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Harmonic Index and its Generalizations: Extremal Results and Bounds

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Abstract

The general sum–connectivity index χ_α of a graph G is defined as $\chi_\alpha(G) = \sum_{uv\in E(G)}(d_u + d_v)^\alpha$, where uv is the edge connecting the vertices u and v, d_u is the degree of the vertex u, and α is a real number. Research on χ_α began in 1972, when the first Zagreb index χ_1 was introduced within a study of total π-electron energy. Later, in 1987, the harmonic index $H(= 2\chi_{-1})$ appeared in connection with some conjectures, generated by the computer program Graffiti. The sum–connectivity index $\chi_{-1/2}$, was proposed in 2009 and eventually extended to the general sum–connectivity index χ_α, which not only includes all the aforementioned graph invariants but also the hyper–Zagreb index χ_2. In this survey, we outline extremal results and bounds involving the mentioned invariants.

1 Introduction

Throughout this survey paper, the term "graph" refers to a simple and finite graph, unless stated otherwise. Let G be such a graph, $V(G)$ its vertex set and $E(G)$ its edge set. The number of vertices, $|V(G)| = n$ is the order of G. The number of edges $|E(G)| = m$ is the size of G. A graph with n vertices and m edges is referred to as an (n, m)-graph. The edge connecting the two vertices u and v will be denoted by uv. The degree of a vertex

u, denoted by d_u, is the number of vertices adjacent to u. If $d_u = 0$, then u is an isolated vertex. If $d_u = 1$ then u is a pendent vertex, whereas uv is a pendent edge.

Additional definitions are found in Section 2. For notation and terminology the readers may also consult the books [27, 86, 91, 184].

The graphs representing molecules are said to be molecular graphs. In these graphs, vertices correspond to the atoms while edges represent the covalent bonds between atoms in the underlying molecule [86, 184]. Graph invariants that found applications in chemistry, especially in QSPR and QSAR studies, are usually referred to as topological indices [46, 58, 174, 175].

The *Platt index*, proposed for predicting properties of paraffins [146], is one of the oldest degree–based topological index. It is defined as

$$Pl(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)\,.$$

Note that $d_u + d_v - 2$ is the degree of the edge uv, namely the number of edges incident to uv.

The Platt index can be written [62, 138] as

$$Pl(G) = M_1(G) - 2m\,, \tag{1}$$

where m is the size of the graph G and $M_1(G)$ is the *first Zagreb index*,

$$M_1(G) = \sum_{u \in V(G)} d_u^2 = \sum_{uv \in E(G)} (d_u + d_v)\,.$$

It was introduced in 1972 within the study of total π-electron energy of alternant hydrocarbons [89]. Certainly, both the topological indices M_1 and Pl have same properties, due to the identity (1).

The first Zagreb index is one of the most thoroughly examined degree–based graph invariants. Details about the (chemical and mathematical) properties of the first Zagreb index can be found in the surveys [13, 28, 29, 83, 84, 87, 138] and in the references quoted therein.

Inspired by the work done on the first Zagreb index M_1, Zhou and Trinajstić [214] proposed the following generalized version of M_1:

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha$$

where α is a real number. It is customary to require that α be non-zero, because the case $\alpha = 0$ is trivial: $\chi_0(G) = m$ for all graphs G.

The topological index χ_α generalizes also the so called *sum–connectivity index* X (which is equal to $\chi_{-1/2}$), introduced in [213], and hence the name *general sum–connectivity index*.

The sum–connectivity index is also a variant of the well–known Randić index [155], which was proposed for measuring the extent of branching of certain chemical compounds. The Randić index of a graph G is defined as

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2} .$$

The sum–connectivity index and Randić index correlate well among themselves and the predictive abilities of these topological indices are practically same in most of the cases; for example, see [81, 118–121, 139, 188]. It should be mentioned here that the topological index χ_2 was proposed in [167], under the name *hyper–Zagreb index*.

In 1987, the so called *harmonic index* appeared within some conjectures, generated by the computer program Graffiti [73]. The harmonic index is usually denoted by H and this topological index coincides with the graph invariant $2\,\chi_{-1}$. Till 2011, the harmonic index attracted little attention. But, after the paper [202] was published, the situation changed and many publications on this topological index resulted and are still appearing.

At this point it should be noted that in the literature there is another topological index [136], which was also proposed under the name harmonic index, but whose definition is different from that of H.

Three fundamental and most studied problems in the theory of topological indices, considered in mathematical chemistry, ask for the

- extremal structures, under certain constraints, that maximize or minimize the given topological index;
- best possible lower and upper bounds for the given topological index;
- relations between different topological indices.

In this survey, we attempt to gather results pertaining to the above mentioned issues, involving the harmonic index H, sum–connectivity index X, hyper–Zagreb index χ_2 and general sum–connectivity index χ_α. Certainly, several result concerning the topological index χ_α recovers also the results regarding the first Zagreb index (and hence the Platt index). Moreover, due to the recently published updated surveys on the first Zagreb index [13, 28, 29], we do not include results that are concerned only with the first Zagreb index.

The remaining part of this survey is organized as follows. The main definitions are given in the next section. Sections 3, 4, and 5 are devoted, respectively, to results on the harmonic index H, sum–connectivity index X, and general sum–connectivity index χ_α (including the hyper–Zagreb index χ_2).

2 Preliminaries

Most of the well–known degree–based topological indices can be obtained from the following general setting [95, 187]:

$$BID(G) = \sum_{uv \in E(G)} f(d_u, d_v), \tag{2}$$

where f is a non-negative real valued symmetric function of d_u and d_v. The topological indices of the form (2) will be referred to as *bond incident degree indices* [185], BID indices in short. In Table 2, we list some choices of the function f for which Eq. (2) corresponds to topological indices considered in the current literature.

The *first Zagreb coindex* is defined [61] as

$$\overline{M}_1(G) = \sum_{uv \notin E(G); u \neq v} (d_u + d_v)$$

which can also be obtained from (2) because of the identity [45]:

$$\overline{M}_1(G) = \sum_{uv \in E(G)} \left[2\left(|V(G)| - 1\right) - (d_u + d_v)\right].$$

The *average distance* $\mu(G)$ of a connected graph G is defined [63] as

$$\mu(G) = \frac{1}{\binom{n}{2}} \sum_{\{u,v\} \subseteq V(G)} d(u, v) \tag{3}$$

where $d(u, v)$ denotes the distance (that is, length of the shortest path) between the vertices u and v.

The *sum–connectivity matrix* $S(G)$ of a non-trivial graph G is defined [215] as

$$S(G) = [s_{i,j}]_{n \times n}$$

The function $f(d_u, d_v)$	Eq. (2) corresponds to	symbol
$d_u + d_v$	first Zagreb index [89]	M_1
$2(d_u + d_v)^{-1}$	harmonic index [73]	H
$(d_u + d_v)^{-1/2}$	sum–connectivity index [213]	X
$(d_u + d_v)^2$	hyper–Zagreb index [167]	χ_2
$(d_u + d_v)^\alpha$	general sum–connectivity index [214]	χ_α
$(d_u)^{-3/2} + (d_v)^{-3/2}$	zeroth–order connectivity/Randić index [106]	${}^0R$
$(d_u)^2 + (d_v)^2$	forgotten topological index [78]	F
$(d_u)^{\alpha-1} + (d_v)^{\alpha-1}$	general zeroth–order Randić index [98]	${}^0R_\alpha$
$d_u\, d_v$	second Zagreb index [88]	M_2
$(d_u\, d_v)^{-1/2}$	Randić index [155]	R
$(d_u\, d_v)^{-1}$	modified second Zagreb index [138]	M_2^*
$(d_u\, d_v)^\alpha$	general Randić index [25]	R_α
$\sqrt{\frac{d_u+d_v-2}{d_u\, d_v}}$	atom–bond connectivity index [72]	ABC
$2\sqrt{d_u\, d_v}(d_u + d_v)^{-1}$	first geometric–arithmetic index [186]	GA
$d_u\, d_v(d_u + d_v)^{-1}$	inverse sum indeg index [187]	ISI

Table 1: Some topological indices considered in the present survey paper. The parameter α is a non-zero real number. Here, it should be mentioned that the modified second Zagreb index M_2^* coincides with the first–order overall index [26, 138], R_α is also referred to as variable second Zagreb index (see [131]), and ${}^0R_\alpha$ coincides with both the first general Zagreb index [110] and variable first Zagreb index [131].

where

$$s_{i,j} = \begin{cases} (d_{v_i} + d_{v_j})^{-1/2} & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

It should be mentioned that trace of the matrix $S(G)^2$ coincides with the harmonic index [215].

The sum $S_i = \sum_{j=1}^{n} s_{i,j}$ is known as the sum of the i-th row of the sum–connectivity matrix $S(G)$ of an n-vertex graph G [198].

The sum of absolute values of all eigenvalues of the sum–connectivity matrix $S(G)$ is referred to as the *sum–connectivity energy* (SE) [215].

If G is an n-vertex graph, then the *sum–connectivity Estrada index* (SEE) of G is defined [198] as

$$SE(G) = \sum_{i=1}^{n} e^{\mu_i}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of the sum–connectivity matrix $S(G)$.

The *eccentricity* of a vertex v in a graph is the distance from v to a vertex farthest from v. The *radius* of a graph G is the minimal vertex eccentricity in G. The *average eccentricity* of a graph G, denoted by $avec(G)$, is the mean value of eccentricities of all vertices of G.

The *diameter* of a graph G is the greatest distance between any pair of vertices of G.

The minimum number of edges of a (connected) graph G whose removal makes G acyclic is known as the *cyclomatic number* and it is denoted by ν.

The *chromatic number* of a graph G, denoted by $\chi(G)$, is the minimum number of colors needed to color the vertices of G so that no two adjacent vertices have the same color. The *total chromatic number* of a graph G is the minimum number of colors needed to color the elements (that is, the vertices and edges) of G so that incident elements as well as the adjacent elements have distinct colors.

The *clique number* of a graph G, denoted by $\omega(G)$, is the maximal order of a complete subgraph of G.

If D is the diagonal matrix of vertex degrees of a graph G and A is the adjacency matrix of G, then the matrix $D + A$ is called *signless Laplacian matrix.*

A *matching* in a graph is a set of pairwise non-adjacent edges.

In a graph G, a set $D \subseteq V(G)$ is a *dominating set* if every vertex of the set $V(G) \setminus D$ has a neighbor in D. A *minimal dominating set* is one which consists of a least number of vertices. The *domination number* is the number of vertices in a minimal dominating set.

Any subset V' of the vertex set of a graph G is said to be an *independent set* if the vertices of V' are pairwise non-adjacent. The *independence number* of a graph G is defined as the cardinality of a maximal independent set in G.

A tree resulting in a path after deletion of all its pendent vertices is known as a *caterpillar.* Let $d \geq 3$, $p_i \geq 0$ for $2 \leq i \leq d-2$ and p_1, $p_{d-1} \geq 1$. Denote by $MS(p_1, p_2, \ldots, p_{d-1})$ the caterpillar consisting of a path $v_1 v_2 \cdots v_{d-1}$ with p_i pendent vertices attached at v_i for $1 \leq i \leq d-1$.

A tree containing exactly one branching vertex is said to be a *starlike tree.* Denote by

$S_n(r_1, r_2, \ldots, r_k)$ the n-vertex starlike tree whose pendent paths have lengths $r_1, r_2, \ldots, r_k$, where $r_1 \geq r_2 \geq \cdots \geq r_k$ and $r_1 + r_2 + \cdots + r_k + 1 = n$.

Following Hosseini *et al.* [97], we define a *proper Kragujevac tree*: a tree possessing a central vertex of degree at least 3, to which branches of the form B_1 and/or B_2 and/or B_3 and/or ... B_k are attached, where the branches B_1, B_2, ..., B_k are depicted in Figure 1.

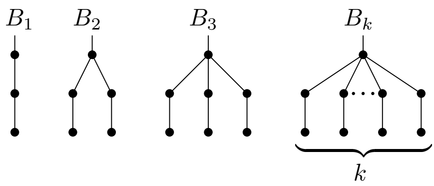

Figure 1: The branches of a proper Kragujevac tree.

Denote by $S_{n,p}$ the tree obtained from the path P_{n-p+1} by attaching $p-1$ pendent vertices to one pendent vertex of P_{n-p+1}.

With given vertex degrees, the *greedy tree* is achieved through the following "greedy algorithm" [189]:

(i) Label the vertex with the largest degree as v (the root);

(ii) Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degrees available to them such that $d_{v_1} \geq d_{v_2} \geq \cdots$;

(iii) Label the neighbors of v_1 (except v) as $v_{1,1}, v_{1,2}, \ldots$ such that they take all the largest degrees available and that $d_{v_{1,1}} \geq d_{v_{1,2}} \geq \cdots$, then do the same for $v_2, v_3, \ldots$;

(iv) Repeat (iii) for all the newly labeled vertices, always start with the neighbors of the labeled vertex with the largest degree whose neighbors are not labeled yet.

Given a non-increasing degree sequence $(d_1, d_2, \ldots, d_m)$ of internal vertices, the *alternating greedy tree* is constructed through the following recursive algorithm [189]:

(i) If $m-1 \leq d_m$, then the alternating greedy tree is simply obtained by a tree rooted at r with d_m children, $d_m - m + 1$ of which are pendents and the rest with degrees $d_1, \ldots, d_{m-1}$;

(ii) Otherwise, $m-1 \geq d_m + 1$. We produce a subtree T_1 rooted at r with $d_m - 1$ children with degrees $d_1, \ldots, d_{d_m - 1}$;

(iii) Consider the alternating greedy tree S with degree sequence $(d_{d_m}, \ldots, d_{m-1})$, let v be a pendent vertex with the smallest neighbor degree. Identify the root of T_1 with v.

A *quasi–tree* is a graph obtained from a tree T by adding one vertex u and edges joining u to some positive number of vertices in T.

A connected graph G is a *cactus* if and only if every edge of G lies on at most one cycle.

Denote by $H(n,k;n_1,n_2,\ldots,n_k)$ the unicyclic graph obtained from a cycle C_k with n_i pendent vertices attached at v_i for $1 \le i \le k$, where $C_k = v_1v_2\cdots v_kv_1$, $n_i \ge 0$ and $n_1+\cdots+n_k = n-k$.

For $3 \le k \le n-2$, let $U_{n,k}^{k_1,k_2,\ldots,k_t}$ be the unicyclic graph obtained from the cycle C_k by attaching t paths of lengths $k_1,k_2,\ldots,k_t$ to one vertex of C_k such that $k_1+k_2+\cdots+k_t = n-k$. Let

$$\mathcal{F}_1 = \{U_{n,3}^{k_1,k_2,\ldots,k_{\Delta-2}} : 1 \le k_1,k_2,\ldots,k_{\Delta-2} \le 2\}$$

and

$$\mathcal{F}_2 = \{U_{n,k}^{k_1,k_2,\ldots,k_{\Delta-2}} : k \ge 3 \ \text{ and } \ k_1,k_2,\ldots,k_{\Delta-2} \ge 2\}.$$

Let u be a fixed pendent vertex of the n-vertex star graph S_n, $n \ge 4$. Denote by $H_{n,r}$ the graph obtained from S_n by adding r edges between u and r other pendent vertices.

Let $K_{1,n-1}^* \cong K_{1,n-1}$ and for $k \ge 2$, let $K_{k,n-k}^*$ be the graph obtained from the complete bipartite graph $K_{k,n-k}$ by adding an edge between every pair of (different) vertices of degree $n-k$.

A graph $\mu^*(G)$ obtained from a graph G by applying the transformation introduced in [135] is known as *Mycielskian* of G. The vertex set of $\mu^*(G)$ consists of the disjoint union $V(G) \cup V'(G) \cup \{w\}$, where $V'(G) = \{v' : v \in V(G)\}$, and the edge set of $\mu^*(G)$ is the set $E(G) \cup \{v'u : vu \in E(G)\} \cup \{v'w : v' \in V'(G)\}$.

Let $(d_0,d_1,\ldots,d_{n-1})$ be a non-increasing degree sequence of a connected graph G with vertex set $V(G) = \{v_0,v_1,\ldots,v_{n-1}\}$, where $d_i = d_{v_i}$ for $i = 0,1,\ldots,n-1$. Following Li *et al.* [108], we introduce an ordering of the vertices of G induced by breadth–first search (BFS): create a sorted list of vertices beginning with v_0; append all neighbors $u_1,u_2,\ldots,u_{d_0}$ of v_0 sorted by decreasing degrees; then append all neighbors of u_1 that are not already in the list, also sorted by decreasing degrees; continue recursively with $u_2,u_3,\ldots$, until all vertices of G are processed. In this way, we get a rooted graph, with root v_0. The distance $d(v,v_0)$ is called the height $h(v)$ of a vertex $v \in V(G)$.

Let G be a connected rooted graph with root v_0. A well ordering $\prec$ of the vertices is called *breadth–first searching ordering* [24,200] with non-increasing degrees (BFS ordering for short) if the following conditions hold for all vertices $u,v \in V(G)$:

(i) $u \prec v$ implies $h(u) \leq h(v)$;

(ii) $u \prec v$ implies $d(u) \geq d(v)$;

(iii) let $uv, xy \in E(G)$ and $uy, xv \notin E(G)$ with $h(u) = h(x) = h(v) - 1 = h(y) - 1$. If $u \prec x$, then $v \prec y$.

A graph having a BFS ordering of its vertices is known as a *BFS graph.*

Denote by $x_{a,b}$ the number of edges, in a graph G, connecting the vertices of degrees a and b.

A *k-polygonal system* is a connected geometric figure obtained by concatenating congruent regular k-polygons side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and a number of finite (internal) regions, and all internal regions must be congruent regular k-polygons. In a k-polygonal system, two polygons are said to be adjacent if they share a side. The *characteristic graph* (or *dualist* or *inner dual*) of a given k-polygonal system consists of vertices corresponding to k-polygons of the system; two vertices are adjacent if and only if the corresponding k-polygons are adjacent. A k-polygonal system whose characteristic graph is the path (respectively, tree) is called *k-polygonal chain* (respectively, *k-polygonal catacondensed system*). In a k-polygonal chain, a k-polygon having one (respectively two) neighboring k-polygon(s) is called *terminal* (respectively, *non-terminal*) *k-polygon.* Any k-polygonal system can be represented by a graph, in which the edges represent sides of a k-polygon while the vertices correspond to the points where two sides of a k-polygon meet. In what follows, by a k-polygonal system we always mean the graph corresponding to the k-polygonal system.

A 3-polygonal (triangular) chain in which every vertex has degree at most 4 is said to be a *linear triangular chain.*

In a 4-polygonal (polyomino) chain, a non-terminal square having a vertex of degree 2 is known as a kink. In a 5-polygonal (pentagonal) chain, a kink is a non-terminal pentagon which contains an edge connecting the vertices of degree 2. A *linear polyomino/pentagonal chain* is the one, without kinks. A *zigzag polyomino/pentagonal chain* is the one, consisting of only kinks and terminal squares. A *segment* in a polyomino/pentagonal chain is a maximal linear sub–chain, including the kinks and/or terminal squares at its ends. The number of squares/pentagons in a segment is called its *length.* A segment is said to be *external* (*internal*, respectively) segment if it contains (does not contain, respectively) terminal square/pentagon.

The 6-polygonal (hexagonal) systems with equal number of hexagons and equal number of internal vertices are known as *isomeric*. Isomeric hexagonal systems have also equal number of vertices and equal number of edges. Paths along the perimeter of a hexagonal system having degree sequences (2, 3, 2), (2, 3, 3, 2), (2, 3, 3, 3, 2), (2, 3, 3, 3, 3, 2) are known as *fissure, bay, cove, fjord,* respectively. Sum of the number of fissures, bays, coves, and fjords of a hexagonal system S is called the *number of inlets* of S.

In a hexagonal system, let b, c, f be the numbers of bays, coves, fjords, respectively.

3 The Harmonic Index

In this section, we collect results concerning the harmonic index H which are related to the bounds and extremal properties of H. Because of the fact that $H = 2\chi_{-1}$, various such type of results follow from Section 5, concerning general sum–connectivity index χ_α, which covers the value $\alpha = -1$.

3.1 Harmonic index on trees

To the best of our knowledge, [202] is the first paper on extremal properties of the harmonic index H. Zhong [202] identified the unique graphs with extremal H values among n-vertex trees.

Theorem 1. [202] *If $n \geq 3$, then among n-vertex connected graphs (and hence, among n-vertex trees) the star is the unique graph with minimal H value, equal to $2(n-1)/n$.*

If we replace "connected graphs" with "graphs without isolated vertices" in Theorem 1 then the resulting (generalized) statement remains true [211]. Theorem 1 was proven also in [38] independently. Tomescu and Kanwal [182] determined trees with first five minimum H values among n-vertex trees, see Theorem 134. Trees with first two (respectively, first four) minimum H values were determined also in [109] (respectively, [53]).

Theorem 2. [202] *If $n \geq 4$, then only the path graph P_n has maximum H value (which is equal to $\frac{n-3}{2} + \frac{4}{3}$) among n-vertex trees.*

Theorem 2 was proved by an alternative way in [99,109]. Ilić [100] proved Theorem 2 in a short way and determined the trees with second maximum H value among n-vertex trees, using a graph transformation which may be helpful in characterizing the graphs with maximum H value among connected (n, m)-graphs. Deng *et al.* [52] characterized the trees with third, fourth and fifth maximum H values from the class of all n-vertex trees (for sufficiently large n).

Theorem 3. [100] *If $n \geq 7$, then only the starlike trees of the form $S_n(r_1, r_2, r_3)$, where $r_1 \geq r_2 \geq r_3 \geq 2$, have second maximum H value (which is equal to $\frac{n-7}{4} + \frac{3}{5} + 1$) among n-vertex trees.*

From Theorem 3, it follows that only the starlike trees of the form $S_n(r_1, r_2, r_3)$, where $r_1 \geq r_2 \geq r_3 \geq 2$, have maximum H value among n-vertex starlike trees. This fact was proved also in [22].

Fan *et al.* [76] determined the graphs with extremal H values from several classes of trees. The next three results were proved in [76, 108] independently.

Theorem 4. [76, 108] *Among n-vertex trees with domination number γ, only the tree $T^0(n, \gamma)$ has minimum H value, where $T^0(n, \gamma)$ is the tree obtained from the star $S_{n-\gamma+1}$ by attaching a pendent edge to each of $\gamma - 1$ pendent vertices of $S_{n-\gamma+1}$.*

Theorem 5. [76, 108] *For $n \geq 4$, among n-vertex trees with domination number $\lceil n/3 \rceil$, only the path P_n has maximum H value.*

Theorem 6. [76, 108] *For $n \geq 5$, among n-vertex trees with domination number 2, only $P_4(\lceil (n-4)/2 \rceil, \lfloor (n-4)/2 \rfloor)$ has maximum H value, where $P_4(\lceil (n-4)/2 \rceil, \lfloor (n-4)/2 \rfloor)$ is the tree obtained from the path P_4 $(= v_1 v_2 \cdots v_\ell)$ by attaching $\lceil (n-4)/2 \rceil$ (respectively, $\lfloor (n-4)/2 \rfloor$) pendent vertices to v_1 (respectively, v_ℓ) of P_4.*

Theorem 7. [76] *If $|V_1| = p, |V_2| = q$ and $n \geq 4$, then among n-vertex trees with bipartition (V_1, V_2), only the tree $B'_{p,q}$ has minimum H value, where the tree $B'_{p,q}$ is obtained from the path P_2 by attaching $p - 1$ pendent vertices to one end vertex of P_2 and $q - 1$ pendent vertices to the other end vertex of P_2.*

The next result was proved independently in [76, 116, 166, 182].

Theorem 8. [76, 116, 166, 182] *For $n \geq 5$ and $3 \leq k \leq n - 2$, among n-vertex trees with k pendent vertices, only the tree $S_{n,k}$ has minimum H value.*

Deng *et al.* [53] characterized the graphs having second minimum H value from the family of n-vertex trees with fixed pendent vertices.

Shi [166] solved the problem of finding trees having maximum harmonic index from the class of trees with fixed order as well as pendent vertices.

Theorem 9. [166] *If* $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$, *then among* n*-vertex trees with* k *pendent vertices, only trees which have* $k-2$ *vertices of maximum degree 3 such that every vertex of degree 3 is adjacent to either another vertex of degree 3 or a vertex of degree 2, have maximum* H *value.*

Theorem 9 can be considered as a particular case of Theorem 136. Since the extremal trees specified in Theorem 9 are chemical trees, these trees also have the maximum H value in the family of n-vertex chemical trees with k pendent vertices under the constrains given in the aforementioned theorem and this fact was proven also in [41, 116]. Graphs with minimum H value in the family of n-vertex chemical trees with fixed number of pendent vertices were determined in [116]. Graphs with first three minimum (respectively, maximum) H values from the family of n-vertex chemical trees were characterized in [116, 205] (respectively, [205]) .

The following theorem was proven in [53, 76, 182] independently.

Theorem 10. [53, 76, 182] *If* $n \geq 3$ *and* $2 \leq d \leq n-1$, *then among* n*-vertex trees with diameter* d, *the tree* $T_d^1(n-d-1)$ *has minimum* H *value, where the tree* $T_d^1(n-d-1)$, *is obtained from the path* P $(= v_0 v_1 \cdots v_d)$ *by attaching* $n-d-1$ *pendent vertices to the vertex* v_1.

Trees with second minimum H value and trees with third to $(\lceil (n-d+1)/2 \rceil + 1)$ −th minimum H values were also determined in [53, 76, 182] and [182], respectively, among n-vertex trees with diameter d. Some extremal results concerning the harmonic index H for multigraphs can be found in [182].

Theorem 11. [158] *If* $n \geq 5$, *then among* n*-vertex trees with maximum degree* Δ,

- *the starlike tree* $S_n(r_1, r_2, \ldots, r_k)$, *with* $r_1 \geq r_2 \geq \cdots \geq r_k \geq 2$, *has maximum* H *value for* $3 \leq \Delta \leq \frac{n-1}{2}$
- *the starlike tree* $S_n(r_1, r_2, \ldots, r_k)$, *with* $1 \leq r_k \leq r_{k-1} \leq \cdots \leq r_1 \leq 2$, *has maximum* H *value for* $\Delta > \frac{n-1}{2}$.

Theorem 12. [189] *Among trees with a given degree sequence, the greedy tree has maximum H value and the alternating greedy tree has minimum H value.*

Theorem 13. [37] *Among proper Kragujevac n-vertex trees with the central vertex of degree r (where $r \geq 3$) and no branches of type B_1, the tree V (respectively, U) has maximum (respectively, minimum) H value, where the trees U and V are depicted in Figure 2.*

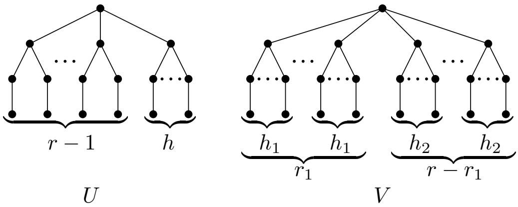

Figure 2: The trees U and V mentioned in Theorems 13 and 88, where $h = \frac{n-5r+3}{2}$, $h_1 = \lfloor \frac{n-r-1}{2r} \rfloor$, $h_2 = \lceil \frac{n-r-1}{2r} \rceil$ and $r_1 = \frac{(3+2h_1)m-n+1}{2}$.

Theorem 14. [158] *If T is an n-vertex tree with maximum degree Δ and $n \equiv r$ (mod $\Delta - 1$), then*

$$H(T) \geq \begin{cases} \frac{2(n-1)^2}{(\Delta+2)n-4(\Delta-1)} & \text{if } r = 0 \\ \frac{2(n-1)^2}{(\Delta+2)n-3\Delta} & \text{if } r = 1 \\ \frac{2(n-1)^2}{(\Delta+2)n-2(\Delta+1)} & \text{if } r = 2 \\ \frac{2(n-1)^2}{(\Delta+2)n-2\Delta-3+r(r-2)} & \text{if } r \geq 3. \end{cases}$$

Theorem 15. [157] *If T is an n-vertex tree with maximum degree Δ and $n \equiv r$ (mod*

$\Delta - 1$), where $\Delta \geq 3$, then

$$H(G) \geq \begin{cases} \frac{2}{\Delta-1}\left(\frac{n(\Delta-2)}{\Delta+1} + \frac{\Delta-2}{2} + \frac{n-(\Delta-1)^2}{2\Delta}\right) & \text{if } r = 0 \text{ and } n > (\Delta-1)(\Delta-2) \\ 2\left(\frac{(\Delta-1)^2-n}{(\Delta-1)^2} + \frac{n-\Delta+1}{\Delta+1} + \frac{n-\Delta+1}{2(\Delta-1)^2}\right) & \text{if } r = 0 \text{ and } n \leq (\Delta-1)(\Delta-2) \\ 2\left(\frac{n(\Delta-2)+1}{\Delta^2-1} + \frac{\Delta-1}{2\Delta-1} + \frac{n-1-\Delta(\Delta-1)}{2\Delta(\Delta-1)}\right) & \text{if } r = 1 \text{ and } n > (\Delta-1)^2+1 \\ 2\left(\frac{\Delta(\Delta-1)-n+1}{\Delta(\Delta-1)} + \frac{n-\Delta}{\Delta+1} + \frac{n-\Delta}{(2\Delta-)(\Delta-1)}\right) & \text{if } r = 1 \text{ and } n \leq (\Delta-1)^2+1 \\ \frac{2}{\Delta-1}\left(\frac{n(\Delta-2)+2}{\Delta+1} + \frac{n-\Delta-1}{2\Delta}\right) & \text{if } r = 2 \\ 2\left(\frac{n(\Delta-2)+r-\Delta+1}{\Delta^2-1} + \frac{r-1}{\Delta+r-1} + \frac{n-(r-1)\Delta-1}{2\Delta(\Delta-1)}\right) & \text{if } r \geq 3 \text{ and } n \geq \Delta(r-1)+1 \\ 2\left(\frac{(r-1)\Delta-n+1}{r(\Delta-1)} + \frac{n-r}{\Delta+1} + \frac{n-r}{(\Delta+r-1)(\Delta-1)}\right) & \text{if } r \geq 3 \text{ and } n < \Delta(r-1)+1. \end{cases}$$

3.2 Harmonic index of unicyclic and bicyclic graphs

The graphs with extremum H values from the collections of all n-vertex connected unicyclic and bicyclic graphs were determined independently in [99, 203] and [99, 210, 220], respectively.

Theorem 16. [99, 203] *If $n \geq 4$, then among n-vertex connected unicyclic graphs, only the graph $H_{n,1}$ has minimum H value and only the cycle C_n has maximum H value.*

It should be mentioned that Li and Shiu [109] proved Theorem 16 by an alternative way.

For sufficiently large n, graphs with second to fourth (respectively, second to fifth) maximum H values were characterized in [209] (respectively, [52]), from the family of connected unicyclic n-vertex graphs.

Tomescu and Kanwal [183] determined the graphs with first three minimum H values from the family of n-vertex connected unicyclic graphs having girth at least 4, see Theorem 141.

Theorem 17. [209] *Let $\mathcal{U}_{n,k}$ be the set of connected unicyclic n-vertex graphs with girth k.*

(i). If $n \geq k \geq 3$, then $H(n,k;n-k,0,\ldots,0)$ is the unique graph with minimum H value

in the set $\mathcal{U}_{n,k}$.

(ii). If $n \geq k = 3$*, then* $H(n, 3; n-4, 1, 0)$ *is the only graph with second minimum* H *value in the set* $\mathcal{U}_{n,k}$.

(iii). If $n \geq k+2 \geq 6$*, then members of* $A(n, k)$ *are the only graphs with second minimum* H *value in the set* $\mathcal{U}_{n,k}$*, where* $A(n, k)$ *is the set of* n*-vertex unicyclic graphs consisting of a cycle* C_k*,* $n-k-1$ *pendent edges incident to a vertex* $x \in V(C_k)$ *and one pendent edge incident to a vertex* $y \in V(C_k)$*, such that the distance between* x *and* y *is at least 2.*

Theorem 17 also follows from Theorem 140(v) and Theorem 141.

Theorem 18. [209] *Let* $\mathcal{U}_{n,k}$ *be the set of connected unicyclic* n*-vertex graphs with girth* k.

(i). If $n-2 \geq k \geq 3$*, then the graph obtained from the cycle* C_k *by attaching a path of length* $n-k$ *to one vertex of* C_k*, is the unique graph with maximum* H *value in the set* $\mathcal{U}_{n,k}$.

(ii). If $n-4 \geq k \geq 3$*, then the members of* $B(n, k)$ *are the only graphs with second maximum* H *value in the set* $\mathcal{U}_{n,k}$*, where* $B(n, k)$ *is the set of* n*-vertex unicyclic graphs obtained either by attaching two paths of length at least 2 to two adjacent vertices of* C_k *or by connecting an edge between a vertex of* C_k *and a vertex* v *of a path of length* $n-k-1$ *such that* v *is not adjacent to any pendent vertex.*

(iii). If $k = n-3$*, then* $U_{n,n-3}$ *is the only graph with second maximum* H *value in the set* $\mathcal{U}_{n,k}$*, where* $U_{n,n-3}$ *is the graph obtained by attaching a path of length 2 and a path of length 1 to two adjacent vertices* u, v *of* C_{n-3}*, respectively.*

(iv). If $k = n-2$*, then* $U_{n,n-2}$ *is the only graph with second maximum* H *value in the set* $\mathcal{U}_{n,k}$*, where* $U_{n,n-2}$ *is the graph obtained from* C_{n-2} *by attaching two pendent edges, one at* $u \in V(C_{n-2})$ *and the other at* $v \in V(C_{n-2})$ *provided that* $uv \in E(C_{n-2})$.

The next result can be considered as an extended version of Theorem 17(i).

Theorem 19. [204] *If* $k \geq 3$*, then* $H(n, k; n-k, 0, \ldots, 0)$ *is the unique graph with minimum* H *value in the set of connected* n*-vertex graphs with girth at least* k.

Theorem 20. [208] *If* $4 \leq d \leq n-2$*, then among* n*-vertex connected unicyclic graphs with diameter* d*, the unique graph obtained by attaching* $n-d-1$ *pendent edges and a path of length* $d-3$ *to two non-adjacent vertices of* C_4*, respectively, has minimum* H *value.*

Theorem 21. [156] *If* $n \geq 5$ *and* G *is the graph with maximum* H *value among connected unicyclic* n*-vertex graphs having maximum degree* Δ*, where* $\frac{n+2}{2} \leq \Delta$ *or* $\Delta \leq \frac{n+1}{2}$*, then* $G \in \mathcal{F}_1 \cup \mathcal{F}_2$.

Theorem 22. [164] *If* G *is a connected unicyclic molecular* n*-vertex graph with* p *pendent vertices, then*

$$H(G) \geq \frac{n}{4} + \frac{3p}{20}$$

with equality if and only if G *contains only vertices of degrees 1 and 4.*

Theorem 23. [99,210,220] *If* $n \geq 4$*, then among* n*-vertex connected bicyclic graphs, only the graph* $H_{n,2}$ *has minimum* H *value.*

Theorem 24. [99,210,220] *If* $n \geq 6$*, then among* n*-vertex connected bicyclic graphs, only the following graphs have maximum* H *value:*

- *the graph obtained from two disjoint cycles by joining them with an edge,*
- *the graph obtained from a cycle by adding an edge between any two non-adjacent vertices.*

Deng *et al.* [52] characterized the graphs with first four maximum H values from the class of all n-vertex connected bicyclic graphs (for sufficiently large n).

3.3 Harmonic index of general graphs

Theorem 25. [108] *Among connected* n*-vertex graphs with fixed degree sequence, there exists a BFS graph with maximum* H *value.*

Theorem 26. [164] *If* $n \geq 3$ *and* G *is a connected* n*-vertex graph with maximum degree* Δ*, then*

$$H(G) \geq \frac{2n\Delta}{(\Delta+1)^2}$$

with equality if and only if G *is the star graph.*

Chang *et al.* [31] extended Theorem 1 for the n-vertex connected graphs with minimum degree at least 2.

Theorem 27. [31] *If* $n \geq 4$*, then among* n*-vertex connected graphs with minimum degree at least 2, only the graph* $K^*_{2,n-2}$ *has minimum* H *value which is equal to*

$$4\left(1 - \frac{3}{n+1}\right) + \frac{1}{n-1}\,.$$

Theorem 27 was proved also by Wu *et al.* [193] independently. The next result was proved independently in [31, 166].

Theorem 28. [31,166] *If $n \geq 3$, then among triangle-free connected n-vertex graphs with minimum degree $k \geq 1$, only the complete bipartite graph $K_{k,n-k}$ has minimum H value (which is equal to $\frac{2k(n-k)}{n}$).*

For $k = 2$ (respectively, for $1 \leq k \leq \frac{n}{2}$), Theorem 28 was proved also by Wu *et al.* [193] (respectively, by Liu [114]) independently. Cheng and Wang [33] extended Theorem 27 to the n-vertex connected graphs with minimum degree at least 3.

Theorem 29. [33] *If $n \geq 6$, then among n-vertex connected graphs with minimum degree at least 3, only the graph $K^*_{3,n-3}$ has minimum H value which is equal to*

$$6\left(1 - \frac{5}{n+2}\right) + \frac{3}{n-1}.$$

Theorem 30. [122] *Among n-vertex connected graphs having k (where $1 \leq k \leq n-2$) vertices of degree $n-1$ (which implies that the minimum degree in G is at least k), $K^*_{k,n-k}$ is the unique graph with minimum H value, which is equal to*

$$\frac{2k(n-k)}{n+k-1} + \frac{k(k-1)}{2(n-1)}.$$

Since $K^*_{k,n-k}$ is the unique extremal graph in Theorem 30 and also for $k = 1, 2, 3$, the only graph $K^*_{k,n-k}$ has minimum harmonic index among n-vertex connected graphs with minimum degree at least k, see Theorems 1, 27, 29, respectively. Thereby, Cheng and Wang [33] proposed the following conjecture:

Conjecture 31. [33] *If $n \geq 4$ and $1 \leq k \leq \lfloor n/2 \rfloor + 1$, then among all n-vertex connected graphs with minimum degree at least k, only the graph $K^*_{k,n-k}$ has minimum H value.*

Generally, Conjecture 31 is not true, as some counterexamples were reported in [7] for $k = \lfloor n/2 \rfloor + 1$. However, Conjecture 31 is true when $1 \leq k \leq n/2$ and this fact was recently proved in [111]. The problem of characterizing graphs with minimum harmonic index from the family of n-vertex connected graphs having minimum degree at least k, for $n/2 < k \leq n-2$, was solved in [111, 113].

Theorem 32. [123] *If $n \geq 4$, then among n-vertex quasi-trees which contain at least one cycle, only the graph $H_{n,1}$ has minimum H value which is equal to*

$$\frac{2(n-3)}{n} + \frac{4}{n+1} + \frac{1}{2}.$$

Theorem 33. [16] *If $n \geq 5$, then among connected n-vertex cacti with k cycles, the graph containing a vertex of degree $n-1$ is the unique graph with minimum H value.*

Several extremal results concerning harmonic index can be found in the book chapter [163]. Next, we state some results concerning specific k-polygonal chain graphs.

Theorem 34. [9] *If $h \geq 4$, then among triangular chains with h triangles and maximum degree 5, only the linear triangular chain has maximum H value.*

Theorem 35. [149] *If $h \geq 3$, then among polyomino chains with h squares, only the linear polyomino chain has maximum H value.*

Theorem 35 was proved also in [14].

Theorem 36. [14, 50] *Among the members of Ω_h, only the zigzag polyomino chain has minimum H value, where Ω_h is the collection of polyomino chains having h squares, in which no internal segment of length 3 has edge connecting the vertices of degree 3.*

Theorem 37. [39, 152] *If $h \geq 3$, then among polyomino chains with h squares, only the zigzag polyomino chain has minimum H value.*

Clearly, Theorem 36 immediately follows from Theorem 37. The next result is due to Cruz and Rada [40].

Theorem 38. [40] *If $h \geq 3$, then among polyomino catacondensed systems with h squares, only the linear polyomino chain has maximum H value.*

Theorem 39. [15] *If $h \geq 3$, then among members of Ω'_h, only the zigzag (respectively, linear) pentagonal chain has minimum (respectively, maximum) H value, where Ω'_h is the collection of pentagonal chains, having h pentagons, in which no internal segment of length 3 has edge connecting the vertices of degree 3.*

Cruz *et al.* [36] characterized the hexagonal systems having extremum H value from the collection of isomeric hexagonal systems.

Theorem 40. [36] *Among isomeric hexagonal systems, those having minimum (respectively, maximum) number of inlets have maximum (respectively, minimum) H value.*

Theorem 41. [153] *Among catacondensed hexagonal systems with h hexagons, the linear hexagonal chain L_h (respectively, E_h) has minimum (respectively, maximum) H value, where E_h is described in Figure 6 of Ref.* [153].

Further extremal results concerning harmonic index of certain hexagonal systems can be found in [21, 34, 35, 92, 92, 150, 151, 154].

Recall that the numbers of bays, coves, and fjords of a hexagonal system are denoted by b, c, and f.

Theorem 42. [57] *If there is a hexagonal system S_0 with $h \geq 3$ hexagons, $2h + 1 + \lceil \sqrt{12h-3} \rceil$ vertices such that S_0 satisfies the equation $b + 2c + 3f = 0$, then among hexagonal systems with h hexagons, S_0 has the minimal H value, which is equal to*

$$\frac{7\lceil \sqrt{12h-3} \rceil}{15} + h + \frac{3}{5}.$$

Further extremal results related to Theorem 42 can be found in [57, 85].

Brewster *et al.* [30] disproved two conjectures posed in [74] concerning the bounds of H. The next result is due to Ilić [100].

Theorem 43. [100] *If $n = a + b \geq 3$ and G is a triangle–free connected (n, m)-graph, then*

$$H(G) \geq \frac{2m}{n} = \frac{2ab}{n}$$

with equality if and only if $G \cong K_{a,b}$.

Theorem 43 also follows from Theorem 161. Theorem 43 was proved also in [114] independently. It is interesting to note that the extremal graphs in both Theorems 28 and 43 are the complete bipartite graphs.

Theorem 44. [48] *For $n \geq 3$, if G is a connected n-vertex graph and λ_1 is the largest eigenvalue of G, then*

$$H(G) \geq \frac{2(n-1)^{3/2}}{\lambda_1 n}$$

with equality if and only if $G \cong S_n$;

$$H(G) \geq 1 + \lambda_1 - \frac{n}{2}$$

with equality if and only if $G \cong K_n$;

$$\begin{aligned} H(G) &\geq 3\sqrt[3]{\frac{(n-1)^2}{2n}} - \lambda_1 \\ H(G) &\geq \frac{\lambda_1 n}{2}. \end{aligned}$$

Zhong [202] established a simple but elegant upper bound, given in the next theorem.

Theorem 45. [202] *If G is an n-vertex graph then*

$$H(G) \leq \frac{n}{2}$$

with equality if and only if G is regular.

The bound given in Theorem 45 was derived also in [38, 99, 114] independently.

Theorem 46. [196] *If G is a non-trivial connected (n,m)-graph, then*

$$H(G) \geq \frac{m}{n - r(G)}$$

where $r(G)$ is the radius of G. If $G \cong K_n$ then the bound is attained.

Theorem 47. [196] *If G is a non-trivial connected (n,m)-graph with p pendent vertices, then*

$$H(G) \geq \frac{p}{n-1} + \frac{m-p}{\left(n-1-\frac{p}{2}\right)^2}\,.$$

Theorem 48. [112] *If $n \geq 4$ and G is a connected n-vertex graph with diameter $D(G)$, then*

$$H(G) \leq D(G) + \frac{n}{2} - 1 \qquad \text{and} \qquad H(G) \leq \frac{1}{2}\, n\, D(G)$$

where the equality sign in any of the above inequalities holds if and only if $G \cong K_n$.

Theorem 49. [112] *If $n \geq 4$ and T is an n-vertex tree with diameter $D(T)$, then*

$$H(T) \geq D(T) + \frac{5}{6} - \frac{n}{2} \qquad \text{and} \qquad H(T) \geq \left(\frac{1}{2} + \frac{1}{3(n-1)}\right) D(T)$$

where the equality sign in any of the above inequalities holds if and only if $G \cong P_n$.

Liu [112] thought that Theorem 49 is true for any connected n-vertex graph, $n \geq 4$, and thereby proposed the following conjecture.

Conjecture 50. [112] *If $n \geq 4$ and G is a connected n-vertex graph with diameter $D(G)$, then*

$$H(G) \geq D(G) + \frac{5}{6} - \frac{n}{2} \qquad \text{and} \qquad H(G) \geq \left(\frac{1}{2} + \frac{1}{3(n-1)}\right) D(G)$$

where the equality sign in any of the above inequalities holds if and only if $G \cong P_n$.

Jerline and Michaelraj [104] proved the first inequality of Conjecture 50 for unicyclic graphs by giving a better bound, given in the next theorem.

Theorem 51. [104] *If $n \geq 7$ and G is a connected n-vertex unicyclic graph with diameter $D(G)$, then*

$$H(G) \geq D(G) + \frac{5}{3} - \frac{n}{2}$$

with equality if and only if G is isomorphic to the graph obtained from the cycle C_4 by attaching one pendent edge and a path of length $n-5$ to two diametrically nonadjacent vertices of C_4.

Jerline and Michaelraj [105] proved the second inequality of Conjecture 50 for unicyclic graphs by establishing the following better bound:

Theorem 52. [105] *If $n \geq 7$ and G is a connected n-vertex unicyclic graph with diameter $D(G)$, then*

$$H(G) \geq \left(\frac{1}{2} + \frac{2}{3(n-2)}\right) D(G)$$

with equality if and only if G is isomorphic to the graph obtained from the cycle C_4 by attaching one pendent edge and a path of length $n-5$ to two diametrically nonadjacent vertices of C_4.

Jerline and Michaelraj [105] proposed the following stronger version of Conjecture 50.

Conjecture 53. [105] *If $n \geq 4$ and G is a connected n-vertex graph, different from tree, with diameter $D(G)$, then*

$$H(G) \geq D(G) + \frac{5}{3} - \frac{n}{2} \qquad \text{and} \qquad H(G) \geq \left(\frac{1}{2} + \frac{2}{3(n-2)}\right) D(G)$$

where the equality sign in any of the above inequalities holds if and only if G is isomorphic to the graph obtained from the cycle C_4 by attaching one pendent edge and a path of length $n-5$ to two diametrically nonadjacent vertices of C_4.

Theorem 54. [49] *If χ is the chromatic number of an n-vertex graph G then*

$$H(G) \geq \frac{\chi}{2}$$

with equality if and only if $G \cong K_a \cup bK_1$ where K_a and K_1 are disjoint complete graphs, and b is a non-negative integer satisfying $a + b = n$.

The next result is an immediate consequence of Theorem 54.

Corollary 55. [49] *If χ is the chromatic number of an n-vertex graph G then*

$$H(G) \geq \chi - \frac{n}{2}$$

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

Deng *et al.* [56] established two lower bounds on H in order to prove a conjecture concerning Randić index and radius of a graph. They also proposed a conjecture concerning lower bound on H.

Theorem 56. [56] *If T is a tree different from the even path, then*

$$H(T) > r(T) + \frac{1}{15}$$

where $r(T)$ is the radius of T.

Theorem 57. [56] *If G is a connected graph with radius $r(G)$ and cyclomatic number $\nu \geq 1$, then*

$$H(G) \geq r(G) - \frac{31}{105}(\nu - 1)\,.$$

For $\nu = 1$, the equality sign in the above inequality holds if and only if G is isomorphic to an even cycle.

Deng *et al.* [56] posed the following conjecture.

Conjecture 58. [56] *If G is a connected graph different from the even path, then*

$$H(G) \geq r(G)$$

where $r(G)$ is the radius of G.

If G is a connected triangle-free n-vertex graph with minimum degree δ satisfying $\delta \geq \sqrt{\frac{n}{2}} + 7$, where n is sufficiently large, then Conjecture 58 is true [166].

Theorem 59. [109] *If G is a connected (n,m)-graph with maximum degree Δ and p pendent vertices, then*

$$H(G) \geq \frac{2p}{\Delta + 1} + \frac{m - p}{\Delta}$$

with equality if and only if $G \cong S_n$ or G is a regular graph or G is a $(\Delta, 1)$-semiregular graph.

Theorem 60. [211] *(i) If $m \geq 1$ and G is a graph of size m such that G contains no isolated vertex, then*

$$H(G) \geq \frac{2m}{m+1}$$

with equality if and only if either $G \cong S_{m+1}$ or $G \cong K_3$.

(ii) If G is a triangle- and quadrangle-free (n,m)-graph, where $m \geq 1$, then

$$H(G) \geq \frac{2m^2}{n(n-1)}$$

with equality if and only either $G \cong S_n$ or G is a Moore graph of diameter 2 (regular graph with diameter two and girth five [94, 212]).

(iii) If G is an (n,m)-graph with minimum degree δ and maximum degree Δ, where $m \geq 1$, then

$$H(G) \geq \frac{2m^2}{2m(\Delta+\delta) - n\delta\Delta}$$

with equality if and only $d_u = \Delta$, $d_v = \delta$ for every edge $uv \in E(G)$.

Theorem 61. [166] *If G is either a tree or a connected triangle-free n-vertex graph with minimum degree δ satisfying $\delta \geq \sqrt{\frac{n}{3}}+5$, where n is sufficiently large, then $H(G) \geq \mu(G)$, where $\mu(G)$ is the average distance of G, Eq. (3). Equality holds if and only if G is the star.*

Theorem 62. [166] *If G is a connected (n,m)–graph with minimum degree δ and maximum degree Δ, then*

$$\frac{n}{2} - \frac{m(\delta-\Delta)^2}{2\delta\Delta(\delta+\Delta)} \leq H(G) \leq \frac{n}{2}$$

with left (respectively, right) equality if and only if G is a biregular (respectively, regular) graph.

Some bounds on the harmonic index, in terms of total chromatic number of a graph, were obtained in [80].

Various bounds on the Harmonic index in terms of different graph parameters, including several other topological indices, were derived in [115, 134, 162, 207, 219].

Theorem 63. [51] *If $n \geq 5$ and G is a connected n-vertex graph, then*

$$H(G) \geq 4 - \frac{3}{n} - avec(G)$$

with equality if and only if $G \cong S_n$. *Also, if* $n \geq 7$ *then*

$$H(G) \geq \frac{2(n-1)(2n-1)}{n^2 \cdot avec(G)}$$

with equality if and only if $G \cong S_n$. *Furthermore, if* $n \geq 3$ *and* q_1 *is the largest signless Laplacian eigenvalue of* G *then*

$$H(G) \geq q_1 - \frac{3n}{2} + 2$$

with equality if and only if $G \cong K_n$. *Finally, if* m *is the size of* G *and* λ_1 *is the largest eigenvalue of* G *then*

$$H(G) \geq \frac{2m^2}{\lambda_1^2 n}$$

with equality if and only if there exist some numbers r_1 *and* r_2 *such that* $d_u + d_v = r_1$ *for every edge* $uv \in E(G)$ *and* $\sum_{v \in N_G(u)} d_v = r_2$ *for every vertex* $v \in V(G)$, *where* $N_G(u)$ *is the set of vertices adjacent to* u.

An upper bound on the harmonic index in terms of different graph parameters was derived in [132].

Theorem 64. [164] *If* $n \geq 3$ *and* G *is a connected molecular* (n,m)*-graph, then*

$$\frac{3m+4n}{20} \leq H(G) \leq \frac{m+2n}{6}$$

with left equality if and only if G *contains only vertices of degrees 1 and 4, and the right equality holding if and only if either* $G \cong P_n$ *or* $G \cong C_n$.

Theorem 65. [164] *If* G *is a connected non-trivial* (n,m)*-graph with maximum degree* Δ *and* p *pendent vertices, then*

$$H(G) \geq \frac{2p}{(\Delta+1)} + \frac{m-p}{\Delta}.$$

with equality if and only if G *contains only vertices of degrees 1 and* Δ.

Theorem 66. [204] *If* G *is a connected non-trivial* n*-vertex graph with girth* $g(G)$ *satisfying the inequality* $g(G) \geq k \geq 3$, *then*

$$\frac{3k}{2} - \frac{6}{n-k+3} + \frac{4}{n-k+4} + 1 - g(G) \leq H(G) \leq \frac{3n}{2} - g(G) \tag{4}$$

$$\frac{k}{g(G)}\left(\frac{k}{2} - \frac{6}{n-k+3} + \frac{4}{n-k+4} + 1\right) \leq H(G) \leq \frac{n^2}{2\,g(G)} \tag{5}$$

$$-\frac{3k}{2} + g(G) \leq H(G) \leq \frac{n}{2} + g(G) - k \tag{6}$$

$$-\frac{g(G)}{2} \leq H(G) \leq \frac{n\,g(G)}{2k}\,. \tag{7}$$

The upper (respectively, lower) bounds in (4) and (5) (respectively, in (6) and (7)) are attained if and only if $G \cong C_n$. The lower bounds in (4) and (5) are attained if and only if $G \cong H(n,k;n-k,0,\dots,0)$. The upper bounds in (6) and (7) are attained if and only if G is a regular graph with $g(G) = k$.

The first two bounds of Theorem 66 generalize the main result of [194].

Theorem 67. [215] *If G is a non-trivial n-vertex graph and μ_1 is the largest eigenvalue of the sum–connectivity matrix $S(G)$, then*

$$H(G) \geq \frac{n}{n-1}\,\mu_1^2$$

with equality if and only if G is isomorphic to either K_n or $\overline{K}_n$.

3.4 Relations between harmonic index and other topological indices

The topological indices occurring in this Subsection are defined in Table 2.

Theorem 68. [202] *If G is a non-trivial connected (n,m)-graph, then*

$$H(G) \leq R(G)$$

where $R(G)$ is the Randić index. Equality holds if and only if G is a $\frac{2m}{n}$-regular graph.

Theorem 68 was proved also in [196,197]. The lower bound, given in the next theorem, is due to Ilić [100].

Theorem 69. [100] *If G is a connected graph with m edges, then*

$$H(G) \geq \frac{2m^2}{M_1(G)}$$

with equality if and only if $d_u + d_v$ is constant for every edge $uv \in E(G)$.

The inequality given in Theorem 69 was also derived in [196, 197]; unfortunately, the authors of [196, 197] made a mistake in the equality case.

Xu [196] derived several bounds on the harmonic index H in terms of some other familiar BID indices.

Theorem 70. [196] *If G is a non-trivial connected graph, then*

$$H(G) \leq \frac{ABC(G)}{2} + R(G)$$

where ABC is the atom–bond connectivity index, see Table 2. Equality holds if and only if $G \cong P_2$.

Lemma 71. [19, 45] *If G is an (n,m)-graph then*

$$\overline{M}_1(G) = 2m(n-1) - M_1(G)\,.$$

From Theorem 69 and Lemma 71, the next result follows.

Theorem 72. *If G is a connected graph with m edges, then*

$$H(G) \geq \frac{2m^2}{2m(n-1) - \overline{M}_1(G)}$$

with equality if and only if $d_u + d_v$ is constant for every edge $uv \in E(G)$.

The inequality given in Theorem 72, without the equality sign, was also derived in [196, 197]. Liu [112] established some bounds on H in terms of order and diameter of a graph.

Theorem 73. [211] *(i) If G is an n-vertex graph, then*

$$\frac{2\sqrt{n-1}}{n}\,R(G) \leq H(G) \leq R(G)$$

with left equality if and only if $G \cong S_n$, and the right equality holding if and only if all components of G are regular. Also, it holds that

$$\frac{n}{2} - H(\overline{G}) \leq H(G) \leq n - H(\overline{G})$$

with left equality if and only if either $G \cong K_n$ or $G \cong \overline{K}_n$, and the right equality holding if and only if G is a k-regular graph with $1 \leq k \leq n-2$.
(ii) If G is a connected n-vertex graph, where $n \geq 3$, then

$$\sqrt{\frac{2}{n-1}}\,X(G) \leq H(G) \leq \frac{2}{\sqrt{3}}\,X(G) \tag{8}$$

with left equality if and only if $G \cong K_n$, and the right equality holding if and only if $G \cong P_3$. If the minimum degree of G is at least $k \geq 2$, then the following bound is better than the upper bound given in (8):

$$H(G) \leq \frac{2}{\sqrt{k}}\,X(G)$$

with equality if and only if G is k-regular.

(iii) If G is a connected n-vertex graph, where $n \geq 7$, then

$$\frac{2}{n}\sqrt{\frac{n-1}{n-2}}\,ABC(G) \leq H(G) < \frac{4}{3\sqrt{2}}\,ABC(G)$$

with left equality if and only if $G \cong S_n$ (see also [90]). If the minimum degree of G is at least $k \geq 2$, then

$$H(G) \leq \frac{ABC(G)}{\sqrt{2k-2}}$$

with equality if and only if G is k-regular.

Theorem 74. [90] *(i) If G is a connected molecular n-vertex graph, where $n \geq 3$, and if*

$$f(x,y) = \sqrt{\frac{x+y-2}{xy}} \cdot \frac{x+y}{2}$$

then

$$\frac{ABC(G)}{f(4,4)} \leq H(G) \leq \frac{ABC(G)}{f(1,2)}\,.$$

The left equality is not possible, but could be satisfied if G is the graph representation of a diamond–like nanostructure [59,60]. The right equality holds if and only if $G \cong P_3$.

(ii) If G is the molecular graph of a benzenoid system, then

$$\frac{ABC(G)}{f(3,3)} \leq H(G) \leq \frac{ABC(G)}{f(2,2)}\,.$$

The left equality is attained if G is the graph representation of nanotubes and nanotoruses, as well as fullerenes [59,60]. The right equality holds if and only if $G \cong C_6$.

Theorem 75. [160] *If G is a graph with minimum degree δ and maximum degree Δ, then*

$$\frac{GA(G)}{\Delta} \leq H(G) \leq \frac{GA(G)}{\delta}$$

where $GA(G)$ is the geometric–arithmetic index, see Table 2. Equality (both left and right) is attained if and only if G is a regular graph.

Several bounds on the harmonic index in terms of other topological indices can be found in the references [11,164].

Iranmanesh and Saheli [102] obtained bounds on the harmonic index of caterpillars with diameter 4.

Bounds on the harmonic index of graphs under various graph operations were obtained in [1,2,140–142,165].

Theorem 76. [161] *If G is a non-trivial graph with minimum degree δ and maximum degree Δ, then*

$$\frac{\delta\, GA(G)^2}{M_2(G)} \leq H(G) \leq \frac{GA(G)^2\,(\delta^2+\Delta^2)^2}{4\delta^2\,\Delta\cdot M_2(G)}$$

where M_2 is the second Zagreb index, see Table 2. Equality (left or right) is attained if and only if G is a regular graph.

Theorem 77. [129] *If G is a non-trivial graph with minimum degree δ and maximum degree Δ, then*

$$\sqrt{\frac{8(\Delta\delta)^{3/2}\,GA(G)\cdot M_2^*(G)}{(\Delta+\delta)^3}} \leq H(G) \leq \sqrt{GA(G)\cdot M_2^*(G)}$$

with (left or right) equality if and only if G is a regular graph.

Theorem 78. [42] *If G is a connected graph with maximum degree Δ and*

$$ID(G) = \sum_{u\in V(G)} \frac{1}{d_u}$$

then

$$H(G) \leq \frac{1}{2}\, ID(G)\,\Delta$$

with equality if and only if G is regular. Also, if $d_u \geq d_v \geq \sqrt{d_u}+1$ for every edge $uv \in E(G)$, then $H(G) > ID(G)$. Furthermore, if G is a tree, then $H(G) < ID(G)$.

Theorem 79. [144] *If G is a connected (n,m)-graph with minimum degree δ and maximum degree Δ, then*

$$\frac{2m}{M_2(G)}\left(ISI(G) - \frac{(\delta-\Delta)(\Delta^2-\delta^2)\left\lceil\frac{m}{2}\right\rceil\left(1-\frac{1}{m}\left\lceil\frac{m}{2}\right\rceil\right)}{2\Delta\delta}\right) \leq H(G) \leq \frac{m(\delta+\Delta)ISI(G)}{\sqrt{\delta\Delta}\,M_2(G)}$$

with (left or right) equality if and only if G is regular.

Theorem 80. [137] *If G is a connected graph of order at least 3, then*

$$H(G) \leq ISI(G)$$

with equality if and only if $G \cong P_3$. If G has minimum degree δ and maximum degree Δ, then

$$\frac{2\,ISI(G)}{\Delta^2} \leq H(G) \leq \frac{2\,ISI(G)}{\delta^2}$$

with (left or right) equality if and only if G is regular.

Theorem 81. [93] *If G is a graph of size m, minimum degree δ and maximum degree Δ, then*

$$\frac{m^2\,\delta}{M_2(G)} \leq H(G) \leq \frac{M_2(G)}{\delta^3}$$

with (left or right) equality if and only if G is regular;

$$\frac{2\sqrt{\delta\Delta}}{\delta+\Delta} \cdot M_2^*(G) \leq H(G) \leq \begin{cases} M_2^*(G) \\ n/2 \end{cases}$$

with left equality if and only if G is regular or biregular, and the right equality holding if and only if G is regular;

$$\frac{M_1(G)}{2\Delta^2} \leq H(G) \leq \frac{M_1(G)}{2\delta^2}$$

with (left or right) equality if and only if G is regular. Also, the following inequality holds

$$m(\delta+2) - \frac{F(G)}{\Delta} \leq H(G) \leq \frac{F(G)}{2\delta^3}\,.$$

Theorem 82. [215] *Let G be a non-trivial n-vertex graph. If μ_n and μ_1 are the smallest and greatest eigenvalues of the sum–connectivity matrix $S(G)$, then*

$$H(G) \geq \frac{(\mu_1-\mu_n)^2}{2}$$

with equality if and only if either G is isomorphic to a complete bipartite graph with possibly isolated vertices or $G \cong \overline{K}_n$;

$$\frac{SE(G)^2}{n} \leq H(G) \leq \frac{SE(G)^2}{2}$$

with left equality if and only if either G is isomorphic to a regular graph of degree one or $G \cong \overline{K}_n$, and the right equality holding if and only if either G is isomorphic to a complete bipartite graph with possibly isolated vertices or $G \cong \overline{K}_n$

Theorem 83. [199] *If G is a non-trivial n-vertex graph, then*

$$\frac{SE(G)^2 - n(\det(S))^{2/n}}{n-1} \leq H(G) \leq SE(G)^2 - n(n-1)\cdot(\det(S))^{2/n}$$

where $\det(S)$ *is the determinant of the sum–connectivity matrix $S(G)$.*

The lower bound given in Theorem 83 is better than the second lower bound mentioned in Theorem 82. Matejić *et al.* [130] obtained several bounds on the harmonic index.

Some inequalities involving the harmonic index and sum–connectivity Estrada index were also derived in [198]. Several bounds concerning harmonic index can be found in the book chapter [163].

4 The Sum–Connectivity Index

Many results for the sum–connectivity index follow as special cases from results for general sum–connectivity index χ_α. In order to avoid repetition, in this section we outline only results pertaining to χ_α for $\alpha = -1/2$.

4.1 Sum–connectivity index of trees

Theorem 84. [213] *Among n-vertex trees, the trees S_n, $MS(n-3,1)$ and $MS(n-4,2)$ have first, second and third, respectively, minimum sum–connectivity index.*

Theorem 85. [213] *If $n \geq 4$, then the path P_n is the unique graph with maximum sum–connectivity index among n-vertex trees. If $n \geq 7$, then only the starlike trees of the form $S_n(r_1, r_2, r_3)$, where $r_1 \geq r_2 \geq r_3 \geq 2$ (respectively, $S_n(r_1, r_2, 1)$, where $r_1 \geq r_2 \geq 2$), have second (respectively, third) maximum sum–connectivity index.*

Betancur *et al* [22] proved that only the starlike trees of the form $S_n(r_1, r_2, r_3)$, where $r_1 \geq r_2 \geq r_3 \geq 2$, have maximum sum–connectivity index among n-vertex starlike trees for $n \geq 7$. This fact also follows from Theorem 85.

Mao and Zhou [128] determined the trees with fourth to seventh maximum sum–connectivity indices and fourth to eighth minimum sum–connectivity indices from the family of n-vertex trees, for sufficiently large n.

Theorem 86. [213] *If $n \geq 5$ and $3 \leq k \leq n-2$, then among n-vertex trees with k pendent vertices, only the tree $S_{n,k}$ has minimum sum–connectivity index.*

The graphs with first three minimum sum–connectivity indices from the family of n-vertex molecular trees were also characterized [213].

Theorem 87. [68] *Among n-vertex trees with maximum degree Δ, only the starlike trees of the form $S_n(\underbrace{2, 2, \ldots, 2}_{n-\Delta-1}, \underbrace{1, 1, \ldots, 1}_{2\Delta-n+1})$, (respectively, $S_n(r_1, r_2, \ldots, r_\Delta)$, $r_1 \geq r_2 \geq \cdots \geq r_\Delta \geq 2$) have maximum sum–connectivity index for $n/2 \leq \Delta \leq n-2$ (respectively, for $3 \leq \Delta \leq \frac{n-1}{2}$).*

Theorem 88. [37] *Among proper Kragujevac n-vertex trees with the central vertex of degree $r \geq 3$ and no branches of type B_1, the tree V (respectively, U) has maximum (respectively, minimum) sum–connectivity index, where the trees U and V are depicted in Figure 2.*

Theorem 89. [195] *If $k \geq 5$ and T is an n-vertex molecular tree with k pendent vertices, then*

$$X(G) \geq \frac{n}{2} + \left(\frac{1}{\sqrt{6}} + \frac{1}{\sqrt{5}} - 1\right) k + \frac{3}{2} - \frac{4}{\sqrt{6}}$$

with equality if and only if $x_{1,4} = k$, $x_{2,4} = k - 4$, $x_{2,2} = n - 2k + 3$ for even k and $6 \leq k \leq \lfloor \frac{n+3}{2} \rfloor$.

Theorem 90. [195] *If k is odd, $9 \leq k \leq \lfloor \frac{n+2}{2} \rfloor$ and T is an n-vertex molecular tree with k pendent vertices, then*

$$X(G) \geq \frac{n}{2} + \left(\frac{1}{\sqrt{6}} + \frac{1}{\sqrt{5}} - 1\right) k + \frac{3}{\sqrt{5}} - \sqrt{6} + 1$$

with equality if and only if $x_{1,4} = k$, $x_{2,4} = k - 6$, $x_{2,2} = n - 2k + 2$, $x_{2,3} = 3$.

Theorem 91. [195] *If $k \geq 3$ and T is an n-vertex molecular tree with k pendent vertices, then*

$$X(G) \leq \frac{n}{2} + \left(\frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}} - \frac{3}{2}\right) k + 1 - \frac{3}{\sqrt{6}}$$

with equality if and only if $x_{1,2} = x_{2,3} = k$, $x_{2,2} = n - 3k + 2$, $x_{3,3} = k - 3$ for $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$.

Theorem 92. [117] *If T is an n-vertex tree with k pendent vertices and $\mu(T)$ is the average distance of T, then*

$$X(G) \geq \begin{cases} \mu(T) + \min\left\{0, \sqrt{k} - 2\right\} & \text{if } k = 2 \\ \mu(T) + \max\left\{0, \frac{k-1}{\sqrt{k+1}} - 2\right\} & \text{if } k \geq 3. \end{cases}$$

Equality is attained if $T \cong S_n$ and $n \to \infty$.

4.2 Sum–connectivity index of unicyclic and bicyclic graphs

Theorem 93. [65] *If $n \geq 5$, then among connected unicyclic n-vertex graphs, the graphs $H(n, 3; n-3, 0, 0)$ and $H(n, 3; n-4, 1, 0)$ are the only species with minimum and second minimum X values (see also [32]).*

Theorem 94. [32, 68] *If $n \geq 4$, then among connected unicyclic n-vertex graphs, the cycle C_n is the unique graph with maximum sum–connectivity index.*

Theorem 95. [68] *If $n \geq 5$, then among connected unicyclic n-vertex graphs, the graphs obtained by attaching a path of length at least 2 to a cycle are the only graphs with the second maximum sum–connectivity index.*

Theorem 96. [32] *If $n \geq 5$ and $1 \leq k \leq n-3$, then among connected unicyclic n-vertex graphs with k pendent vertices, the graph obtained from the cycle C_{n-k} by attaching k pendent vertices to a single vertex, is the unique graph with minimum sum–connectivity index.*

Theorem 97. [68] *Among connected unicyclic n-vertex graphs with maximum degree Δ, only the the unicyclic graph obtained by attaching $2\Delta - n - 1$ pendent vertices and $n - \Delta - 1$ paths of length 2 to a vertex of a triangle, (respectively, the unicyclic graph obtained by attaching $\Delta - 2$ paths of length at least 2 to a vertex of a cycle) have maximum sum–connectivity index for $\frac{n+2}{2} \leq \Delta \leq n-2$ (respectively, for $3 \leq \Delta \leq \frac{n+1}{2}$).*

Theorem 98. [64] *If $n \geq 8$, then among connected bicyclic n-vertex graphs, $H_{n,2}$ (respectively, the bicyclic graph, different from $H_{n,2}$, having a vertex of degree $n-1$) is the unique graph with minimum (respectively, second minimum) sum–connectivity index.*

Graphs with first two maximum sum–connectivity indices in the family of connected bicyclic n-vertex graphs were also characterized in [64].

4.3 Sum–connectivity index of general graphs

Theorem 99. [173] *Among n-vertex quasi-trees, the graph obtained from the cycle C_n by adding chords from one vertex u to c consecutive other vertices, has maximum sum–connectivity index, where $c = n-3$ if $n \leq 32$ and $c = 30$ otherwise.*

Extremal results concerning minimum sum–connectivity index and matching number were obtained in [66] for trees and connected unicyclic graphs, in [64] for connected bicyclic graphs, and in [126] for cacti. Results on trees with given matching number and maximum sum–connectivity index are found in [222]

Theorem 100. [213] *The complete graph K_n is the unique graph with maximum sum–connectivity index among n-vertex graphs. If $n \geq 5$, then the star S_n is the unique graph with minimum sum–connectivity index among n-vertex graphs without isolated vertices.*

Theorem 100 was proven in [38] by an alternative way.

Theorem 101. [126] *If $n \geq 5$, then among connected n-vertex cacti with k cycles, the graph containing a vertex of degree $n-1$ is the unique graph with minimum sum–connectivity index.*

Theorem 102. [192] *If $n \geq 11$, then among n-vertex connected graphs with minimum degree at least 2, only the graph $K^*_{2,n-2}$ has minimum sum–connectivity index.*

Theorem 103. [192] *If $n \geq 11$, then among connected triangle–free n-vertex graphs with minimum degree at least 2, the complete bipartite graph $K_{2,n-2}$ is the unique graph with minimum sum–connectivity index.*

Theorem 104. [9] *If $h \geq 4$, then among triangular chains with h triangles and maximum degree 5, only the linear triangular chain has maximum sum–connectivity index.*

Theorem 105. [149] *If $h \geq 3$, then among polyomino chains with h squares, only the linear polyomino chain has maximum sum–connectivity index.*

Theorem 105 was proven also in [14].

Theorem 106. [14] *Among the members of Ω_h, only the zigzag polyomino chain has minimum sum–connectivity index, where Ω_h is the collection of polyomino chains, having h squares, in which no internal segment of length 3 has an edge connecting vertices of degree 3.*

Theorem 107. [39,152] *If $h \geq 3$, then among polyomino chains with h squares, only the zigzag polyomino chain has minimum sum–connectivity index.*

Clearly, Theorem 106 immediately follows from Theorem 107. The next result concerning sum–connectivity index of polyomino catacondensed systems is due to Cruz and Rada [40].

Theorem 108. [40] *If $h \geq 3$, then among polyomino catacondensed systems with h squares, only the linear polyomino chain has maximum sum–connectivity index.*

Theorem 109. [15] *If $h \geq 3$, then among the members of Ω'_h, only the zigzag (respectively, linear) pentagonal chain has minimum (respectively, maximum) sum–connectivity index, where Ω'_h is the collection of pentagonal chains, having h pentagons, in which no internal segment of length 3 has an edge connecting vertices of degree 3.*

Theorem 110. [36] *Among the isomeric hexagonal systems, those having minimum (respectively, maximum) number of inlets have maximum (respectively, minimum) sum–connectivity index.*

Theorem 111. [153] *Among catacondensed hexagonal systems with h hexagons, the linear hexagonal chain L_h (respectively, E_h) has minimum (respectively, maximum) sum–connectivity index, where E_h is described in Figure 6 of Ref.* [153].

Additional extremal results on the sum–connectivity index of hexagonal systems can be found in [21, 34, 35, 92, 92, 150, 151, 154].

Theorem 112. [57] *If there is a hexagonal system S_0 with $h \geq 3$ hexagons, $2h + 1 + \lceil \sqrt{12h-3} \rceil$ vertices such that S_0 satisfies the equation $b + 2c + 3f = 0$, then among hexagonal systems with h hexagons S_0 has the minimal sum–connectivity index.*

Further extremal results related to Theorem 112 can be found in [57, 85].

The following theorem gives lower bounds on the sum–connectivity index X.

Theorem 113. [213] *(i) If G is a graph without pendent vertices, then $X(G) \geq R(G)$ with equality if and only if all the non-isolated vertices of G have degree 2.*
(ii) If G is a graph with $m \geq 1$ edges, then

$$X(G) \geq \frac{m\sqrt{m}}{\sqrt{M_1(G)}}$$

with equality if and only if there exists a number r_0 such that $d_u + d_v = r_0$ for every edge $uv \in E(G)$;

$$X(G) \geq \frac{m}{\sqrt{m+1}}$$

with equality if and only if G has no two independent edges.
(iii) If $m \geq 1$ and G is an (n, m)-graph, then

$$X(G) \geq \frac{m\sqrt{n-1}}{\sqrt{2m + (n-1)(n-2)}}$$

with equality if and only if G is isomorphic to one of the graphs K_n, S_n, $K_n \cup K_1$;

$$X(G) \geq \frac{m\sqrt{m}}{\sqrt{n(n-1)}}$$

with equality if and only if $G \cong S_n$ or G is isomorphic to a Moore graph of diameter 2 (regular graph with diameter two and girth five). Moreover, if the graph G has minimum degree δ and maximum degree Δ then

$$X(G) \geq \frac{m\sqrt{m}}{\sqrt{2m(\delta+\Delta) - n\delta\Delta}}$$

with equality if and only if $d_u + d_v = \delta + \Delta$ *for every edge* $uv \in E(G)$.

(iv) If $m \geq 1$ *and* G *is a triangle-free* (n, m)*-graph, then*

$$X(G) \geq \frac{m}{\sqrt{n}}$$

with equality if and only if G *is a complete bipartite graph.*

(v) If G *is an* n*-vertex graph, then*

$$X(G) \geq \frac{n\sqrt{n-1}}{2\sqrt{2}} - X(\overline{G})$$

with equality if and only if G *is isomorphic to either* K_n *or* $\overline{K}_n$.

The following theorem gives upper bounds on the sum–connectivity index X.

Theorem 114. [213] *(i) If* G *is a graph with* m *edges, then* $X(G) \leq m/\sqrt{2}$ *with equality if and only if* G *consists of* m *copies of* K_2 *and arbitrary number of isolated vertices.*

(ii) If $m \geq 1$ *and* G *is an* (n, m)*-graph, then*

$$X(G) < \sqrt{\frac{mn}{2}}\,.$$

(iii) If G *is an* n*-vertex graph with maximum degree* Δ*, then*

$$X(G) \leq \frac{n\sqrt{\Delta}}{2\sqrt{2}}$$

with equality if and only if G *is regular of degree* Δ.

The bound given in the first part of the next theorem is an improved version of the one, given in Theorem 114(ii).

Theorem 115. [96] *(i) If* $m \geq 1$ *and* G *is an* (n, m)*-graph, then*

$$X(G) \leq \frac{\sqrt{mn}}{2}$$

with equality holding if and only if G *is regular.*

(ii) If G *is a triangle– and quadrangle-free connected* n*-vertex graph with radius* $r(G)$*, then*

$$X(G) \leq \frac{n}{2}\sqrt{\frac{\sqrt{n - r(G) + 1}}{2}}$$

with equality if and only if either G *is isomorphic to a Moore graph of diameter 2 or* $G \cong C_6$.

Theorem 116. [213] *If* $4 \leq n-1 \leq m \leq 2n$ *and* G *is a connected molecular* (n,m)*-graph, then*

$$\frac{4}{3}\left(\frac{1}{\sqrt{5}} - \frac{1}{2\sqrt{2}}\right) n + \frac{1}{3}\left(\frac{5}{2\sqrt{2}} - \frac{2}{\sqrt{5}}\right) m \leq X(G) \leq \left(\frac{2}{\sqrt{3}} - 1\right) n + \left(\frac{3}{2} - \frac{2}{\sqrt{3}}\right) m$$

with left equality if and only if G *contains only vertices of degrees 1 and 4, and the right equality holding if and only if* G *is either a path or a cycle.*

Theorem 117. [211] *If* G *is a connected* n*-vertex graph with minimum degree at least* k*, where* $k \geq 2$*, and* χ *is the chromatic number of* G*, then*

$$X(G) \geq \chi \sqrt{\frac{k}{8}}$$

with equality if and only if $G \cong K_n$*.*

Several bounds on the sum–connectivity index in terms of other topological indices can be found in [11].

Theorem 118. [43] *If* G *is a connected* n*-vertex graph with* p *pendent vertices, such that every non-pendent vertex has degree at least* δ'*, then*

$$X(G) \geq R(G) - \frac{p}{\sqrt{\delta'(\delta'+1)}(\sqrt{\delta'+1} + \sqrt{\delta'})}$$

with equality if and only if G *is isomorphic to any of the graphs* S_n*,* P_n*,* C_n*.*

Theorem 119. [107] *The sum–connectivity index of almost every* n*-vertex tree is among* $(r \pm \epsilon)n$*, where* r *is some constant and* ϵ *is an arbitrary positive number.*

Theorem 120. [143] *If* G *is an* (n,m)*-graph with maximum degree* Δ *and minimum degree* δ*, then*

$$\frac{n}{\sqrt{n+\Delta+1}} + m\left(\frac{2}{\sqrt{1+3\Delta}} + \frac{1}{2\sqrt{\Delta}}\right) \leq X(\mu^*(G)) \leq \frac{n}{\sqrt{n+\delta+1}} + m\left(\frac{2}{\sqrt{1+3\delta}} + \frac{1}{2\sqrt{\delta}}\right).$$

where $\mu^*(G)$ *is the Mycielskian of* G*.*

Recall that by $S_i = \sum_{j=1}^{n} s_{i,j}$ we denote the sum of the i-th row of the sum–connectivity matrix $S(G)$.

Theorem 121. [198] *If* G *is a connected non-trivial* n*-vertex graph and* μ_1 *is the largest eigenvalue of the sum–connectivity matrix* $S(G)$*, then*

$$X(G) \leq \frac{n\,\mu_1}{2}$$

with equality if and only if $S_1 = S_2 = \cdots = S_n$*.*

An inequality involving the sum–connectivity index and sum–connectivity Estrada index was also derived in [198].

4.4 Relations between sum–connectivity index and other topological indices

Theorem 122. [216] *If G is a graph, then*

$$X(G) \geq \frac{R(G)}{\sqrt{2}}$$

with equality if and only if all non-isolated vertices have degree 1. Also, if G has no component on two vertices, then

$$X(G) \geq \sqrt{\frac{2}{3}}\, R(G)$$

with equality if and only if all non-trivial components of G are paths on 3 vertices.

Theorem 123. [216] *If G is a graph with m edges, then*

$$X(G) \leq \sqrt{\frac{m\, R(G)}{2}}$$

with equality if and only if G is regular. If G has n vertices, then

$$X(G) \leq \frac{n\sqrt{n-1}}{2} - X(\overline{G})$$

with equality if and only if G is regular of degree $(n-1)/2$. Moreover, if G does not contain any isolated vertex but has the clique number ω, then

$$X(G) \leq \frac{1}{2}\sqrt{\frac{m(\omega-1)}{\omega}} \cdot {}^0R(G)$$

with equality if and only if G is a regular complete ω-partite graph.

A lower bound on the sum–connectivity index of strong product of graphs was derived in [2].

Theorem 124. [211] *If G is a connected n-vertex graph, where $n \geq 5$, then*

$$X(G) \leq \sqrt{\frac{n-1}{2}}\, R(G)$$

with equality if and only if $G \cong K_n$;

$$\sqrt{\frac{n-1}{n(n-2)}}\, ABC(G) \leq X(G) < \sqrt{\frac{2}{3}}\, ABC(G)$$

with left equality if and only if $G \cong S_n$.

Some bounds on the sum–connectivity index in terms of harmonic index can be obtained from Theorem 73(ii).

Theorem 125. [160] *If G is a graph with minimum degree δ and maximum degree Δ, then*

$$\frac{GA(G)}{\sqrt{2\Delta}} \leq X(G) \leq \sqrt{\frac{m\,GA(G)}{2\delta}}$$

with (left or right) equality if and only if G is a regular graph;

$$X(G) \leq \sqrt{\frac{R(G)\cdot GA(G)}{2}}$$

with equality if and only if G is either a regular or a biregular graph.

Theorem 126. [44] *If G is a connected (n,m)-graph with maximum degree Δ, then*

$$X(G) \leq \frac{\Delta \cdot {}^0R(G)}{2\sqrt{2}}$$

$$X(G) \leq \frac{\sqrt{\Delta} + \sqrt{(n-1)(2m-\Delta)}}{2\sqrt{2}}\,.$$

The equality sign in either of the above inequalities holds if and only if G is a regular graph.

Theorem 127. [44] *If T is an n-vertex tree, then*

$$X(T) < {}^0R(T)\,.$$

If G is an n-vertex graph such that $d_v \geq 2n^{1/3}$ for all $v \in V(G)$, then

$$X(G) > {}^0R(G)\,.$$

Theorem 128. [137] *If G is a connected graph, then*

$$X(G) \leq \sqrt{ISI(G)\cdot M_2^*(G)}$$

with equality if and only if G is regular or biregular. If G has minimum degree δ, maximum degree Δ and size m, then

$$ISI(G)\cdot\sqrt{\frac{2}{\Delta^3}} \leq X(G) \leq \frac{\sqrt{ISI(G)\cdot m}}{\delta}$$

with (left or right) equality if and only if G is regular.

5 General Sum–Connectivity Index

Throughout this section, whenever the condition on α is not mentioned, it is assumed that α is any real number different from zero.

5.1 General sum–connectivity index of trees

Theorem 129. [214] *If $n \geq 4$, then among n-vertex trees*

• *the star S_n is the only graph with minimum (respectively, maximum) χ_α value for $\alpha < 0$ (respectively, for $\alpha > 0$);*

• *the path P_n is the only graph with minimum (respectively, maximum) χ_α value for $\alpha > 0$ (respectively, for $-1.4094 \approx 1 - \frac{\log 2}{\log(4/3)} \leq \alpha < 0$).*

Theorem 130. [67] *If $n \geq 4$, then among n-vertex trees, the path P_n is the only graph with maximum χ_α value for $x_0 < \alpha < 1 - \frac{\log 2}{\log(4/3)} \approx -1.4094$, where $x_0 \approx -1.7036$ is the unique root of the equation $3^\alpha - 4^\alpha = 2(4^\alpha - 5^\alpha)$.*

Theorem 131. [67] *If $x_1 \approx -4.3586$ is the unique root of the equation $4^\alpha - 5^\alpha = 3(5^\alpha - 6^\alpha)$, $\alpha < x_1$, and $n \geq 4$, then among n-vertex trees, the starlike tree $S_n(\overbrace{2, \ldots, 2}^{(n-1)/2})$ (respectively, $S_n(3, \overbrace{2, \ldots, 2}^{(n-4)/2})$) is the only graph with maximum χ_α value for even n (respectively, for odd n).*

Theorem 132. [182] *If $-1 \leq \alpha < 0$, $n \geq 3$, and $2 \leq d \leq n-1$, then among n-vertex trees with diameter d, the tree $S_{n,n-d+1}$ has minimum χ_α value.*

Theorem 133. [182] *If $-1 \leq \alpha < 0$ and $3 \leq d \leq n-2$, then among n-vertex trees with diameter d, the trees having minimum χ_α values are (in this order): $MS(n-d, 0, \ldots, 0, 1), MS(n-d-1, 0, \ldots, 0, 2), \ldots, MS\left(\left\lceil \frac{n-d+1}{2} \right\rceil, 0, \ldots, 0, \left\lfloor \frac{n-d+1}{2} \right\rfloor\right)$.*

The next result is a generalized version of Theorem 84.

Theorem 134. [182] *If $-1 \leq \alpha < 0$, then among n-vertex trees, the trees S_n, $MS(n-3, 1)$, $MS(n-4, 2)$, $S_{n,n-3}$ and $MS(n-5, 3)$ have first, second, third, fourth and fifth, respectively, minimum χ_α values.*

The next result is a generalized version of Theorems 86 and 8.

Theorem 135. [182] *If $-1 \leq \alpha < 0$, $n \geq 5$ and $3 \leq k \leq n-2$, then among n-vertex trees with k pendent vertices, only the tree $S_{n,k}$ has minimum χ_α value.*

Extremal results concerning general sum–connectivity index for multigraphs can be found in [182].

Theorem 136. [41] *If $-1 \leq \alpha < 0$ and $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$, then among n-vertex trees with k pendent vertices, only the trees having $k-2$ vertices of maximum degree 3 such that every vertex of degree 3 is adjacent to either another vertex of degree 3 or a vertex of degree 2, have maximum χ_α value.*

Since the extremal trees specified in Theorem 136 are chemical trees, these trees also have the maximum χ_α value in the family of n-vertex chemical trees with k pendent vertices under the constrains given in the aforementioned theorem [41].

Theorem 137. [189] *Among trees with given degree sequence, the greedy tree has maximum (respectively, minimum) χ_α value for $\alpha < 0$ or $\alpha > 1$ (respectively, for $0 < \alpha < 1$) and alternating greedy tree has minimum (respectively, maximum) H value for $\alpha < 0$ or $\alpha > 1$ (respectively, for $0 < \alpha < 1$).*

Partial part of Theorem 137 also appeared in [20, 201].

Theorem 138. [181] *If $n \geq 3$, $\alpha \geq 1$, and $n/2 \leq s \leq n-1$, then among n-vertex trees with independence number s, the starlike tree $S_n(\underbrace{2,2,\ldots,2}_{n-s-1},\underbrace{1,1,\ldots,1}_{2s-n+1})$ is the unique tree with maximum χ_α value.*

The next result is a generalized version of Theorem 89.

Theorem 139. [41] *If $-1 \leq \alpha < 0$, $k \geq 5$, and T is an n-vertex molecular tree with k pendent vertices, then*

$$\chi_\alpha(G) \geq 4^\alpha(n-2k+3) + 5^\alpha \cdot k + 6^\alpha(k-4)$$

with equality if and only if $x_{1,4} = k$, $x_{2,4} = k-4$, $x_{2,2} = n-2k+3$ for even k and $6 \leq k \leq \lfloor \frac{n+3}{2} \rfloor$.

5.2 General sum–connectivity index of unicyclic, bicyclic, tricyclic and tetracyclic graphs

Tache and Tomescu [172] characterized the graphs having maximum χ_α value for n-vertex trees and unicyclic graphs with fixed number of pendent vertices. Jamil and Tomescu [103] obtained the graphs with minimum χ_α values in the families of n-vertex trees (for $-1 \le \alpha < 0$) and unicyclic graphs (for $-0.585 \le \alpha < 0$) with fixed matching number, under some constraints.

Theorem 140. [66] *If $n \ge 5$, then among connected unicyclic n-vertex graphs*

(i) for $\alpha > 0$, the cycle C_n is the unique graph with minimum χ_α value;

(ii) for $0 < \alpha < 1$, the graphs obtained by attaching a path on at least two vertices to a vertex of a cycle, are the only graphs with second minimum χ_α value;

(iii) for $\alpha > 1$, the graph obtained by attaching a pendent vertex to a vertex of the cycle C_{n-1}, is the unique graph with second minimum χ_α value;

(iv) for $\alpha = 1$, the extremal graphs mentioned in (ii) and (iii) are the only graphs with second minimum χ_α value.

(v) for $-1 \le \alpha < 0$, $H(n, 3; n-3, 0, 0)$ and $H(n, 3; n-4, 1, 0)$ are, respectively, the only graphs with minimum and second minimum χ_α values.

Theorem 140(v) can be considered as an extended version of Theorem 93. Clearly, the extremal graphs mentioned in Theorem 140(v) have girth equal to 3. Tomescu and Kanwal [183] extended this result to unicyclic graphs of girth at least 4.

Theorem 141. [183] *Let $-1 \le \alpha < 0$ and $\mathcal{U}_{n,k}$ be the set of connected unicyclic n-vertex graphs of girth k.*

(i). If $n \ge k \ge 4$, then $H(n, k; n-k, 0, \ldots, 0)$ is the unique graph with minimum χ_α value in the set $\mathcal{U}_{n,k}$.

(ii). If $n \ge k+2 \ge 6$, then the members of $A(n, k)$ are the only graphs with second minimum χ_α value in the set $\mathcal{U}_{n,k}$, where $A(n, k)$ is the set of n-vertex unicyclic graphs consisting of a cycle C_k, $n-k-1$ pendent edges incident to a vertex $x \in V(C_k)$ and one pendent edge incident to a vertex $y \in V(C_k)$, such that the distance between x and y is at least 2.

(iii). If $n \ge k+4 \ge 8$, then there exists a natural number $n_0(\alpha)$ such that if $n-k \ge n_0(\alpha)$ then $H(n, k; n-k-1, 1, 0, \ldots, 0)$ is the unique graph with third minimum χ_α value in the set $\mathcal{U}_{n,k}$.

The next result is a generalized version of Theorem 96.

Theorem 142. [179] *If* $-1 \leq \alpha < 0$, $n \geq 5$, *and* $1 \leq k \leq n-3$, *then among connected unicyclic* n*-vertex graphs with* k *pendent vertices, the graph obtained from* C_{n-k} *by attaching* k *pendent vertices to a single vertex of* C_{n-k}, *is the unique graph with minimum* χ_α *value.*

Theorem 143. [18] *If* $n \geq 6$ *and* $-1 \leq \alpha < 0$, *then among* n*-vertex connected bicyclic graphs, only the following graphs have maximum* χ_α *value:*

- *the graph obtained from two disjoint cycles by joining them with an edge,*
- *the graph obtained from a cycle by adding an edge between any two non-adjacent vertices.*

Conjecture 144. [6] *If* $-1 \leq \alpha < 0$ *and* $\nu \geq 1$, *then among connected* n*-vertex graphs with cyclomatic number* ν, $H_{n,\nu}$ *is the unique graph with minimum* χ_α *value.*

Theorem 145. [169] *If* $n \geq 5$ *and* $\alpha > 1$, *then among connected bicyclic* n*-vertex graphs, only the graphs consisting only of vertices of degrees 2 and 3, such that no two vertices of degree 3 are adjacent, have minimum* χ_α *value.*

In Theorem 145, if we replace the condition "$\alpha > 1$" with "$\alpha = 1$" then the resulting statement remains true [47, 82].

Theorem 146. [168] *If* $n \geq 5$ *and* $\alpha \geq 1$, *then among connected bicyclic* n*-vertex graphs,* $H_{n,2}$ *is the unique graph with maximum* χ_α *value.*

Ali and Dimitrov [12] gave a short proof of Theorem 146. For $\alpha = 2$, Theorems 129, 140(i), 145 and 146 were also proven in [79].

Tache [171] characterized the graphs having maximum χ_α value, for $\alpha > 1$, from the classes of connected bicyclic n-vertex graphs with (i) fixed number of pendent vertices, and (ii) girth.

Theorem 147. [221] *If* $n \geq 5$ *and* $\alpha \geq 1$, *then among connected tricyclic* n*-vertex graphs, only* $H_{n,3}$ *and/or* K *have/has maximum* χ_α *value and* K *is the graph obtained from* K_4 *by attaching* $n-4$ *pendent vertices to one of the vertices of* K_4.

Theorem 147 was proven in a short way in [8]. Clearly, Theorem 147 does not give precise extremal graphs. This gap was not addressed in [8] either, but was filled in [12]. The unique tetracyclic and unicyclic graphs with maximum χ_α value, for $\alpha \geq 1$, were also identified in [12]. For a recent result on tricyclic graphs see [147].

Theorem 148. [12] *If $n \geq 5$ and $\alpha \geq 1$, then among connected tricyclic n-vertex graphs, only $H_{n,3}$ and/or K have/has maximum χ_α value and K is the graph obtained from K_4 by attaching $n-4$ pendent vertices to one of the vertices of K_4. More precisely,*

$$\chi_\alpha(H_{n,3}) < \chi_\alpha(K) \qquad \text{for} \quad 1 < \alpha < 2$$

$$\chi_\alpha(H_{n,3}) > \chi_\alpha(K) \qquad \text{for} \quad \alpha > 2$$

$$\chi_\alpha(H_{n,3}) = \chi_\alpha(K) \qquad \text{for} \quad \alpha = 1, 2.$$

Also, only the graph $H_{n,4}$ has maximum χ_α value, for $\alpha \geq 1$ and $n \geq 6$, among connected tetracyclic n-vertex graphs. Furthermore, $H_{n,1}$ is the unique graph with maximum χ_α value for $\alpha \geq 1$ among connected unicyclic n-vertex graphs.

The unique unicyclic and bicyclic graphs with maximum χ_2 value were identified also in [79].

5.3 General sum–connectivity index of general graphs

Theorem 149. [54] *Among n-vertex graphs,*

- *K_n is the unique graph with maximum χ_α value for non-zero $\alpha > -1$;*
- *the graphs in which each component is regular of non-zero degree, are the only graphs with maximum χ_α value for $\alpha = -1$;*
- *S_n is the unique graph with minimum χ_α value for $n \geq 6$ (respectively, for sufficiently large n) and for $-1 \leq \alpha \leq \frac{1}{2}$ (respectively, for $\frac{1}{2} < \alpha < 0$).*

Theorem 150. [178] *If $-1 \leq \alpha < 0$, $n \geq 5$, and $3 \leq k \leq n-1$, then among connected n-vertex graphs, containing at least one cycle, with girth at least k, the graph obtained from the cycle C_{n-k} by attaching k pendent vertices to a single vertex of C_{n-k}, is the unique graph with minimum χ_α value.*

Tache [170] determined the graphs with maximum χ_α values from different families of cacti for $\alpha > 1$. The next result is a generalized version of Theorem 101.

Theorem 151. [4] *If $-1 \leq \alpha < 0$ and $n \geq 3$, then among connected n-vertex cacti with k cycles, the graph containing a vertex of degree $n-1$ is the unique graph with minimum χ_α value.*

Theorem 152. [176] *If $-1 \leq \alpha < \alpha_0 \approx -0.867$ and $n \geq 3$, then among connected n-vertex graphs with minimum degree at least 2, $K^*_{2,n-2}$ is the unique graph with minimum χ_α value, where α_0 is the unique root of $4(4^x - 5^x) = 6^x$.*

Theorem 153. [176] *If* $-1 \leq \alpha < \beta_0 \approx -0.817$ *and* $n \geq 4$*, then among connected triangle-free n-vertex graphs with minimum degree at least 2, the complete bipartite graph* $K_{2,n-2}$ *is the unique graph with minimum* χ_α *value, where* β_0 *is the unique root of* $5 \cdot 4^x = 6 \cdot 5^x$.

Since every 2–connected graph has degree at least 2 and both the extremal graphs mentioned in Theorems 152 and 153 are 2–connected, thereby Theorems 152 and 153 remains valid if we replace the condition "connected" with "2–connected".

Conjecture 154. [176] *If* $-1 \leq \alpha < \beta_0 \approx -0.817$ *and* $2 \leq k \leq n/2$*, then among connected triangle-free n-vertex graphs with minimum degree at least* k*, the complete bipartite graph* $K_{k,n-k}$ *is the unique graph with minimum* χ_α *value, where* β_0 *is the unique root of* $5 \cdot 4^x = 6 \cdot 5^x$.

If $m \geq k(n-k)$, then Conjecture 154 holds due to Theorem 161.

Tomescu [177] surveyed extremal results concerning general sum–connectivity index, established till 2014.

Tomescu *et al.* [180] determined the unique species having maximal χ_α value, $\alpha \geq 1$, among graphs with fixed order and connectivity (and with fixed order and edge-connectivity).

Theorem 155. [180] *If* $n \geq 3$ *and* $\kappa \geq 1$*, then among n-vertex graphs with connectivity* κ*,* $K_\kappa + (K_1 \cup K_{n-\kappa-1})$ *is the unique graph with maximal* χ_α *value for* $\alpha \geq 1$.

Corollary 156. [180] *If the connectivity "*κ*" is replaced by the edge-connectivity "*λ*" throughout Theorem 155, then the resulting statement remains true.*

The next result is also due to Tomescu *et al.* [180].

Theorem 157. [180] *Let* G *be a 2-connected or 2-edge-connected graph with* $n \geq 3$ *vertices. Then for* $\alpha > 0$*,* $\chi_\alpha(G)$ *is minimal if and only if* $G \cong C_n$.

The problem of characterizing graphs having extremum χ_α values over the collection of certain polyomino chains, with fixed number of squares, was solved in [17] for $\alpha > 1$. The same problem was also addressed in [14] and its solution for the case $0 < \alpha < 1$ was reported there.

Theorem 158. [57] *If $\alpha > 1$ or $\alpha < 0$ (respectively, if $0 < \alpha < 1$), then among catacondensed benzenoid systems with h hexagons,*

- *the linear benzenoid chain L_h has minimum (respectively, maximum) χ_α value;*
- *the benzenoid system with $\lfloor h/2 \rfloor - 1$ branched hexagons and $\lceil h/2 - \lfloor h/2 \rfloor \rceil$ kinks, has maximum (respectively, minimum) χ_α value.*

Some extremal results concerning general sum–connectivity index of benzenoid systems (not necessarily, catacondensed benzenoid systems) can also be obtained from the results established in [57]. Also, some extremal results related to the general sum–connectivity index of particular systems (e.g., fluoranthenes, phenylenes etc.) can be found in [10, 85, 92, 127, 185].

Theorem 159. [214] *If G is an (n,m)-graph with $m \geq 1$, then*

$$\chi_\alpha(G) \begin{cases} \leq m\left(\frac{2m}{n-1} + n - 2\right)^\alpha & \text{for } 0 < \alpha < 1 \\ \\ \geq m\left(\frac{2m}{n-1} + n - 2\right)^\alpha & \text{for } \alpha < 0. \end{cases}$$

The equality sign in either of the above inequalities holds if and only if G is isomorphic to K_n, S_n or $K_1 \cup K_{n-1}$.

Theorem 160. [214] *If G is an (n,m)-graph and $\alpha > 1$, then*

$$\chi_\alpha(G) \geq m^{1-\alpha}\left[2m\left(2\left\lfloor\frac{2m}{n}\right\rfloor + 1\right) - n\left\lfloor\frac{2m}{n}\right\rfloor\left(\left\lfloor\frac{2m}{n}\right\rfloor + 1\right)\right]^\alpha$$

with equality if and only if G is isomorphic either to a regular graph or a bipartite semiregular graph. Also, the following inequality holds

$$\chi_\alpha(G) \geq 4^\alpha\, m^{\alpha+1}\, n^{-\alpha}$$

with equality if and only if G is isomorphic to a regular graph. Furthermore,

$$\chi_\alpha(G) \leq 2^\alpha m(n-1)^\alpha$$

with equality if and only if G is isomorphic to either K_n or $\overline{K}_n$.

Theorem 161. [214] *If G is an (n,m)-graph with $m \geq 1$, then*

$$\chi_\alpha(G) \begin{cases} \leq mn^\alpha & \text{for } \alpha > 0 \\ \\ \geq mn^\alpha & \text{for } \alpha < 0. \end{cases}$$

The equality sign in either of the above inequalities holds if and only if G is isomorphic to a complete bipartite graph.

Theorem 162. [214] *If G is a non-trivial n-vertex graph, then*

$$\chi_\alpha(G)\begin{cases}\leq 2^{\alpha-1}n(n-1)^{\alpha+1}-\chi_\alpha(\overline{G}) & \text{for } \alpha>0\\ \geq 2^{\alpha-1}n(n-1)^{\alpha+1}-\chi_\alpha(\overline{G}) & \text{for } \alpha<0\\ \geq 2^{-1}n(n-1)^{\alpha+1}-\chi_\alpha(\overline{G}) & \text{for } \alpha\geq 1\\ < 2^{\alpha}n(n-1)-\chi_\alpha(\overline{G}) & \text{for } \alpha<0\\ > 2^{-\alpha}n^{\alpha}(n-1)^{2\alpha}-\chi_\alpha(\overline{G}) & \text{for } 0<\alpha<1.\end{cases}$$

The equality sign in either of the first two inequalities holds if and only if G is isomorphic to either K_n or $\overline{K}_n$. The equality sign in third inequality holds if and only if G is isomorphic to a regular graph of degree $(n-1)/2$.

Theorem 163. [55] *If G is a non-trivial connected n-vertex graph and μ_1 is the largest eigenvalue of the general sum–connectivity matrix $S_\alpha(G)$, then*

$$\chi_{2\alpha}(G)\geq\frac{n(\mu_1)^2}{2(n-1)}\qquad \text{and} \qquad \chi_\alpha(G)\leq\frac{n\mu_1}{2}\,.$$

The equality sign in the first inequality holds if and only if $G\cong K_n$ and the equality sign in second inequality holds if and only if G is a regular graph.

The first inequality in Theorem 163 is an extended version of the one, given in Theorem 67.

Bianchi *et al.* [23] derived an upper bound and a lower bound on the general sum–connectivity index using a majorization technique.

Theorem 164. [55] *Let μ_n and μ_1 be the smallest and largest, respectively, eigenvalues of the general sum–connectivity matrix $S_\alpha(G)$, where G is a non-trivial connected n-vertex graph. The following inequality holds*

$$\chi_{2\alpha}(G)\geq\left(\frac{\mu_1-\mu_n}{2}\right)^2$$

with equality if and only if G is a complete bipartite graph.

Theorem 165. [55] *Let θ_t and θ_1 be the smallest and largest, respectively, positive eigenvalues of the general sum–connectivity Laplacian matrix $L_\alpha(G)$, where G is a non-trivial connected n-vertex graph. The following inequality holds*

$$\frac{n-1}{2}\,\theta_t\leq\chi_\alpha(G)\leq\frac{n-1}{2}\,\theta_1$$

with equality if and only if $G \cong K_n$. If the graph G is bipartite with bipartition (A, B) then it holds that

$$\frac{|A||B|}{|A|+|B|}\,\theta_t \le \chi_\alpha(G) \le \frac{|A||B|}{|A|+|B|}\,\theta_1\,.$$

Réti and Felde [159] derived several bounds on χ_α with some particular values of α. Various bounds on the general sum–connectivity index χ_α, for several graph operations, were reported in [3,5].

Wang *et al.* [190] established bounds on the general sum–connectivity index for several graph transformations.

Theorem 166. [107] *For $\alpha < 0$, the general sum–connectivity index χ_α of almost every n-vertex tree is among $(r_\alpha \pm \epsilon)n$, where r_α is some constant and ϵ is an arbitrary positive number.*

Bounds on χ_2 can bound in the references [70,71,75,101,133,144,145,148,191].

5.4 Relations between the general sum–connectivity index and other topological indices

Theorem 167. [214] *If G is a graph with $m \ge 1$ edges and M_1 is its first Zagreb index, then*

$$\chi_\alpha(G) \begin{cases} \le (M_1)^\alpha\, m^{1-\alpha} & \text{for } 0 < \alpha < 1 \\ \\ \ge (M_1)^\alpha\, m^{1-\alpha} & \text{for } \alpha < 0 \text{ or } \alpha > 1. \end{cases}$$

The equality sign in either of the above inequalities holds if and only if $d_u + d_v$ is a constant for every edge $uv \in E(G)$.

Theorem 168. [214] *If G is a non-trivial n-vertex graph and M_1 is its first Zagreb index, then*

$$\chi_\alpha(G) \begin{cases} \ge (M_1)^\alpha & \text{for } 0 < \alpha < 1 \\ \\ \le 2^{\alpha-1} n(n-1) & \text{for } \alpha < 0. \end{cases}$$

The equality sign in the first inequality holds if and only if G is isomorphic to either $K_2 \cup \overline{K}_{n-2}$ or $\overline{K}_n$. The equality sign in the second inequality holds if and only if $G \cong K_2$.

Various bounds on the general sum–connectivity index in terms of different graph parameters, including several other topological indices, were obtained in [69,134,162].

Theorem 169. [129] *If G is a non-trivial n-vertex graph with minimum degree δ, maximum degree Δ, second Zagreb index M_2, first geometric–arithmetic index GA and size at least 1, then*

$$\frac{(GA)^2}{4M_2} \leq \chi_{-2}(G) \leq \left(\frac{(\Delta^2+\delta^2)GA}{4\delta\Delta\sqrt{M_2}}\right)^2$$

with left equality if and only if there is a constant λ such that $d_u d_v(d_u+d_v)^2 = \lambda$ for every edge $uv \in E(G)$, and the right equality holding if and only if G is regular. Also, it holds that

$$\chi_{-2}(G) \leq \frac{1}{4}\, M_2^*(G)\,.$$

Theorem 170. [44] *If G is an n-vertex graph and $\alpha \geq 1$, then*

$$\chi_\alpha(G) \geq {}^0R_\alpha(G)$$

with equality if and only if $G \cong nK_1$ or $G \cong tK_2 \cup (n-2t)K_1$ ($t \leq \frac{n}{2}$) with $\alpha = 1$.

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