorem 3.1.

$$M_1(S(G)) = \begin{cases} 8n - 10 & \textit{if } G = P_n,\ n \geq 2 \\ 8n & \textit{if } G = C_n,\ n > 2 \\ (n-1)(n+4) & \textit{if } G = S_n,\ n \geq 2 \\ n^3 - n & \textit{if } G = K_n,\ n \geq 2 \\ ts(t+s+4) & \textit{if } G = K_{t,s},\ \forall t, s > 0 \\ 2(4t + 4s + 1) & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$M_2(S(G)) = \begin{cases} 8n - 12 & \textit{if } G = P_n,\ n \geq 2 \\ 8n & \textit{if } G = C_n,\ n > 2 \\ 2n(n-1) & \textit{if } G = S_n,\ n \geq 2 \\ 2n(n-1)^2 & \textit{if } G = K_n,\ n \geq 2 \\ 2ts(t+s) & \textit{if } G = K_{t,s},\ \forall t, s > 0 \\ 4(2t + 2s + 1) & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

In the same paper, [26], the first and second multiplicative Zagreb indices, Zagreb coindices, multiplicative sum Zagreb index, multiplicative Zagreb coindices and total multiplicative sum Zagreb index of the subdivision graph $S(G)$ for the same well-known graph classes were given. For the completeness of the topic, we recall them without proof:

Theorem 3.2.

$$\Pi_1(S(G)) = \begin{cases} 2^{4n-6} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{4n} & \textit{if } G = C_n,\ n > 2 \\ 2^{2n-2}(n-1)^2 & \textit{if } G = S_n,\ n \geq 2 \\ (n-1)^{2n}2^{n^2-n} & \textit{if } G = K_n,\ n \geq 2 \\ t^{2s}s^{2t}2^{2t\cdot s} & \textit{if } G = K_{t,s},\ \forall t, s > 0 \\ 9 \cdot 2^{4(t+s-1)} & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$\Pi_2(S(G)) = \begin{cases} 2^{4n-6} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{4n} & \textit{if } G = C_n,\ n > 2 \\ 2^{2n-2}(n-1)^{n-1} & \textit{if } G = S_n,\ n \geq 2 \\ (2n-2)^{n(n-1)} & \textit{if } G = K_n,\ n \geq 2 \\ (4ts)^{t\cdot s} & \textit{if } G = K_{t,s}, \forall t, s > 0 \\ 27 \cdot 2^{4(t+s-1)} & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

Theorem 3.3. $$\Pi_1^*(S(G)) = \begin{cases} 9 \cdot 2^{4n-8} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{4n} & \textit{if } G = C_n,\ n > 2 \\ 3^{n-1}(n+1)^{n-1} & \textit{if } G = S_n,\ n \geq 2 \\ (n+1)^{n(n-1)} & \textit{if } G = K_n,\ n \geq 2 \\ (t+2)^{t\cdot s}(s+2)^{t\cdot s} & \textit{if } G = K_{t,s},\ \forall t,\ s > 0 \\ 2^{4(t+s-2)} \cdot 3 \cdot 5^3 & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

Theorem 3.4.

$$\overset{T}{\Pi}(S(G)) = \begin{cases} 2^{4n^2-14n+13}3^{4n-6} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{2n(2n-1)} & \textit{if } G = C_n,\ n > 2 \\ 2^{\frac{3}{2}(n-1)(n-2)}3^{(n-1)^2}[n(n+1)]^{n-1} & \textit{if } G = S_n,\ n > 2 \\ 2^{m(m-1)+n(n-1)/2}(n-1)^{n(n-1)/2}(n+1)^{mn} & \textit{if } G = K_n,\ n \geq 2 \\ 2^{t\cdot s(t\cdot s-1)+[t(t-1)+s(s-1)]/2}s^{s(s-1)/2}t^{t(t-1)/2} & \\ (t+2)^{t\cdot s^2}(s+2)^{t^2\cdot s}(s+t)^{s\cdot t} & \textit{if } G = K_{t,s},\ \forall t,\ s > 0 \\ 4(s+t)^2 - 10(s+t) + 8 & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

In [1], the following very useful relation between the first Zagreb index and coindex is given:

$$M_1(G) + \overline{M_1(G)} = 2m(n-1).$$

By means of the last equation, we now prove the following theorem:

Theorem 3.5. *Let* $m,\ n,\ m(S_1),\ n(S_1)$ *be the number of edges and vertices of* G *and* $S(G)$*, respectively. Then the first Zagreb coindex of subdivision graph of path, cycle, star, complete, bipartite and tadpole graphs is given as follows:*

$$\overline{M_1(S(G))} = \begin{cases} 8n^2 - 24n + 18 & \textit{if } G = P_n,\ n \geq 2 \\ 4n(2n-3) & \textit{if } G = C_n,\ n > 2 \\ (n-1)(7n-12) & \textit{if } G = S_n,\ n > 2 \\ n(n-1)(n^2-3) & \textit{if } G = K_n,\ n \geq 2 \\ ts(3t+3s+4ts-8) & \textit{if } G = K_{t,s},\ \forall t,\ s > 0 \\ 8(s+t)^2 - 12(s+t) - 2 & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

Theorem 3.6. *Let $m,\ n,\ m(S_1),\ n(S_1)$ be as above. Then the second Zagreb coindex of the subdivision graph of path, cycle, star, bipartite and tadpole graphs are given as follows:*

$$\overline{M_2(S(G))} = \begin{cases} 8n^2 - 28n + 26 & \text{if } G = P_n,\ n \geq 2 \\ 4n(2n-3) & \text{if } G = C_n,\ n > 2 \\ (n-1)(\frac{11}{2}n - 10) & \text{if } G = S_n,\ n > 2 \\ \frac{n(n-1)}{2}(4n^2 - 9n + 3) & \text{if } G = K_n,\ n \geq 2 \\ st[8st - \frac{5}{2}(s+t) - 2] & \text{if } G = K_{t,s}, \forall t,\ s > 0 \\ 8(s+t)^2 - 12(s+t) - 5 & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

Theorem 3.7.

$$\overline{\Pi_1(S(G))} = \begin{cases} 2^{4n^2-18n+21} \cdot 3^{4n-8} & \text{if } G = P_n,\ n \geq 2 \\ 4^{n(2n-3)} & \text{if } G = C_n,\ n > 2 \\ 2^{3\binom{n-1}{2}} 3^{n-1} n^{n-1} & \text{if } G = S_n,\ n > 2 \\ 2^{\frac{(n-2)(n+1)}{2}} [4(n-1)]^{\binom{n}{2}} (n+1)^{\frac{-n(n-1)}{2}} & \text{if } G = K_n,\ n \geq 2 \\ 4^{\binom{ts}{2}} (2t)^{\binom{t}{2}} (2s)^{\binom{s}{2}} (t+2)^s (s+2)^t (s+t)^{ts} & \text{if } G = K_{t,s}, \forall t,\ s > 0 \\ 2^{2[2(s+t)^2 - 7(s+t) + 8]} 3^{2s+2t-3} 5^{2s+2t-5} & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$\overline{\Pi_2(S(G))} = \begin{cases} 4^{(n-2)(2n-3)} & \text{if } G = P_n,\ n \geq 2 \\ 4^{n(2n-3)} & \text{if } G = C_n,\ n > 2 \\ 4^{(n-1)(n-2)} (n-1)^{n-1} & \text{if } G = S_n,\ n > 2 \\ 2^{\binom{n}{2} \frac{(n-2)(n+3)}{2}} (n-1)^{\frac{n^2(n-1)}{2}} & \text{if } G = K_n,\ n \geq 2 \\ 2^{ts(t+s+ts-3)} t^{s(s+ts-1)} s^{t(t+ts-1)} & \text{if } G = K_{t,s},\ \forall t,\ s > 0 \\ 2^{2(s+t-1)(2s+2t-3)} 3^{2(t+s-2)} & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

The following result gives the relations between the first and second Zagreb indices of the r-subdivision graph $S^r(G)$ and the first Zagreb index of the graph G:

Theorem 3.8. *Let G be a simple graph with n vertices and m edges and let $S^r(G)$ be the r-subgraph of G. Then the first and second Zagreb indices of $S^r(G)$ are related to the first Zagreb index by the relations*

$$\begin{aligned} M_1(S^r(G)) &= M_1(G) + 4mr, \\ M_2(S^r(G)) &= 2M_1(G) + 4m(r-1). \end{aligned}$$

Proof. For a simple graph G, we have

$$\begin{aligned} M_1(S^r(G)) &= \sum_{i=1}^{n+rm} d_i^2 \\ &= \sum_{i=1}^{n} d_i^2 + \sum_{i=n+1}^{n+rm} d_i^2 \\ &= M_1(G) + 4mr \end{aligned}$$

as all degrees $d_{n+1},\ d_{n+2},\ ...,\ d_{n+rm}$ of the added vertices are 2.

Secondly, every edge (i,j) of G is subdivided in $r+1$ parts with weights $2d_i,\ 2d_j$ and $r-1$ times $2 \cdot 2$. Therefore,

$$\begin{aligned} M_2(S^r(G)) &= \sum_{(i,j)\in E} (2d_i + 2d_j + 4(r-1)) \\ &= \sum_{(i,j)\in E} (2d_i + 2d_j) + 4 \sum_{(i,j)\in E} (r-1) \\ &= 2M_1(G) + 4m \cdot (r-1). \end{aligned}$$

■

Looking at the orders of the magnitudes of the first and second Zagreb indices, Caporossi and Hansen conjectured that there is a nice comparision between these two indices, [3]:

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}.$$

This nice inequality which is known as the Zagreb indices inequality is true for many graph types including trees, unicyclic graphs, graphs with only two different vertex degrees, and some other graph classes with vertex degrees satisfying several conditions. Hansen and Vukićević proved that Zagreb indices inequality is true for all molecular graphs, [11].

We have a lower bound for the first Zagreb index of $S^r(G)$ in terms of m, n and r:

Corollary 3.1. *Let G be a simple graph with n vertices and m edges. Then the first Zagreb index of the r-subdivision graph $S^r(G)$ satisfies the following inequality:*

$$M_1(S^r(G)) \geq \frac{4m(m+nr)}{nr}.$$

Proof. Ilic and Stevanovic, [14], gave the sharp bound $M_1(G) \geq \frac{4m^2}{n}$. By using this inequality and previous theorem, we get

$$M_1(S^r(G)) = M_1(G) + 4mr \geq \frac{4m^2}{n} + 4mr = \frac{4m(m+nr)}{n} \geq \frac{4m(m+nr)}{nr} \ .$$

■

We have a similar inequality which we shall call as the Zagreb indices inequality for the r-subdivision graphs:

Corollary 3.2. *Let G be a simple graph with n vertices and m edges. Then the first and second Zagreb indices of $S^r(G)$ satisfy the following inequality:*

$$\frac{M_1(S^r(G))}{m+nr} \leq \frac{M_2(S^r(G)) + 4m(r-1)}{2m}.$$

Proof. By using the previous corollary, we get

$$\begin{aligned} nr \cdot M_1(S^r(G)) &\geq 4m^2 + 4mnr \\ nrM_1(S^r(G)) - 4m^2 - 4mnr + m \cdot M_1(S^r(G)) &\geq m \cdot M_1(S^r(G)) \\ \frac{M_1(S^r(G)) - 4m}{m} &\geq \frac{M_1(S^r(G))}{m + nr}. \end{aligned}$$

Hence

$$\begin{aligned} \frac{M_1(S^r(G))}{m + nr} &\leq \frac{M_1(S^r(G))}{m} - 4 \\ &= \frac{M_1(G) + 4mr}{m} - 4 \\ &= \frac{\frac{M_2(S^r(G)) - 4mr + 4m}{2} + 4mr}{m} - 4 \\ &= \frac{M_2(S^r(G)) + 4mr + 4m - 8m}{2m} \\ &= \frac{M_2(S^r(G)) + 4m(r - 1)}{2m}. \end{aligned}$$

■

Example 3.1. *Let $m, n, m(S_r), n(S_r)$ be the number of edges and vertices of G and $S^r(G)$, respectively. Then the first and second Zagreb indices of the r-subdivision graphs of path, cycle, star, complete, bipartite and tadpole graphs are given as follows:*

$$\begin{aligned} M_1(S^r(P_n)) &= 4nr - 4r + 4n - 6, \\ M_1(S^r(C_n)) &= 4n(r + 1), \\ M_1(S^r(S_n)) &= (n - 1)(4r + n), \\ M_1(S^r(K_n)) &= n(n - 1)^2 + 4rm, \\ M_1(S^r(K_{t,s})) &= ts(t + s + 4r), \\ M_1(S^r(T_{t,s})) &= 2 + 4(r + 1)(t + s), \end{aligned}$$

and

$$\begin{aligned} M_2(S^r(P_n)) &= 4(nr - r + n - 2), \\ M_2(S^r(C_n)) &= 4n(r + 1), \\ M_2(S^r(S_n)) &= 2(n - 1)(n + 2r - 2), \\ M_2(S^r(K_n)) &= 2n(n - 1)(n + r - 2), \\ M_2(S^r(K_{t,s})) &= 2st[(s + t) + 2(r - 1)], \\ M_2(S^r(T_{t,s})) &= 4\left[(r + 1)(s + t) + 1\right]. \end{aligned}$$

The following result gives the relations between the first and second multiplicative Zagreb indices of the r-subdivision graph $S^r(G)$ and the first and second multiplicative Zagreb indices of the graph G:

Theorem 3.9. *Let G be a simple graph with n vertices and m edges and let $S^r(G)$ be the r-subgraph of G. Then the first and the second multiplicative Zagreb indices of $S^r(G)$ are*

$$\begin{aligned}\Pi_1(S^r(G)) &= 2^{2rm} \cdot \Pi_1(G),\\ \Pi_2(S^r(G)) &= 2^{2rm} \cdot \Pi_2(G).\end{aligned}$$

Proof. For a simple graph G,

$$\Pi_1(S^r(G)) = \prod_{i=1}^{n+rm} d_i^2 = \prod_{i=1}^{n} d_i^2 \cdot \prod_{i=n+1}^{n+rm} d_i^2 = \Pi_1(G) \cdot 2^{2rm}$$

as all degrees $d_{n+1}, d_{n+2}, ..., d_{n+rm}$ of the newly added vertices are 2.

Secondly, every edge (i,j) of G is subdivided in $r+1$ parts with weights $2d_i,\ 2d_j$ and $r-1$ times $2 \cdot 2$. Therefore,

$$\begin{aligned}\Pi_2(S^r(G)) &= \prod_{(i,j)\in E} \left[2d_i \cdot 2d_j \cdot (2\cdot 2)^{(r-1)}\right]\\ &= \prod_{(i,j)\in E} (2d_i \cdot 2d_j) \cdot \prod_{(i,j)\in E} 4^{(r-1)}\\ &= 2^{2m} \prod_{(i,j)\in E} d_i d_j \cdot 4^{m(r-1)}\\ &= 2^{2mr} \cdot \Pi_2(G).\end{aligned}$$

■

Reti and Gutman gave some bounds and inequalities for multiplicative Zagreb indices in [23]. Applying these formulae to the multiplicative Zagreb indices of r-subgraphs by using previous theorem, we obtain some results for r-subgraphs:

Corollary 3.3. *For a simple graph G with n vertices and m edges, we have*

$$\Pi_1(S^r(G)) \le 2^{2(n+rm)} \cdot \left(\frac{m}{n}\right)^{2n}.$$

Proof. By [23], we know that

$$\Pi_1(G) \le \left(\frac{2m}{n}\right)^{2n},$$

so using previous theorem, we get

$$\begin{aligned}\frac{\Pi_1(S^r(G))}{2^{2rm}} &\le \left(\frac{2m}{n}\right)^{2n}\\ \Pi_1(S^r(G)) &\le 2^{2rm} \cdot \left(\frac{2m}{n}\right)^{2n}\\ \Pi_1(S^r(G)) &\le 2^{2(n+rm)} \cdot \left(\frac{m}{n}\right)^{2n}.\end{aligned}$$

■

Corollary 3.4. *For a simple graph G with n vertices and m edges, it holds that*

$$\Pi_1(S^r(G)) \le 2^{2rm} \cdot \left(\frac{M_1(G)}{n}\right)^n .$$

Proof. By [23], we know that

$$\Pi_1(G) \le \left(\frac{M_1(G)}{n}\right)^n ,$$

so using Theorem 3.9, we get

$$\begin{aligned} \frac{\Pi_1(S^r(G))}{2^{2rm}} &\le \left(\frac{M_1(G)}{n}\right)^n \\ \Pi_1(S^r(G)) &\le 2^{2rm} \cdot \left(\frac{M_1(G)}{n}\right)^n . \end{aligned}$$

■

Corollary 3.5. *For a simple graph G with n vertices and m edges, it holds that*

$$\Pi_2(S^r(G)) \ge 2^{2m(r+1)} \cdot \left(\frac{m}{n}\right)^{2m} .$$

Proof. By [23],

$$\Pi_2(G) \ge \left(\frac{2m}{n}\right)^{2m} .$$

Using Theorem 3.9, we have

$$\begin{aligned} \frac{\Pi_2(S^r(G))}{2^{2mr}} &\ge \left(\frac{2m}{n}\right)^{2m} \\ \Pi_2(S^r(G)) &\ge 2^{2mr} \cdot \left(\frac{2m}{n}\right)^{2m} \\ \Pi_2(S^r(G)) &\ge 2^{2m(r+1)} \cdot \left(\frac{m}{n}\right)^{2m} . \end{aligned}$$

■

Corollary 3.6. *For a simple graph G with n vertices and m edges, it holds that*

$$\Pi_2(S^r(G)) \le 2^{2rm} \cdot \left(\frac{M_2(G)}{m}\right)^m .$$

Proof. Similarly, by [23], we know that

$$\Pi_2(G) \le \left(\frac{M_2(G)}{m}\right)^m ,$$

so by Theorem 3.9, we get the desired result:

$$\begin{aligned} \frac{\Pi_2(S^r(G))}{2^{2rm}} &\le \left(\frac{M_2(G)}{m}\right)^m \\ \Pi_2(S^r(G)) &\le 2^{2rm} \cdot \left(\frac{M_2(G)}{m}\right)^m . \end{aligned}$$

■

Example 3.2. *Let* $m,\ n,\ m(S_r),\ n(S_r)$ *be the number of edges and vertices of* G *and* $S^r(G)$*, respectively. Then the first and second Zagreb indices of the* r*-subdivision graphs of path, cycle, star, complete, bipartite and tadpole graphs are given as follows:*

$$\begin{aligned}
\Pi_1(S^r(P_n)) &= 2^{2(nr-r+n-2)},\\
\Pi_1(S^r(C_n)) &= 2^{2n(r+1)},\\
\Pi_1(S^r(S_n)) &= 2^{2r(n-1)} \cdot (n-1)^2,\\
\Pi_1(S^r(K_n)) &= (n-1)^{2n} \cdot 2^{rn(n-1)},\\
\Pi_1(S^r(K_{t,s})) &= ts^{2t} \cdot t^{2s} \cdot 2^{2rts},\\
\Pi_1(S^r(T_{t,s})) &= 3^2 \cdot 2^{2(rt+t+rs+s-2)},
\end{aligned}$$

and

$$\begin{aligned}
\Pi_2(S^r(P_n)) &= 2^{2(nr-r+n-2)},\\
\Pi_2(S^r(C_n)) &= 2^{2n(r+1)},\\
\Pi_2(S^r(S_n)) &= 2^{2r(n-1)} \cdot (n-1)^{(n-1)}),\\
\Pi_2(S^r(K_n)) &= (n-1)^{n(n-1)} \cdot 2^{nr(n-1)},\\
\Pi_2(S^r(K_{t,s})) &= (ts)^{ts} \cdot 2^{2tsr},\\
\Pi_2(S^r(T_{t,s})) &= 2^{2[(t+s)(r+1)-2]} \cdot 3^3.
\end{aligned}$$

The other 6 types of Zagreb indices of the r-subdivision graphs of the above graph classes were calculated in [27].

Although we have concentrated on several versions of Zagreb indices in this section, there are many other vertex degree based topological indices. We shall recall some of them below and give some inequalities for these indices of the r-subdivision graphs.

The Randić index, also known as the connectivity index, of a graph is the sum of bond contributions $1/(d_u d_v)^{1/2}$ where d_u and d_v are the degrees of the vertices making bond $u \sim v$:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^{1/2}}.$$

The Randić index was introduced as a structural descriptor which initially was called branching index that later became Randić connectivity index, one of the most used molecular descriptor in the QSPR and QSAR modeling, [20]. Later this index was generalized by Bollobás and Erdős to the following form for any real number α, and named the general Randić index, [2]:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

There are a lot of variants of the Randić index amongst topological indices. The sum connectivity index was defined as a slight variant of the Randić index and it is exactly the additive version of the Randić index, [32]:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{(d_u + d_v)^{1/2}}.$$

This index was extended to the general sum-connectivity index in [33] in 2010:

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

The harmonic index was defined as another variant of the Randić index, [9]:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

The following result gives some inequalities for Randic, sum-connectivity and harmonic indices of $S^r(G)$:

Theorem 3.10. *Let G be a simple graph with n vertices and m edges and Δ, and δ be the maximum and minimum degrees of G, respectively. Then the inequalities for Randic, sum-connectivity and harmonic indices of $S^r(G)$ are given as follows:*

$$\frac{2m}{\sqrt{2\Delta}} + \frac{m(r-1)}{2} \leq R(S^r G)) \leq \frac{2m}{\sqrt{2\delta}} + \frac{m(r-1)}{2},$$

$$\frac{2m}{\sqrt{2+\Delta}} + \frac{m(r-1)}{2} \leq \chi(S^r(G)) \leq \frac{2m}{\sqrt{2+\delta}} + \frac{m(r-1)}{2},$$

$$\frac{4m}{2+\Delta} + \frac{m(r-1)}{4} \leq H(S^r(G)) \leq \frac{4m}{2+\delta} + \frac{m(r-1)}{4}.$$

Proof. The proof is given for the sum-connectivity index. Similar combinatorial methods can be used for others. There are two types of entries in $\chi(S^r(G))$:

i) $u \in V(G)$ and v is a newly added vertex of degree 2 in $S^r(G)$: For each u, there are d_u added vertices v forming and edge with u, so each vertex pair adds $\frac{1}{\sqrt{2+d_u}}$ to $\chi(S^r(G))$.

ii) Both u and v are middle vertices (of degree 2) which form an edge: There are $r-1$ vertex pairs in each edge of $S^r(G)$, so $\frac{m(r-1)}{2}$ is added to $\chi(S^r(G))$. Finally, adding all these together, we get

$$\chi(S^r(G)) = \sum_{u \in V} \frac{1}{\sqrt{2+d_u}} + \frac{m(r-1)}{2}.$$

If the maximum degree Δ is taken in place of each d_u, it can be easily seen that

$$\chi(S^r(G)) \geq \frac{2m}{\sqrt{2+\Delta}} + \frac{m(r-1)}{2}.$$

Similarly

$$\chi(S^r(G)) \leq \frac{2m}{\sqrt{2+\delta}} + \frac{m(r-1)}{2}.$$

■

Another topological index based on the connectivity between atoms and bonds of a molecule was defined in [8]. This topological index which is used to describe the heats of formation of alkanes is called the atom-bond connectivity index (ABC index) and given by the formula

$$ABC(G) = \sum_{uv\in E(G)} (\frac{1}{d_u} + \frac{1}{d_v} - \frac{2}{d_u d_v})^{1/2}.$$

For the atom-bond connectivity index of the r-subdivision graph, we have an exact formula which can be proven similarly:

Lemma 3.11. *Let G be a simple graph with n vertices and m edges and Δ, and δ be the maximum and minimum degrees of G, respectively. Let $S^r(G)$ be the r-subgraph of G. Then the atom-bond connectivity index of $S^r(G)$ is*

$$ABC(S^r(G)) = \frac{m(r+1)}{\sqrt{2}}.$$

Another interesting problem is to explore the relationship between topological index of a composite graph and that of its building blocks. In 2011, Ranjini at all calculated the Zagreb indices of the line graphs of the tadpole graphs, wheel graphs and ladder graphs by using the subdivision concept in [21]. The line graph $L(G)$ of a graph G is the graph whose vertices are the edges of G, and two edges e and f are incident if and only if they have a common end vertex in G. Inspired by the results of [21], Su and Xu calculated the topological indices of the graphs $L[S(T_{r,s})]$:

Proposition 1. *Let G be the line graph of the subdivision graph of the tadpole graph $T_{r,s}$. Then*
i) $M_\alpha(G) = 2^{\alpha+1}(r+s-2) + 3^{\alpha+1} + 1$
ii) $R_\alpha(G) = 2^{2\cdot\alpha+1}(r+s-3) + 3\cdot 6^\alpha + 3^{2\cdot\alpha+1} + 2^\alpha$
iii) $\chi_\alpha(G) = 2^{2\cdot\alpha+1}(r+s-3) + 3\cdot 6^\alpha + 3\cdot 5^\alpha + 3^\alpha$.

Proof. The subdivision graph $S(T_{r,s})$ contains $2(r+s)$ edges, so its line graph contains $2(r+s)$ vertices, out of which 3 vertices are of degree 3 and one vertex of degree 1. The remaining $2r+2s-4$ vertices are all of degree 2. so the M_α value of G is equal to $2^{\alpha+1}(r+s-2)+3^{\alpha+1}+1$. this completes the proof of (i).

The line graph $L[S(T_{r,s})]$ contains a path of length $2\cdot s-1$ and let x_1 be the unique vertex of degree 3 attached to this path. Hence $\sum_{uv\in E(G)}(d_u d_v)^\alpha$ which respect to the path is $4^\alpha(2s-3)+6^\alpha+2^\alpha$. Let x_2 and x_3 be the neighbors of x_1 which are of degree 3 in the line graph $L[S(T_{r,s})]$. The vertices x_2 and x_3 have two neighbors of degree 3 and one neighbor of degree 2 in $L[S(C_r)+e]$, where e is the edge adjacent to $S(C_r)$. The vertex x_1 has two adjacent vertices of degree 3 and one vertex of degree 2 in the path. Hence $\sum_{uv\in E(G)}(d_ud_v)^\alpha$ corresponding to the vertices is $3^{2\alpha+1}+6^\alpha$. Among the remaining $2r-2$ vertices, there exist $2r-3$ vertices with neighbors of degree 2 and one vertex with a neighbor of degree 3. Hence $\sum_{uv\in E(G)}(d_ud_v)^\alpha$ with respect to $2r-2$ vertices is $2^{2\alpha}(2r-3)+6^\alpha$. Hence the R_α-value of G is $2^{2\alpha+1}(r+s-3)+3\cdot 6^\alpha+3^{2\alpha+1}+2^\alpha$. This completes the proof of (ii).

By the similar arguments as the proof of (i) and (ii), we can obtain the proof of (iii). ■

Corollary 3.7. *[21] Let G be the line graph of the subdivision graph of the tadpole graph $T_{r,s}$. Then $M_1(G)=8r+8s+12$ and $M_2(G)=8r+8s+23$.*

Corollary 3.8. *[21] Let G be the line graph of the subdivision graph of the tadpole graph $T_{r,s}$. Then $\chi_1(G)=8r+8s+12$ and $\overline{M_1}(G)=8(n+k)^2-8(n+2k)-6$.*

4. Applications to double graphs

For a graph G with vertex set $V(G)=\{v_1,\ v_2,\ \ldots,\ v_n\}$, we take another copy of G with vertices labelled by $\{v_1,\ v_2,\ \ldots,\ v_n\}$ this time, where v_i corresponds to v_i for each i. If we connect v_i at one copy to the neighbours of v_i for each i at the other copy, we obtain a new graph called the double graph of G. It is denoted by $D(G)$. The double graphs of the cyclic graph C_4 and path graph P_6 are shown in Figures 8 and 9:

Double graphs were first introduced by Indulal and Vijayakumari, [15], in the study of equienergetic graphs. Later Munarini et al., [19], calculated the double graphs of N_n and $K_{t,s}$ as N_{2n} and $K_{2m,2n}$, respectively. Here we first calculate double graphs of other simple graph types such as cycle graph C_n, path graph P_n, star graph S_n, complete graph K_n, tadpole graph $T_{t,s}$.

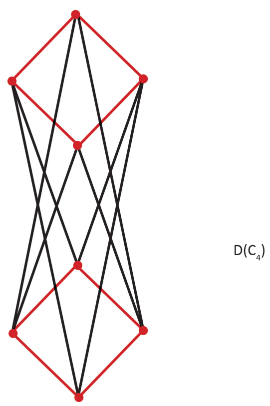

Figure 8. Double graph of cyclic graph C_4

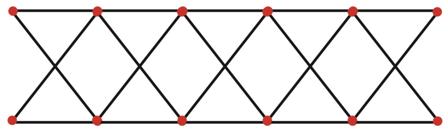

Figure 9. Double graph of path graph P_6

For convenience, we shall denote the number of vertices and edges of $G,\ D(G)$ and $S(D(G))$ by $n,\ m,\ n^d,\ m^d$ and $n^d(S_1)$, $m^d(S_1)$, respectively. The following relations are obvious and will be used in the rest of the chapter:

Lemma 4.1. *With the above notation, we have*
i) $n^d = 2n$
ii) $m^d = 4m$
iii) $n^d(S_1) = m^d + n^d = 2n + 4m,$
iv) $m^d(S_1) = 2m^d = 8m.$

Proof. **i)** $n^d = 2n$ by definition.
ii) $m^d = 2m + \sum_{i=1}^{n} d_{v_i} = 2m + 2m = 4m.$
iii) $n^d(S_1) = m^d + n^d$ by definition. Also by i) and ii), $n^d(S_1) = 2n + 4m.$
iv) $m^d(S_1) = 2m^d = 8m$ by the definition of subdivision graph. ■

In this section, the first and second Zagreb indices and the first and second multiplicative Zagreb indices for the double graphs of some graph types will be calculated. First we have

Theorem 4.2. *The First and second Zagreb indices of double graphs of some well-known graphs are given by*

$$M_1((D(G)) = \begin{cases} 32n - 48 & \text{if } G = P_n,\ n \geq 2 \\ 32n & \text{if } G = C_n,\ n > 2 \\ 8n(n-1) & \text{if } G = S_n,\ n \geq 2 \\ 8n(n-1)^2 & \text{if } G = K_n,\ n \geq 2 \\ 16[2(t+s)+1] & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$M_2(D(G)) = \begin{cases} 64(n-2) & \text{if } G = P_n,\ n\ \geq 2 \\ 64n & \text{if } G = C_n,\ n > 2 \\ 16(n-1)^2 & \text{if } G = S_n,\ n \geq 2 \\ 8n(n-1)^3 & \text{if } G = K_n,\ n \geq 2 \\ 16(3t+4s+4) & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

Proof. We prove the theorem for star graphs. Similar methods can be used for others. Let G be a star graph S_n. Its double graph has $n^d = 2n$ and $m^d = 2m + 2(n-1) = 4(n-1)$. In $D(S_n)$, we have two vertices with degree $2(n-1)$ in the centers of stars, $2(n-1)$ vertices of degree 2 at the end points of stars. So if we use the definition of $M_1(G)$, we have

$$\begin{aligned} M_1(D(S_n)) &= 2^2 \cdot 2(n-1) + 2 \cdot [2(n-1)]^2 \\ &= 16(n-1). \end{aligned}$$

There is only one type of entry in $M_2(D(S_n))$ forming an edge: If u is an endpoint (pendant vertice) of degree 2 and v is the central vertex of degree $2(n-1)$ in $D(S_n)$ then, for each u and v there are $4(n-1)$ edges so each vertex pair adds $2 \cdot 2(n-1) \cdot 4(n-1)$ is added to $M_2(D(S_n))$. By the definition of $M_2(G)$ we get

$$\begin{aligned} M_2(D(S_n)) &= 2(n-1) \cdot 2 \cdot 4(n-1) \\ &= 16(n-1) + 16(n-1)^2 \\ &= 16n(n-1). \end{aligned}$$

■

Theorem 4.3. *First and second multiplicative Zagreb indices of double graphs of some well-known graphs are given by*

$$\Pi_1((D(G)) = \begin{cases} 2^{8(n-1)} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{8n} & \textit{if } G = C_n,\ n > 2 \\ 2^{4n} \cdot (n-1)^4 & \textit{if } G = S_n,\ n \geq 2 \\ [2(n-1)]^{4n} & \textit{if } G = K_n,\ n \geq 2 \\ 2^{8(t+s-1)} \cdot 3^4 & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

and

$$\Pi_2(D(G)) = \begin{cases} 2^{16(n-1)} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{16n} & \textit{if } G = C_n,\ n > 2 \\ [4(n-1)]^{4(n-1)} & \textit{if } G = S_n,\ n \geq 2 \\ [2(n-1)]^{4n(n-1)} & \textit{if } G = K_n,\ n \geq 2 \\ 2^{2(6t+8s-5)} \cdot 3^{10} & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

In [31], Zagreb indices and multiplicative Zagreb indices of some well-known graph types were given. Here, they are recalled without proof:

Theorem 4.4. *Let* $m,\ n,\ m(S_1),\ n(S_1),\ m^d(S_1),\ n^d(S_1)$ *be the number of edges and vertices of* $G,\ S(G)$ *and* $S(D(G))$*, respectively. Then the first and second Zagreb indices of the subdivision graph of double graphs of path, cycle, star, complete and tadpole graphs are given as follows:*

$$M_1(S(D(G))) = \begin{cases} 16(3n-4) & \textit{if } G = P_n,\ n \geq 2 \\ 48n & \textit{if } G = C_n,\ n > 2 \\ 8(n-1)(n+2) & \textit{if } G = S_n,\ n \geq 2 \\ 8n^2(n-1) & \textit{if } G = K_n,\ n \geq 2 \\ 16(3(t+s)+1) & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$M_2(S(D(G))) = \begin{cases} 32(2n-3) & \textit{if } G = P_n,\ n \geq 2 \\ 64n & \textit{if } G = C_n,\ n > 2 \\ 16n(n-1) & \textit{if } G = S_n,\ n \geq 2 \\ 16n(n-1)^2 & \textit{if } G = K_n,\ n \geq 2 \\ 32(2(t+s)+1) & \textit{if } G = T_{t,s},\ t \geq 3,\ r \geq 1. \end{cases}$$

Theorem 4.5. *The first and second multiplicative Zagreb indices of the subdivision graphs of double graphs of several graph types*

$$\Pi_1(S(D(G))) = \begin{cases} 2^{16(n-1)} & \textit{if } G = P_n,\ n \geq 2 \\ 2^{16n} & \textit{if } G = C_n,\ n > 2 \\ (n-1)^4 \cdot 2^{4(3n-2)} & \textit{if } G = S_n,\ n \geq 2 \\ (n-1)^{4n} \cdot 2^{4n^2} & \textit{if } G = K_n,\ n \geq 2 \\ 2^{8[2(t+s)-1]} \cdot 3^4 & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

and

$$\Pi_2(S(D(G))) = \begin{cases} 2^{8(3n-4)} & \textit{if } G = P_n,\ n\ geq 2 \\ 2^{24n} & \textit{if } G = C_n,\ n > 2 \\ 2^{16(n-1)} \cdot (n-1)^{4(n-1)} & \textit{if } G = S_n,\ n \geq 2 \\ [4(n-1)]^{4n(n-1)} & \textit{if } G = K_n,\ n \geq 2 \\ 2^{24(t+s)-16} \cdot 3^{12} & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

We conclude this chapter by the following two theorems which give the first and second Zagreb and also multiplicative Zagreb indices of the r-subdivision graph of the double graph of some graphs:

Theorem 4.6. *Let $m,\ n,\ m(S_r),\ n(S_r),\ m^d(S_r),\ n^d(S_r)$ be the number of edges and vertices of $G,\ S^r(G)$ and $S^r(D(G))$, respectively. Then the first and the second Zagreb indices of r-subdivision graphs of double graphs of path, cycle, star, complete and tadpole graphs are given as follows:*

$$M_1(S^r(D(G))) = \begin{cases} 16(nr-r+1)+32(n-2) & \textit{if } G = P_n,\ n \geq 2 \\ 32n+16nr & \textit{if } G = C_n,\ n > 2 \\ 8(n-1)\left[1+2r+(n-1)\right] & \textit{if } G = S_n,\ n \geq 2 \\ 8n(n-1)\left[(n-1)+r\right] & \textit{if } G = K_n,\ n \geq 2 \\ 16\left[(s+t)(r+2)+1\right] & \textit{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$M_2(S^r(D(G))) = \begin{cases} 32+16(n-1)(r-1)+64(n-2) & \textit{if } G = P_n,\ n \geq 2 \\ 64n+16n(r-1) & \textit{if } G = C_n,\ n > 2 \\ 8(n-1)\left[2n+r-1\right] & \textit{if } G = S_n,\ n \geq 2 \\ 8n(n-1)\left[2(n-1)+(r-1)\right] & \textit{if } G = K_n,\ n \geq 2 \\ 16\left[(s+t)(r^2+3)+2\right] & \textit{if } G = T_{t,s},\ t \geq 3,\ r \geq 1. \end{cases}$$

Theorem 4.7. *The first and second multiplicative Zagreb indices of the r-th subdivision of double graphs of several graph types are given by*

$$\Pi_1(S^r(D(G))) = \begin{cases} 2^{8[1+r(n-1)+(n-2)]} & \text{if } G = P_n,\ n \geq 2 \\ 2^{8n(r+1)} & \text{if } G = C_n,\ n > 2 \\ 2^{4(n-1)[1+2r]}\,[2(n-1)]^4 & \text{if } G = S_n,\ n \geq 2 \\ [2(n-1)]^{4n}\,2^{4nr(n-1)} & \text{if } G = K_n,\ n \geq 2 \\ 2^{8[(t+s)(r+1)-1]}3^4 & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1 \end{cases}$$

and

$$\Pi_2(S^r(D(G))) = \begin{cases} 2^{2[(r-1)(n-1)+4(3n-4)]} & \text{if } G = P_n,\ n \geq 2 \\ 2^{8n(r+2)} & \text{if } G = C_n,\ n > 2 \\ 2^{8(n-1)(r+1)}(n-1)^{4(n-1)} & \text{if } G = S_n,\ n \geq 2 \\ (n-1)^{4n(n-1)}2^{4n(n-1)(r+1)} & \text{if } G = K_n,\ n \geq 2 \\ 2^{8[(t+s)(r+2)-2]}3^{12} & \text{if } G = T_{t,s},\ t \geq 3,\ s \geq 1. \end{cases}$$

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