

Received July 5, 2019, accepted August 26, 2019, date of publication September 4, 2019, date of current version October 2, 2019.

Digital Object Identifier 10.1109/ACCESS.2019.2939510

# On the Minimal General Sum-Connectivity Index of Connected Graphs Without Pendant Vertices

AKBAR ALI<sup>1,2</sup>, SHAHZAD AHMED<sup>1</sup>, ZHIBIN DU<sup>3</sup>, WEI GAO<sup>4</sup>,  
AND MUHAMMAD ASLAM MALIK<sup>5</sup>

<sup>1</sup>Knowledge Unit of Science, University of Management and Technology, Sialkot 51310, Pakistan<sup>2</sup>College of Sciences, University of Hail, Hail 81451, Saudi Arabia<sup>3</sup>School of Mathematics and Statistics, Zhaoqing University, Zhaoqing 526061, China<sup>4</sup>School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China<sup>5</sup>Department of Mathematics, University of the Punjab, Quaid-i-Azam Campus, Lahore 54590, Pakistan

Corresponding authors: Akbar Ali (akbarali.maths@gmail.com) and Wei Gao (gaowei@ynnu.edu.cn)

This work was supported in part by the National Natural Science Foundation of China under Grant 11761083.

**ABSTRACT** The general sum-connectivity index of a graph  $G$ , denoted by  $\chi_\alpha(G)$ , is defined as  $\sum_{uv \in E(G)} (d(u) + d(v))^\alpha$ , where  $uv$  is the edge connecting the vertices  $u, v \in V(G)$ ,  $d(w)$  denotes the degree of a vertex  $w \in V(G)$ , and  $\alpha$  is a non-zero real number. For  $\alpha = -1/2$  and  $n \geq 11$ , Wang *et al.* [On the sum-connectivity index, *Filomat* 25 (2011) 29–42] proved that  $K_2 + \bar{K}_{n-2}$  is the unique graph with minimum  $\chi_\alpha$  value among all the  $n$ -vertex graphs having minimum degree at least 2, where  $K_2 + \bar{K}_{n-2}$  is the join of the 2-vertex complete graph  $K_2$  and the edgeless graph  $\bar{K}_{n-2}$  on  $n - 2$  vertices. Tomescu [2-connected graphs with minimum general sum-connectivity index, *Discrete Appl. Math.* 178 (2014) 135–141] proved that the result of Wang *et al.* holds also for  $n \geq 3$  and  $-1 \leq \alpha < -0.867$ . In this paper, it is shown that the aforementioned result of Wang *et al.* remains valid if the graphs under consideration are connected,  $n \geq 6$  and  $-1 \leq \alpha < \alpha_0$ , where  $\alpha_0 \approx -0.68119$  is the unique real root of the equation  $\chi_\alpha(K_2 + \bar{K}_4) - \chi_\alpha(C_6) = 0$ , and  $C_6$  is the cycle on 6 vertices.

**INDEX TERMS** Chemical graph theory, general sum-connectivity index, topological index.

## I. INTRODUCTION

Throughout this paper, the term “graph” refers to a non-trivial, simple, finite and connected graph. Vertex set and edge set of a graph  $G$  will be denoted, respectively, by  $V(G)$  and  $E(G)$ . The degree of a vertex  $u \in V(G)$  and the edge connecting the two vertices  $u, v \in V(G)$  will be denoted by  $d(u)$  and  $uv$ , respectively. A graph with  $n$  vertices will be referred as an  $n$ -vertex graph. Minimum degree of a graph  $G$  is the least number among all the vertex degrees of  $G$ . A vertex  $v \in V(G)$  of degree 1 is called pendant vertex. Those graph-theoretic notation and terminology which are not defined here, can be found in some standard books of graph theory, like [12], [25].

Finding graph(s) from a certain graph family with extremal values of those graph invariants which found some application(s) in chemistry, is the topic of many publications, appeared in chemical graph theory [22], [46]. The *first Zagreb index*, appeared within the study of total  $\pi$ -electron energy

of alternant hydrocarbons [24], and *Randić index*, proposed for measuring the extent of branching of certain chemical compounds [38], are perhaps the most studied graph invariants regarding the aforementioned extremal graph-theoretic problem. Details about the mathematical aspects of the first Zagreb index (respectively, Randić index) can be found in the recent surveys [6], [13], [14], recent papers [8], [11], [21], [28]–[30], [39], [40] (respectively, [5], [17]–[20], [23], [26], [32], [35]) and related references listed therein.

Inspired by the work done on the Randić index and the first Zagreb index, Zhou and Trinajstić proposed the *sum-connectivity index* (a variant of the both Randić index and first Zagreb index) [47] and *general sum-connectivity index* (the generalized version of the both first Zagreb index and sum-connectivity index) [48]. The general sum-connectivity index of a graph  $G$  is defined as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha,$$

where  $\alpha$  is a non-zero real number. The choice  $\alpha = -1/2$

The associate editor coordinating the review of this manuscript and approving it for publication was Aniruddha Datta.

corresponds to the sum-connectivity index. It needs to be mentioned here that  $2\chi_{-1}$  coincides with the well-studied harmonic index; see [7]. Details about  $\chi_\alpha$  can be found in the recent survey [7], recent papers [1]–[4], [9], [10], [16], [27], [33], [36], [37], [43] and related references cited therein.

The Randić index is actually the most widely applied graph invariant in chemistry and pharmacology [23]. The chemical applicability of the sum-connectivity index was tested in [31], [34] and it was concluded that the predictive ability of the sum-connectivity index and Randić index is practically same. Consequently, we may say that the sum-connectivity index is as much important as the Randić index is. But, why should one consider the general sum-connectivity index in chemistry, particularly in quantitative structure-property and structure-activity relations? Actually, the main advantage of using the general sum-connectivity index is that the value of  $\alpha$  can be determined during the regression procedure in such a way that the standard error of estimate for a particular studied property of molecules is as small as possible and the corresponding correlation coefficient is as large as possible. Thus, it is meaningful to explore the mathematical aspects of the general sum-connectivity index.

In this paper, we prove that the graph which attains minimum sum-connectivity index [44] for  $n \geq 11$  (minimum harmonic index [15], [45] for  $n \geq 4$  and minimum general sum-connectivity index  $\chi_\alpha$  [42] for  $-1 \leq \alpha < -0.867$ ,  $n \geq 3$ ) in the family of all  $n$ -vertex graphs having minimum degree at least 2, also attains the minimum general sum-connectivity index  $\chi_\alpha$  in the aforementioned graph class for  $-1 \leq \alpha < -0.68119$  and  $n \geq 6$ . Since all the graphs considered in this paper are non-trivial and connected (unless otherwise stated), the class of graphs with minimum degree at least 2 is actually equal to the class of graphs without pendant vertices.

## II. STATEMENT OF THE MAIN RESULT AND SOME PRELIMINARY LEMMAS

In order to state the main result, we need some definitions. By disjoint graphs  $G$  and  $H$ , we mean the graphs  $G$  and  $H$  are vertex-disjoint as well as edge-disjoint. The join of two disjoint graphs  $G_1$  and  $G_2$  is denoted by  $G_1 + G_2$  and is defined as the graph with the vertex set  $V(G_1) \cup V(G_2)$  and the edge set  $E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1) \text{ and } v \in V(G_2)\}$ . Throughout this paper, join will be taken over disjoint graphs. Complement of a graph  $G$  is the graph  $\bar{G}$  with the vertex set  $V(G)$  and the edge set  $\{uv : uv \notin E(G) \text{ where } u \neq v\}$ . As usual the  $n$ -vertex complete graph and  $n$ -vertex cycle graph will be denoted as  $K_n$  and  $C_n$ , respectively. Throughout this paper, we denote by  $\alpha_0 \approx -0.68119$  the unique real root of the equation  $\chi_\alpha(K_2 + \bar{K}_4) - \chi_\alpha(C_6) = 0$ . Now, we can state our main result.

**Theorem II-A:** *If  $-1 \leq \alpha < \alpha_0$  and  $n \geq 6$  then among all  $n$ -vertex connected graphs having minimum degree at least 2,  $K_2 + \bar{K}_{n-2}$  is the unique graph with minimum  $\chi_\alpha$  value, which*

*is equal to*

$$2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha.$$

For a non-empty set  $A \subset V(G)$ , denote by  $G - A$  the graph obtained from  $G$  by removing all the vertices of  $A$  as well as all the edges incident to these vertices. A non-trivial connected graph  $G$  is  $k$ -connected if and only if  $G - X$  is a non-trivial connected graph for every  $X \subset V(G)$  with  $|X| < k$ . Bearing in mind the facts that the graph  $K_2 + \bar{K}_{n-2}$  is 2-connected and that every 2-connected graph has minimum degree at least 2, we have the next result as a direct consequence of Theorem II-A.

**Corollary II-B:** *If  $-1 \leq \alpha < \alpha_0$  and  $n \geq 6$  then among all  $n$ -vertex 2-connected graphs,  $K_2 + \bar{K}_{n-2}$  is the unique graph with minimum  $\chi_\alpha$  value, which is equal to*

$$2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha.$$

In the remaining part of this section, some lemmas are given, which play a vital role in proving Theorem II-A. The first such lemma is related to the removal of an edge from a graph.

**Lemma II-C:** [42] *If  $v_1v_2$  is an edge of a graph  $G$  such that  $d(v_1) + d(v_2) \leq d(u) + d(v)$  for all  $uv \in E(G)$ , then*

$$\chi_\alpha(G - v_1v_2) < \chi_\alpha(G)$$

*for  $-1 \leq \alpha < 0$ , where  $G - v_1v_2$  is the graph deduced from  $G$  by removing the edge  $v_1v_2$ .*

The proof of the next lemma is straightforward and hence omitted.

**Lemma II-D:** *If  $\alpha < 0$ , then the function  $f$  defined by*

$$f(x, y) = (x+2)^\alpha + (y+2)^\alpha - (x+y)^\alpha, \quad \text{where } x, y \geq 3,$$

*is strictly decreasing in both  $x$  and  $y$ , on the interval  $[3, \infty)$ .*

As mentioned before, in the remaining part of this paper, we take  $\alpha_0 \approx -0.68119$  as the unique root of the equation  $\chi_\alpha(K_2 + \bar{K}_4) - \chi_\alpha(C_6) = 0$  where  $C_6$  is the cycle on 6 vertices.

**Lemma II-E:** *If  $n \geq 7$  and  $-1 \leq \alpha < \alpha_0$  then the function  $f$  defined by*

$$f(\alpha, n) = (2n-4)(n^\alpha - (n+1)^\alpha) - (2n-2)^\alpha$$

*is positive-valued.*

*Proof:*

By using Lagrange's mean value theorem, we have

$$(2n-4)(n^\alpha - (n+1)^\alpha) = -(2n-4)\alpha\epsilon^{\alpha-1} > -(2n-4)\alpha(n+1)^{\alpha-1},$$

where  $n < \epsilon < n+1$ . So,

$$f(\alpha, n) = (2n-4)(n^\alpha - (n+1)^\alpha) - (2n-2)^\alpha > -(2n-4)\alpha(n+1)^{\alpha-1} - (2n-2)^\alpha.$$

Now, we need only to show that

$$-(2n-4)\alpha(n+1)^{\alpha-1} > (2n-2)^\alpha,$$

which is equivalent to

$$-\alpha \left( 2 - \frac{6}{n+1} \right) > \left( 2 - \frac{4}{n+1} \right)^\alpha.$$

Let

$$g(\alpha, n) = -\alpha \left( 2 - \frac{6}{n+1} \right) - \left( 2 - \frac{4}{n+1} \right)^\alpha.$$

Clearly,  $g$  is strictly increasing in  $n$ , because

$$\frac{\partial g}{\partial n} = -\frac{\alpha}{(n+1)^2} \left( 4 \left( 2 - \frac{4}{n+1} \right)^{\alpha-1} + 6 \right) > 0.$$

Consequently, for  $-1 \leq \alpha < \alpha_0$ , it holds that

$$g(\alpha, n) \geq g(\alpha, 7) = -\frac{5\alpha}{4} - \left( \frac{3}{2} \right)^\alpha > 0.$$

because

$$-\alpha > 0.61 \approx \frac{4}{5} \left( \frac{2}{3} \right)^{0.68} > \frac{4}{5} \left( \frac{2}{3} \right)^{-\alpha}.$$

This completes the proof of the lemma.  $\square$

*Lemma II-F:* If  $x, y \geq 3$  and  $-1 \leq \alpha < 0$ , then the function  $f$  defined by

$$f(x, y) = (x-1)(x+2)^\alpha + (y-1)(y+2)^\alpha - (x-2)(x+1)^\alpha - (y-2)(y+1)^\alpha + (x+y)^\alpha - (x+y-2)^\alpha$$

is strictly decreasing in both  $x$  and  $y$ .

*Proof:* Throughout this proof, we assume that  $-1 \leq \alpha < 0$  and  $x, y \geq 3$ . One obtains

$$f_x(x, y) = (x + \alpha x - \alpha + 2)(x+2)^{\alpha-1} - (x + \alpha x - 2\alpha + 1)(x+1)^{\alpha-1} + \alpha(x+y)^{\alpha-1} - \alpha(x+y-2)^{\alpha-1}$$

and

$$f_{xy}(x, y) = \alpha(\alpha - 1)[(x+y)^{\alpha-2} - (x+y-2)^{\alpha-2}],$$

where  $f_x = \frac{\partial f}{\partial x}$  and  $f_{xy} = \frac{\partial^2 f}{\partial x \partial y}$ . Obviously, the function  $f_{xy}$  is negative-valued. Hence, the function  $f_x$  is decreasing in  $y$ , which implies that

$$f_x(x, y) \leq f_x(x, 3) = h(x+1) - h(x) + g(x) - g(x+1), \quad (1)$$

where

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

and

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

Cauchy's mean value theorem guaranties that for every real number  $x$ , there exists a number  $c_x$  in the open interval  $(x, x+1)$  such that

$$\frac{h(x+1) - h(x)}{g(x+1) - g(x)} = \frac{h'(c_x)}{g'(c_x)}.$$

But,

$$\frac{h'(c_x)}{g'(c_x)} = \left( \frac{c_x + 1}{c_x + 2} \right)^{\alpha-2} \left( \frac{2 + (\alpha + 1)c_x}{1 - \alpha} + 1 \right),$$

which is greater than 1 and hence

$$h(x+1) - h(x) + g(x) - g(x+1) < 0,$$

because the function  $g$  is strictly decreasing. Therefore, from Equation (1), it follows that the function  $f_x$  is negative-valued and hence  $f$  is strictly decreasing in  $x$ . Because of the symmetry, we also conclude that  $f$  is strictly decreasing in  $y$ .  $\square$

*Lemma II-G:* If  $-1 \leq \alpha < 0$ , then the function  $f$  defined by

$$f(x) = x(x+2)^\alpha - (x-2)x^\alpha,$$

is decreasing in  $x \geq 2$ .

*Proof:* One obtains

$$\frac{df}{dx} = g(x) - g(x-2), \quad (2)$$

where  $g(y) = (y + \alpha y + 2)(y+2)^{\alpha-1}$ ,  $y \geq 0$ . But, under the given constraint on  $\alpha$ , the following inequality holds

$$\frac{dg}{dy} = \alpha(y(\alpha + 1) + 4)(y+2)^{\alpha-2} < 0,$$

for all  $y \geq 0$ , which implies that the function  $g$  is decreasing in  $y$  on the interval  $[0, \infty)$  and hence from Equation (2), the desired result follows.  $\square$

*Lemma II-H:* Let

$$f(\alpha, n) = (n-5)(n-1)^\alpha - (n-3)(n+1)^\alpha + 2^\alpha [(n-3)^\alpha - (n-1)^\alpha] + 4^\alpha.$$

If  $-1 \leq \alpha < \alpha_0$  and  $n$  is an integer with  $n \geq 9$ , then  $f(\alpha, n) > 0$ .

*Proof:* If  $n \geq 13$ , then due to the assumption  $-1 \leq \alpha < \alpha_0$ , we have

$$n > 1 + 4 \cdot 2^{(-1/\alpha_0)} > 1 + 4 \cdot 2^{-1/\alpha},$$

which implies that

$$4^\alpha - 2(n-1)^\alpha > 0 \quad (3)$$

for  $-1 \leq \alpha < \alpha_0$ . Also, the inequalities

$$(n-3)[(n-1)^\alpha - (n+1)^\alpha] > 0 \quad (4)$$

and

$$2^\alpha [(n-3)^\alpha - (n-1)^\alpha] > 0 \quad (5)$$

hold for all  $n \geq 13$  and  $\alpha$  satisfying  $-1 \leq \alpha < \alpha_0$ . By adding (3)–(5), we get the desired result for  $n \geq 13$ . In the remaining proof, we assume that  $9 \leq n \leq 12$  and  $-1 \leq \alpha < \alpha_0$ . We note that the function  $\Phi$ , defined by

$$\Phi(\alpha) = \left( \frac{4}{n+1} \right)^\alpha + \left( \frac{n-1}{n+1} \right)^\alpha,$$

is strictly decreasing. Thus,

$$\left( \frac{4}{n+1} \right)^\alpha + \left( \frac{n-1}{n+1} \right)^\alpha > \left( \frac{4}{n+1} \right)^{\alpha_0} + \left( \frac{n-1}{n+1} \right)^{\alpha_0} > 3,$$

(for  $n = 9, 10, 11, 12$  and  $-1 \leq \alpha < \alpha_0$ ) which implies that  $4^\alpha + (n - 1)^\alpha - 3 \cdot (n + 1)^\alpha > 0$ , adding it to the inequality  $(n - 6)[(n - 1)^\alpha - (n + 1)^\alpha] + 2^\alpha[(n - 3)^\alpha - (n - 1)^\alpha] > 0$  yield  $f(\alpha, n) > 0$ .  $\square$

In the proofs of some upcoming lemmas, we will write directly the inequalities related to (3) because their derivations are fully analogous to that of (3).

*Lemma II-I:* If  $\alpha < 0$ , then the function  $f$  defined by

$$f(x) = (x + 2)^\alpha - (x + 3)^\alpha,$$

is decreasing in  $x \geq 2$ .

*Lemma II-J:* The function  $f$  is defined by

$$f(\alpha, n) = (2^\alpha + 1)[(n - 2)^\alpha - (n - 1)^\alpha] + 2[(n - 3)n^\alpha - (n - 2)(n + 1)^\alpha] + 5^\alpha.$$

If  $-1 \leq \alpha < \alpha_0$  and  $n$  is an integer greater than 6, then  $f(\alpha, n)$  is positive-valued.

*Proof:* Clearly, the inequality  $f(\alpha, n) > 0$ , for  $n \geq 14$ , can be obtained by adding the following inequalities

$$5^\alpha - 2n^\alpha > 0, \quad (2^\alpha + 1)[(n - 2)^\alpha - (n - 1)^\alpha] > 0, \\ 2(n - 2)[n^\alpha - (n + 1)^\alpha] > 0,$$

which hold for all  $n \geq 14$  and  $\alpha$  satisfying  $-1 \leq \alpha < \alpha_0$ . In what follows, it is assumed that  $7 \leq n \leq 13$  and  $-1 \leq \alpha < \alpha_0$ . We note that

$$2(n - 3) \left( \frac{n}{n + 1} \right)^\alpha + \left( \frac{5}{n + 1} \right)^\alpha \\ > 2(n - 3) \left( \frac{n}{n + 1} \right)^{\alpha_0} + \left( \frac{5}{n + 1} \right)^{\alpha_0} > 2(n - 2),$$

(for  $n = 7, 8, \dots, 13$  and  $-1 \leq \alpha < \alpha_0$ ) which implies that

$$2[(n - 3)n^\alpha - (n - 2)(n + 1)^\alpha] + 5^\alpha > 0, \quad (6)$$

adding it to the inequality

$$(2^\alpha + 1)[(n - 2)^\alpha - (n - 1)^\alpha] > 0$$

give  $f(\alpha, n) > 0$ .  $\square$

*Lemma II-K:* If  $-1 \leq \alpha < 0$ , then the function  $f$  defined by

$$f(x) = (x + 3)^\alpha + (x - 1)[(x + 2)^\alpha - (x + 1)^\alpha],$$

is decreasing in  $x \geq 3$ .

*Proof:* Here, we have

$$\frac{df}{dx} = g(x) - g(x + 1) + h(x + 1) - h(x) \quad (7)$$

where

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

and

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

We note that the functions  $g$  and  $h$  are the same as used in the proof of Lemma II-F, and hence by using the same reasoning given there, we have

$$g(x) - g(x + 1) + h(x + 1) - h(x) < 0,$$

under the given constraints. Therefore, from Equation (7), it follows that  $\frac{df}{dx} < 0$  for all  $x \geq 3$  and  $\alpha$  satisfying  $-1 \leq \alpha < 0$ .  $\square$

*Lemma II-L:* If  $n$  is an integer greater than 8 and  $-1 \leq \alpha < \alpha_0$  then the function  $f$  defined by

$$f(\alpha, n) = (n - 6)(n - 2)^\alpha + 2^\alpha[(n - 4)^\alpha - (n - 1)^\alpha] \\ + (n - 4)(n - 1)^\alpha - 2(n - 2)(n + 1)^\alpha \\ + n^\alpha + 2 \cdot 5^\alpha + 4^\alpha,$$

is positive-valued.

*Proof:* Under the given constraints, it is evident that

$$f(\alpha, n) > (n - 6)(n - 2)^\alpha + 2^\alpha[(n - 4)^\alpha - (n - 1)^\alpha] \\ + (n - 4)(n - 1)^\alpha - 2(n - 2)(n - 1)^\alpha \\ + 3 \cdot 5^\alpha \quad (8) \\ = (n - 6)(n - 2)^\alpha + 2^\alpha[(n - 4)^\alpha - (n - 1)^\alpha] \\ - n(n - 1)^\alpha + 3 \cdot 5^\alpha. \quad (9)$$

Also, we note that the right hand side of (8) is positive for  $n \geq 16$  because the inequalities

$$3[5^\alpha - 2(n - 2)^\alpha] > 0, \quad 2^\alpha[(n - 4)^\alpha - (n - 1)^\alpha] > 0, \\ n[(n - 2)^\alpha - (n - 1)^\alpha] > 0,$$

hold for all  $n \geq 16$  and  $\alpha$  satisfying the given condition. In the rest of the proof, we take  $9 \leq n \leq 15$  and  $-1 \leq \alpha < \alpha_0$ . Here, we have

$$2 \left( \frac{5}{n + 1} \right)^\alpha + \left( \frac{4}{n + 1} \right)^\alpha > 2 \left( \frac{5}{n + 1} \right)^{\alpha_0} + \left( \frac{4}{n + 1} \right)^{\alpha_0} > 5,$$

(for  $n = 9, 10, \dots, 15$  and  $-1 \leq \alpha < \alpha_0$ ) which implies that  $2 \cdot 5^\alpha + 4^\alpha - 5(n + 1)^\alpha > 0$ , adding it to the inequality

$$[n^\alpha - (n + 1)^\alpha] + (n - 4)[(n - 1)^\alpha - (n + 1)^\alpha] \\ + (n - 6)[(n - 2)^\alpha - (n + 1)^\alpha] + 2^\alpha[(n - 4)^\alpha - (n - 1)^\alpha] > 0,$$

yield  $f(\alpha, n) > 0$ .  $\square$

*Lemma II-M:* Let

$$f(\alpha, n) = 2[(n - 3)n^\alpha - (n - 2)(n + 1)^\alpha] \\ + 2^\alpha[(n - 2)^\alpha - (n - 1)^\alpha] + 4^\alpha.$$

If  $n$  is an integer greater than 6 and  $-1 \leq \alpha < \alpha_0$  then  $f(\alpha, n) > 0$ .

*Proof:* Clearly, the inequality  $f(\alpha, n) > 0$ , for  $n > 12$ , can be obtained by adding the inequalities

$$4^\alpha - 2n^\alpha > 0, \quad 2^\alpha[(n - 2)^\alpha - (n - 1)^\alpha] > 0, \\ 2(n - 2)[n^\alpha - (n + 1)^\alpha] > 0,$$

which hold for all  $n > 12$  and  $\alpha$  satisfying  $-1 \leq \alpha < \alpha_0$ . In what follows, we assume that  $7 \leq n \leq 12$  and  $-1 \leq \alpha < \alpha_0$ .

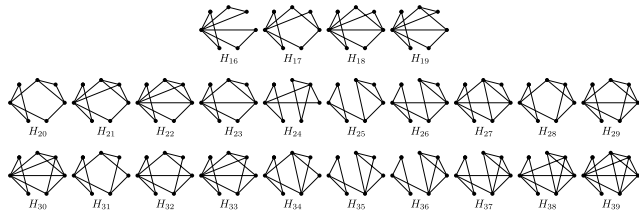


FIGURE 1. All those non-isomorphic graphs on 7 vertices with minimum degree 2 which satisfy other constraints of Lemma III-B.

From (6), it follows that  $2[(n-3)n^\alpha - (n-2)(n+1)^\alpha] + 4^\alpha > 0$ , adding it to the inequality  $2^\alpha[(n-2)^\alpha - (n-1)^\alpha] > 0$  give  $f(\alpha, n) > 0$ . □

III. PROOF OF THEOREM I-A

Lemma III-A: Theorem II-A is true for  $n = 6$ .

Proof: There are 61 non-isomorphic connected 6-vertex graphs with minimum degree at least 2. We generate these graphs by using SageMath [41]. We calculate the general sum-connectivity indices of these 61 graphs and then we compare these indices with  $\chi_\alpha(K_2 + \bar{K}_4)$ , which gives the desired result. □

Lemma III-B: Let  $G$  be an  $n$ -vertex connected graph with minimum degree at least 2. Suppose that  $G$  contains at least one pair of adjacent vertices of degree 2. Also, suppose that if  $u, v \in V(G)$  is an arbitrary pair of adjacent vertices of degree 2 then

- (i) either  $u, v$  have a common neighbor of degree more than 3,
- (ii) or  $u, v$  have a common neighbor of degree 3, which is adjacent to a branching vertex (a vertex with degree greater than 2).

If  $-1 \leq \alpha < \alpha_0$  and  $n = 7$  or  $8$ , then it holds that

$$\chi_\alpha(G) > 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha. \tag{10}$$

Proof: If the minimum degree of  $G$  is at least 3, then we may choose an edge  $v_1v_2 \in E(G)$  satisfying the inequality  $d(v_1) + d(v_2) \leq d(u) + d(v)$  for all  $uv \in E(G)$ . Clearly, the graph  $G - v_1v_2$  still has minimum degree at least 2, and by using Lemma II-C, we have  $\chi_\alpha(G) > \chi_\alpha(G - v_1v_2)$  for  $-1 \leq \alpha < \alpha_0$ . Thereby, it is enough to prove the lemma when  $G$  has minimum degree 2.

All those non-isomorphic graphs on 7 vertices with minimum degree 2 are depicted in Figure 1, which satisfy other constraints of this lemma. Routine calculations yield

$$\begin{aligned} \chi_\alpha(H_{16}) &= 3(4^\alpha + 2 \cdot 8^\alpha), \\ \chi_\alpha(H_{17}) &= 4^\alpha + 3 \cdot 5^\alpha + 5 \cdot 7^\alpha, \\ \chi_\alpha(H_{18}) &= 4^\alpha + 3 \cdot 6^\alpha + 5 \cdot 8^\alpha + 10^\alpha, \\ \chi_\alpha(H_{19}) &= 4^\alpha + 6^\alpha + 2(5^\alpha + 2 \cdot 8^\alpha + 9^\alpha), \\ \chi_\alpha(H_{20}) &= 4^\alpha + 3 \cdot 5^\alpha + 4 \cdot 6^\alpha + 7^\alpha, \\ \chi_\alpha(H_{21}) &= 4^\alpha + 5^\alpha + 2 \cdot 8^\alpha + 3(6^\alpha + 7^\alpha), \\ \chi_\alpha(H_{22}) &= 4^\alpha + 3 \cdot 8^\alpha + 10^\alpha + 2(6^\alpha + 7^\alpha + 9^\alpha), \end{aligned}$$

$$\begin{aligned} \chi_\alpha(H_{23}) &= 4^\alpha + 5^\alpha + 8^\alpha + 9^\alpha + 2(6^\alpha + 2 \cdot 7^\alpha), \\ \chi_\alpha(H_{24}) &= 2(4^\alpha + 3 \cdot 6^\alpha) + 8^\alpha, \\ \chi_\alpha(H_{25}) &= 4^\alpha + 4(5^\alpha + 6^\alpha), \\ \chi_\alpha(H_{26}) &= 4^\alpha + 5^\alpha + 4 \cdot 6^\alpha + 3 \cdot 7^\alpha + 8^\alpha, \\ \chi_\alpha(H_{27}) &= 4^\alpha + 2(6^\alpha + 2 \cdot 7^\alpha + 8^\alpha + 9^\alpha), \\ \chi_\alpha(H_{28}) &= 4^\alpha + 7 \cdot 6^\alpha + 2 \cdot 7^\alpha, \\ \chi_\alpha(H_{29}) &= 4^\alpha + 5 \cdot 7^\alpha + 9^\alpha + 2(6^\alpha + 8^\alpha), \\ \chi_\alpha(H_{30}) &= 4^\alpha + 3 \cdot 8^\alpha + 2(2 \cdot 7^\alpha + 9^\alpha + 10^\alpha), \\ \chi_\alpha(H_{31}) &= 4^\alpha + 2(2 \cdot 5^\alpha + 6^\alpha + 7^\alpha), \\ \chi_\alpha(H_{32}) &= 4^\alpha + 3 \cdot 8^\alpha + 2(5^\alpha + 6^\alpha + 7^\alpha), \\ \chi_\alpha(H_{33}) &= 4^\alpha + 2(2 \cdot 6^\alpha + 8^\alpha + 2 \cdot 9^\alpha), \\ \chi_\alpha(H_{34}) &= 4^\alpha + 3(2 \cdot 6^\alpha + 8^\alpha), \\ \chi_\alpha(H_{35}) &= 4^\alpha + 2(2 \cdot 5^\alpha + 6^\alpha + 7^\alpha), \\ \chi_\alpha(H_{36}) &= 4^\alpha + 3 \cdot 6^\alpha + 2(5^\alpha + 2 \cdot 7^\alpha), \\ \chi_\alpha(H_{37}) &= 4^\alpha + 4 \cdot 7^\alpha + 3(6^\alpha + 8^\alpha), \\ \chi_\alpha(H_{38}) &= 4^\alpha + 5 \cdot 7^\alpha + 3(8^\alpha + 9^\alpha), \\ \chi_\alpha(H_{39}) &= 4^\alpha + 4(2 \cdot 8^\alpha + 10^\alpha). \end{aligned}$$

It is not difficult to verify that  $\chi_\alpha(H_i) > 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha$  for every  $i \in \{16, 17, \dots, 39\}$  and  $-1 \leq \alpha < \alpha_0$ .

Now, we consider the case  $n = 8$ . It is clear that  $G$  contains at least one cut-vertex (a vertex whose removal disconnects  $G$ ), which implies that the vertex connectivity (minimum number of vertices whose removal disconnects  $G$ ) of  $G$  is 1. Also, we note that  $G$  must not be triangle-free. By using SageMath [41], we generate all those non-isomorphic connected 8-vertex graphs with minimum degree 2 and vertex connectivity 1, which contain at least one triangle. There are totally 307 graphs. From these 307 graphs, we observe that exactly 192 satisfy the constraints of the lemma. We calculate the general sum-connectivity indices of the desired 192 graphs and then we compare these indices with  $\chi_\alpha(K_2 + \bar{K}_6)$ , which gives the desired result. □

The set formed by neighbors of a vertex  $v \in V(G)$  is denoted by  $N(v)$ . For non-empty sets  $A \subset V(G)$  and  $B \subseteq E(\bar{G})$ , denote by  $G - A + B$  the graph deduced from  $G - A$  by adding the edges of  $B$ . Let  $G'$  be a graph obtained from another graph  $G$  by applying some graph transformation such that  $V(G') \subseteq V(G)$ . Throughout this section, whenever such two graphs are under discussion, by the vertex degree  $d(u)$ ,  $u \in V(G')$ , we always mean that it is degree of the vertex  $u$  in  $G$ .

The next lemma is proved for  $n = 7$ . But, throughout the proof of this lemma, we use  $n$  instead of 7, for the purpose of referring it afterwards for other values of  $n$ .

Lemma III-C: Let  $G$  be an  $n$ -vertex connected graph with minimum degree at least 2. Suppose that  $G$  satisfies at least one of the following conditions:

- (i)  $G$  does not contain any pair of adjacent vertices of degree 2;
- (ii)  $G$  contains at least one pair of adjacent vertices of degree 2 having a common neighbor of degree 3, which is adjacent to only vertices of degree 2;

(iii)  $G$  contains at least one pair of adjacent vertices of degree 2 without common neighbor.

If  $n = 7$  and  $-1 \leq \alpha < \alpha_0$ , then it holds that

$$\chi_\alpha(G) \geq 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha \quad (11)$$

with equality if and only if  $G \cong K_2 + \bar{K}_{n-2}$ .

*Proof:* Bearing in mind the first paragraph of the proof of Lemma III-B, it is enough to prove the result when minimum degree of  $G$  is 2.

*Case 1:*  $G$  has no pair of adjacent vertices of degree 2.

Let  $u \in V(G)$  be a vertex of degree 2 having neighbors  $v$  and  $w$ .

*Subcase 1.1:* There is no edge between  $v$  and  $w$ .

Clearly, it holds that  $3 \leq d(v) \leq n-2$  and  $3 \leq d(w) \leq n-2$ . If we take  $G_1 \cong G - \{u\} + \{vw\}$  (noting that  $G_1$  has six vertices), then by using Lemmas II-D, III-A and II-E, we have

$$\begin{aligned} \chi_\alpha(G) &= \chi_\alpha(G_1) + (2+d(v))^\alpha + (2+d(w))^\alpha \\ &\quad - (d(v)+d(w))^\alpha \\ &\geq \chi_\alpha(G_1) + 2 \cdot n^\alpha - 2^\alpha(n-2)^\alpha \\ &\geq 2(n-2)n^\alpha \\ &> 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha. \end{aligned}$$

*Subcase 1.2:* There is an edge between  $v$  and  $w$ .

In this case, the vertex degrees  $d(v)$  and  $d(w)$  satisfy the inequalities  $3 \leq d(v) \leq n-1$  and  $3 \leq d(w) \leq n-1$ . By setting  $G_2 \cong G - \{u\}$  and utilizing Lemmas II-F and III-A, we obtain

$$\begin{aligned} \chi_\alpha(G) &= \chi_\alpha(G_2) + (2+d(v))^\alpha + (2+d(w))^\alpha \\ &\quad + (d(v)+d(w))^\alpha - (d(v)+d(w)-2)^\alpha \\ &\quad + \sum_{t \in N(v) \setminus \{u,w\}} \left[ (d(v)+d(t))^\alpha \right. \\ &\quad \left. - (d(v)-1+d(t))^\alpha \right] \\ &\quad + \sum_{z \in N(w) \setminus \{v,u\}} \left[ (d(w)+d(z))^\alpha \right. \\ &\quad \left. - (d(w)-1+d(z))^\alpha \right] \\ &\geq \chi_\alpha(G_2) + (2+d(v))^\alpha + (2+d(w))^\alpha \\ &\quad + (d(v)+d(w))^\alpha - (d(v)+d(w)-2)^\alpha \\ &\quad + (d(v)-2) \left[ (d(v)+2)^\alpha - (d(v)+1)^\alpha \right] \\ &\quad + (d(w)-2) \left[ (d(w)+2)^\alpha - (d(w)+1)^\alpha \right] \\ &= \chi_\alpha(G_2) + (d(v)-1)(2+d(v))^\alpha \\ &\quad + (d(w)-1)(2+d(w))^\alpha + (d(v)+d(w))^\alpha \\ &\quad - (d(v)+d(w)-2)^\alpha - (d(v)-2)(d(v)+1)^\alpha \\ &\quad - (d(w)-2)(d(w)+1)^\alpha \\ &\geq \chi_\alpha(G_2) + 2(n-2)(n+1)^\alpha \\ &\quad + 2^\alpha[(n-1)^\alpha - (n-2)^\alpha] - 2(n-3)n^\alpha \\ &\geq 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha. \end{aligned} \quad (12)$$

We note that the equality sign holds throughout in (12) if and only if all the members of the sets  $N(v) \setminus \{u, w\}$ ,  $N(w) \setminus \{v, u\}$  have degree 2, both the vertices  $v, w$  have degree  $n-1$  and  $G_2 \cong K_2 + \bar{K}_{n-3}$ . This shows that the equality sign holds throughout in (12) if and only if  $G \cong K_2 + \bar{K}_{n-2}$ .

*Case 2:*  $G$  contains at least one pair of adjacent vertices of degree 2 having a common neighbor of degree 3, which is adjacent to only vertices of degree 2.

Let  $u, u' \in V(G)$  be two adjacent vertices of degree 2, denote by  $u_1$  the common neighbor of  $u$  and  $u'$ , and let  $N(u_1) = \{u, u', u_2\}$  where  $d(u_2) = 2$ . Let  $u_3$  be the neighbor of  $u_2$  different from  $u_1$ . Clearly, the vertex  $u_3$  may be adjacent to at most  $n-4$  vertices. If  $G_3 \cong G - \{u_2\} + \{u_1u_3\}$ , then by using Lemmas II-I, III-A and II-J, we have

$$\begin{aligned} \chi_\alpha(G) &= \chi_\alpha(G_3) + 5^\alpha + (2+d(u_3))^\alpha - (3+d(u_3))^\alpha \\ &\geq \chi_\alpha(G_3) + 5^\alpha + (n-2)^\alpha - (n-1)^\alpha \\ &\geq 2(n-3)n^\alpha + (2^\alpha+1)(n-2)^\alpha - (n-1)^\alpha + 5^\alpha \\ &> 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha. \end{aligned}$$

*Case 3:*  $G$  contains at least one pair of adjacent vertices of degree 2 without common neighbor.

Let  $u, u' \in V(G)$  be a pair of adjacent vertices of degree 2 having no common neighbor. Let  $u_1$  be the neighbor of  $u$  different from  $u'$ . By setting  $G_4 \cong G - \{u\} + \{u'u_1\}$ , using Lemmas III-A and II-M, we get

$$\begin{aligned} \chi_\alpha(G) &= \chi_\alpha(G_4) + 4^\alpha \\ &\geq 2(n-3)n^\alpha + 2^\alpha(n-2)^\alpha + 4^\alpha \\ &> 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha. \end{aligned}$$

This completes the proof.  $\square$

From Lemmas III-B and III-C, the next result follows.

*Lemma III-D:* Theorem II-A is true for  $n = 7$ .

*Remark III-E:* If we replace  $n = 8$  in Lemma III-C, then the resulting statement remains true due to Lemma III-D (more precisely, in the proof of Lemma III-C, all the using of Lemma III-A are replaced by Lemma III-D).

The next lemma follows directly from Lemma III-B and Remark III-E.

*Lemma III-F:* Theorem II-A is true for  $n = 8$ .

**Proof of Theorem II-A.** We prove the result by induction on  $n$ . The result is true for  $n = 6, 7, 8$  and  $-1 \leq \alpha < \alpha_0$  because of Lemmas III-A, III-D and III-F. Now, we suppose that  $n \geq 9$ ,  $-1 \leq \alpha < \alpha_0$  and the result is true for all those graphs of order at most  $n-1$  whose minimum degree is at least 2.

Let  $G$  be an  $n$ -vertex graph with minimum degree at least 2. If the minimum degree of  $G$  is at least 3, then we may choose an edge  $v_1v_2 \in E(G)$  satisfying  $d(v_1) + d(v_2) \leq d(u) + d(v)$  for all  $uv \in E(G)$ . Clearly, the graph  $G - v_1v_2$  (obtained from  $G$  by removing the edge  $v_1v_2$ ) still has minimum degree at least 2, and by using Lemma II-C, we have  $\chi_\alpha(G) > \chi_\alpha(G - v_1v_2)$  for  $-1 \leq \alpha < \alpha_0$ . Thus, we assume that the minimum degree of  $G$  is 2.

If  $G$  does not contain any pair of adjacent vertices of degree 2, then the proof is fully analogous to that of

Case 1 in Lemma III-C (more precisely, in the proof of Lemma III-C, we would use “induction hypothesis” instead of Lemma III-A).

Suppose that  $G$  contains at least one pair of adjacent vertices of degree 2. Let  $u, v \in V(G)$  be adjacent vertices of degree 2. Then there are four possibilities:

- (i)  $u$  and  $v$  have no common neighbor;
- (ii)  $u$  and  $v$  have a common neighbor of degree 3, which is adjacent to only vertices of degree 2;
- (iii)  $u$  and  $v$  have a common neighbor of degree 3, which is adjacent to a branching vertex (a vertex with degree greater than 2);
- (iv)  $u$  and  $v$  have a common neighbor of degree more than 3.

The proof of (i) and (ii) are, respectively, fully analogous to that of Cases 3 and 2 in Lemma III-C.

For (iii) and (iv), denote by  $u_1$  the common neighbor of  $u$  and  $v$ . Obviously, it holds that  $3 \leq d(u_1) \leq n - 1$ .

First suppose that  $u_1$  has degree 3. Let  $u_2$  be the neighbor of  $u_1$  different from  $u$  and  $v$ . Due to the given constraints, it holds that  $3 \leq d(u_2) \leq n - 3$ . If  $G_5 \cong G - \{u, v, u_1\}$ , then by using Lemma II-K, induction hypothesis and Lemma II-L, we have

$$\begin{aligned} \chi_\alpha(G) &= \chi_\alpha(G_5) + 4^\alpha + 2 \cdot 5^\alpha + (3 + d(u_2))^\alpha \\ &\quad + \sum_{z \in N(u_2) \setminus \{u_1\}} \left[ (d(u_2) + d(z))^\alpha \right. \\ &\quad \left. - (d(u_2) - 1 + d(z))^\alpha \right] \\ &\geq \chi_\alpha(G_5) + 4^\alpha + 2 \cdot 5^\alpha + (3 + d(u_2))^\alpha \\ &\quad + (d(u_2) - 1) \left[ (d(u_2) + 2)^\alpha - (d(u_2) + 1)^\alpha \right] \\ &\geq \chi_\alpha(G_5) + 4^\alpha + 2 \cdot 5^\alpha + n^\alpha \\ &\quad + (n - 4) \left[ (n - 1)^\alpha - (n - 2)^\alpha \right] \\ &\geq (n - 6)(n - 2)^\alpha + 2^\alpha(n - 4)^\alpha + n^\alpha \\ &\quad + (n - 4)(n - 1)^\alpha + 4^\alpha + 2 \cdot 5^\alpha \\ &> 2(n - 2)(n + 1)^\alpha + 2^\alpha(n - 1)^\alpha. \end{aligned}$$

Next suppose that  $u_1$  has degree greater than 3. If  $G_6 \cong G - \{u, v\}$ , then simple computations give

$$\begin{aligned} \chi_\alpha(G) &= \chi_\alpha(G_6) + 4^\alpha + 2(2 + d(u_1))^\alpha \\ &\quad + \sum_{z \in N(u_1) \setminus \{u, v\}} \left[ (d(u_1) + d(z))^\alpha \right. \\ &\quad \left. - (d(u_1) - 2 + d(z))^\alpha \right] \\ &\geq \chi_\alpha(G_6) + 4^\alpha + 2(2 + d(u_1))^\alpha \\ &\quad + (d(u_1) - 2) \left[ (d(u_1) + 2)^\alpha - (d(u_1))^\alpha \right] \\ &= \chi_\alpha(G_6) + 4^\alpha + d(u_1)(2 + d(u_1))^\alpha \\ &\quad - (d(u_1) - 2)(d(u_1))^\alpha. \end{aligned}$$

By using the induction hypothesis, Lemmas II-G and II-H, we have

$$\begin{aligned} \chi_\alpha(G) &\geq \chi_\alpha(G_6) + 4^\alpha + (n - 1)(n + 1)^\alpha \\ &\quad - (n - 3)(n - 1)^\alpha \end{aligned}$$

$$\begin{aligned} &\geq (n - 5)(n - 1)^\alpha + 2^\alpha(n - 3)^\alpha \\ &\quad + (n - 1)(n + 1)^\alpha + 4^\alpha \\ &> 2(n - 2)(n + 1)^\alpha + 2^\alpha(n - 1)^\alpha. \end{aligned}$$

This completes the proof of Theorem II-A.

#### IV. CONCLUSION

We have proved that the graph  $K_2 + \overline{K}_{n-2}$  which attains minimum sum-connectivity index [44] for  $n \geq 11$  (minimum harmonic index [15], [45] for  $n \geq 4$  and minimum general sum-connectivity index  $\chi_\alpha$  [42] for  $-1 \leq \alpha < -0.867$ ,  $n \geq 3$ ) in the family of all  $n$ -vertex graphs having minimum degree at least 2, also attains the minimum general sum-connectivity index  $\chi_\alpha$  in the aforementioned graph class for  $-1 \leq \alpha < -0.68119$  and  $n \geq 6$  (see Theorem II-A). For sufficiently large  $n$ , we expect that the same graph  $K_2 + \overline{K}_{n-2}$  has minimum general sum-connectivity index  $\chi_\alpha$  in the above-mentioned graph class also for  $-0.68119 \leq \alpha < 0$ ; it would be interesting, in future, to prove this assertion. But, we remark that the technique (mathematical induction) adopted in the present paper would not work well in this regard, because the verification of the induction-base-step would be much more tedious (as  $n$  would be increased when we considerably increase  $\alpha$  in the interval  $(-0.68119, 0)$ ).

#### ACKNOWLEDGMENT

The authors would like to thank the anonymous referees for their valuable comments and suggestions, which led to a number of improvements in the earlier version of the manuscript.

#### REFERENCES

- [1] S. Akhter, M. Imran, and Z. Raza, “Bounds for the general sum-connectivity index of composite graphs,” *J. Inequal. Appl.*, vol. 2017, Apr. 2017, Art. no. 76.
- [2] A. Ali, “An alternative but short proof of a result of Zhu and Lu concerning general sum-connectivity index,” *Asian-Eur. J. Math.*, vol. 11, no. 2, 2018, Art. no. 1850030.
- [3] A. Ali and D. Dimitrov, “On the extremal graphs with respect to bond incident degree indices,” *Discrete Appl. Math.*, vol. 238, pp. 32–40, Mar. 2018.
- [4] A. Ali, D. Dimitrov, Z. Du, and F. Ishfaq, “On the extremal graphs for general sum-connectivity index ( $\chi_\alpha$ ) with given cyclomatic number when  $\alpha > 1$ ,” *Discrete Appl. Math.*, vol. 257, pp. 19–30, Mar. 2019.
- [5] A. Ali and Z. Du, “On the difference between atom-bond connectivity index and Randić index of binary and chemical trees,” *Int. J. Quantum Chem.*, vol. 117, no. 23, 2017, Art. no. e25446.
- [6] A. Ali, I. Gutman, E. Milovanović, and I. Milovanović, “Sum of powers of the degrees of graphs: Extremal results and bounds,” *MATCH Commun. Math. Comput. Chem.*, vol. 80, pp. 5–84, Jan. 2018.
- [7] A. Ali, L. Zhong, and I. Gutman, “Harmonic index and its generalizations: Extremal results and bounds,” *MATCH Commun. Math. Comput. Chem.*, vol. 81, pp. 249–311, Jan. 2019.
- [8] M. An and K. C. Das, “First Zagreb index,  $k$ -connectivity,  $\beta$ -deficiency and  $k$ -hamiltonicity of graphs,” *MATCH Commun. Math. Comput. Chem.*, vol. 80, pp. 141–151, Jan. 2018.
- [9] M. An and L. Xiong, “Extremal polyomino chains with respect to general sum-connectivity index,” *Ars Comb.*, vol. 131, pp. 255–271, Jan. 2017.
- [10] M. Arshad and I. Tomescu, “Maximum general sum-connectivity index with  $-1 \leq \alpha < 0$  for bicyclic graphs,” *Math. Rep.*, vol. 19, pp. 93–96, Jan. 2017.
- [11] L. Bedratyuk and O. Savenko, “The star sequence and the general first Zagreb index,” *MATCH Commun. Math. Comput. Chem.*, vol. 79, pp. 407–414, Jun. 2018.
- [12] J. A. Bondy and U. S. R. Murty, *Graph Theory*. London, U.K.: Springer, 2008.

- [13] B. Borovičanić, K. Das, B. Furtula, and I. Gutman, "Bounds for Zagreb indices," *MATCH Commun. Math. Comput. Chem.*, vol. 78, pp. 17–100, Jan. 2017.
- [14] B. Borovičanić, K. C. Das, B. Furtula, and I. Gutman, "Zagreb indices: Bounds and extremal graphs," in *Bounds in Chemical Graph Theory*, I. Gutman, B. Furtula, K. C. Das, E. Milovanović, and I. Milovanović, Eds. Kragujevac, Serbia: Univ. Kragujevac, 2017, pp. 67–153.
- [15] R. Chang and Y. Zhu, "On the harmonic index and the minimum degree of a graph," *Romanian J. Inform. Sci. Technol.*, vol. 15, pp. 335–343, Jan. 2012.
- [16] Q. Cui and L. Zhong, "On the general sum-connectivity index of trees with given number of pendent vertices," *Discrete Appl. Math.*, vol. 222, pp. 213–221, May 2017.
- [17] Q. Cui and L. Zhong, "The general Randić index of trees with given number of pendent vertices," *Appl. Math. Comput.*, vol. 302, pp. 111–121, Jun. 2017.
- [18] K. C. Das, S. Balachandran, and I. Gutman, "Inverse degree, Randić index and harmonic index of graphs," *Appl. Anal. Discrete Math.*, vol. 11, pp. 304–313, Oct. 2017.
- [19] W. Gao, M. R. Farahani, and M. Imran, "About the Randić connectivity, modify Randić connectivity and sum-connectivity indices of titania nanotubes  $\text{TiO}_2(m,n)$ ," *Acta Chim. Slovenica*, vol. 64, pp. 256–260, Mar. 2017.
- [20] A. Ghalavand and A. R. Ashrafi, "Ordering chemical graphs by Randić and sum-connectivity numbers," *Appl. Math. Comput.*, vol. 331, pp. 160–168, Aug. 2018.
- [21] A. Ghalavand and A. R. Ashrafi, "Some inequalities between degree- and distance-based topological indices of graphs," *MATCH Commun. Math. Comput. Chem.*, vol. 79, pp. 399–406, Jan. 2018.
- [22] I. Gutman, "Degree-based topological indices," *Croatica Chem. Acta.*, vol. 86, no. 4, pp. 351–361, 2013.
- [23] I. Gutman, B. Furtula, and V. Katanić, "Randić index and information," *AKCE Int. J. Graphs Combinatorics*, vol. 15, no. 3, pp. 307–312, 2018. doi: 10.1016/j.akcej.2017.09.006.
- [24] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total  $\phi$ -electron energy of alternant hydrocarbons," *Chem. Phys. Lett.*, vol. 17, pp. 535–538, Dec. 1972.
- [25] F. Harary, *Graph Theory*. Reading, MA, USA: Addison-Wesley, 1969.
- [26] N. H. M. Husin, R. Hasni, Z. Du, and A. Ali, "More results on extremum Randić indices of (molecular) trees," *Filomat*, vol. 32, pp. 3581–3590, 2018.
- [27] M. K. Jamil and I. Tomescu, "Minimum general sum-connectivity index of trees and unicyclic graphs having a given matching number," *Discrete Appl. Math.*, vol. 222, pp. 143–150, May 2017.
- [28] S. Ji and S. Wang, "On the sharp lower bounds of Zagreb indices of graphs with given number of cut vertices," *J. Math. Anal. Appl.*, vol. 458, pp. 21–29, Feb. 2018.
- [29] J.-B. Liu, C. Wang, S. Wang, and B. Wei, "Zagreb indices and multiplicative Zagreb indices of Eulerian graphs," *Bull. Malaysian Math. Sci. Soc.*, vol. 42, no. 1, pp. 67–78, Jan. 2019. doi: 10.1007/s40840-017-0463-2.
- [30] Z. H. Liu, Q. Ma, and Y. Chen, "New bounds on Zagreb indices," *J. Math. Inequal.*, vol. 11, pp. 167–179, Jan. 2017.
- [31] B. Lucic, I. Sovic, J. Batista, K. Skala, D. Plavsic, D. Vikić-Topić, D. Beslo, S. Nikolic, and N. Trinajstić, "The sum-connectivity index—An additive variant of the randić connectivity index," *Current Comput. Aided Drug Des.*, vol. 9, no. 2, pp. 184–194, 2013.
- [32] T. Mansour, M. A. Rostami, S. Elumalai, and B. A. Xavier, "Correcting a paper on the Randić and geometric-arithmetic indices," *Turkish J. Math.*, vol. 41, no. 1, pp. 27–32, 2017.
- [33] I. V. Z. Milovanović, E. I. Milovanović, and M. Matejić, "Some inequalities for general sum-connectivity index," *MATCH Commun. Math. Comput. Chem.*, vol. 79, pp. 477–489, Jan. 2018.
- [34] S. Nikolić, N. Trinajstić, and S. I. Turk, "On the additive version of the connectivity index," in *Proc. AIP Conf.*, vol. 1504, Dec. 2012, pp. 342–350.
- [35] S. O and Y. Shi, "Sharp bounds for the Randić index of graphs with given minimum and maximum degree," *Discrete Appl. Math.*, vol. 247, pp. 111–115, Oct. 2018. doi: 10.1016/j.dam.2018.03.064.
- [36] Q. Qin and Y. Shao, "Minimum general sum-connectivity index of tricyclic graphs," *Oper. Res. Trans.*, vol. 22, no. 1, pp. 142–150, 2018.
- [37] H. S. Ramane, V. V. Manjapur, and I. Gutman, "General sum-connectivity index, general product-connectivity index, general Zagreb index and coindices of line graph of subdivision graphs," *AKCE Int. J. Graphs Combinatorics*, vol. 14, pp. 92–100, Apr. 2017.
- [38] M. Randić, "Characterization of molecular branching," *J. Amer. Chem. Soc.*, vol. 97, no. 23, pp. 6609–6615, 1975.
- [39] J. M. Rodríguez, J. L. Sánchez, and J. M. Sigarreta, "CMMSE-on the first general Zagreb index," *J. Math. Chem.*, vol. 56, pp. 1849–1864, Aug. 2018.
- [40] M. Sababheh, "Graph indices via the AM–GM inequality," *Discrete Appl. Math.*, vol. 230, pp. 100–111, Oct. 2017.
- [41] *SageMath*. Accessed: May 17, 2019. [Online]. Available: <http://www.sagemath.org/>
- [42] I. Tomescu, "2-Connected graphs with minimum general sum-connectivity index," *Discrete Appl. Math.*, vol. 178, pp. 135–141, Dec. 2014.
- [43] H. Wang, J.-B. Liu, S. Wang, W. Gao, S. Akhter, M. Imran, and M. R. Farahani, "Sharp bounds for the general sum-connectivity indices of transformation graphs," *Discrete Dyn. Nature Soc.*, vol. 2017, Dec. 2017, Art. no. 2941615.
- [44] S. Wang, B. Zhou, and N. Trinajstić, "On the sum-connectivity index," *Filomat*, vol. 25, no. 3, pp. 29–42, 2011.
- [45] R. Wu, Z. Tang, and H. Deng, "A lower bound for the harmonic index of a graph with minimum degree at least two," *Filomat*, vol. 27, no. 1, pp. 49–53, 2013.
- [46] K. Xu, M. Liu, K. C. Das, I. Gutman, and B. Furtula, "A survey on graphs extremal with respect to distance-based topological indices," *MATCH Commun. Math. Comput. Chem.*, vol. 71, pp. 461–508, Feb. 2014.
- [47] B. Zhou and N. Trinajstić, "On a novel connectivity index," *J. Math. Chem.*, vol. 46, pp. 1252–1270, Nov. 2009.
- [48] B. Zhou and N. Trinajstić, "On general sum-connectivity index," *J. Math. Chem.*, vol. 47, pp. 210–218, Jan. 2010.

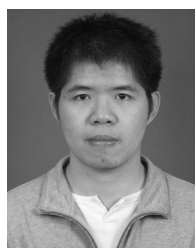


**AKBAR ALI** received the M.Phil. degree from the University of the Punjab, Pakistan, in 2011, and the Ph.D. degree from the National University of Computer and Emerging Sciences, Pakistan, in 2016. He is currently an Assistant Professor with the University of Hail, Hail, Saudi Arabia. Before joining the University of Hail, he was serving as an Assistant Professor with the University of Management and Technology, Sialkot, Pakistan, where the first draft of the article was prepared.

His research interest includes discrete mathematics, especially (chemical) graph theory. He is currently a member of the Editorial Boards of the journals *MATCH Communications in Mathematical and in Computer Chemistry* and the *Iranian Journal of Mathematical Chemistry*. He is also the Managerial Secretary of the journal *Discrete Mathematics Letters*.



**SHAHZAD AHMED** received the M.Sc. degree in mathematics from the University of the Punjab, Lahore, Pakistan, in 2008, and the M.S. degree in mathematics from the University of Management and Technology, Sialkot, Pakistan, in 2018. His research interests include mathematical chemistry and discrete mathematics, especially (chemical) graph theory.



**ZHIBIN DU** was born in Zhaoqing, China, in 1985. He received the B.S. degree in mathematics and applied mathematics from Huizhou University, Huizhou, China, in 2007, the M.S. degree in operational research and cybernetics from South China Normal University, Guangzhou, China, in 2010, and the Ph.D. degree in applied mathematics from Tongji University, Shanghai, China, in 2013. He is currently a Postdoctoral Fellow with the Institute of Mathematics, Academia Sinica, Taipei, Taiwan, and an Associate Professor with Zhaoqing University, Zhaoqing, China.

He has authored more than 70 articles. His research interests mainly include chemical graph theory, spectral graph theory, and combinatorial matrix theory. He is an Associate Editor of two journals. He is a reviewer of *Mathematical Reviews* of the American Mathematical Society.

Dr. Du's awards and honors mainly include the Doctoral Graduate Academic New-talent Award from the Ministry of Education of China, the Doctoral Graduate National Scholarship from the Ministry of Education of China, and the Excellent Doctoral Thesis Award from Tongji University.





**WEI GAO** received the Ph.D. degree from the Mathematical Department, Soochow University, China, in 2012. After that, he was with the School of Information Science and Technology, Yunnan Normal University. His research interests include graph theory, theoretical chemistry, statistical learning theory, computation topics on energy and environmental science, and artificial intelligence. He is a Committee Member of the China Society of Industrial and Applied Mathematics (CSIAM) Graph Theory and Combinatorics with Applications Committee, the International Association of Engineers (IAENG), and the Asia Society of Applied Mathematics and Engineering (Asia-SAME), and act as an Academic Adviser of the Center for Energy Research, Iran. He is the Chair of ICED 2017 and ISGTCTC 2018. He is an Editor of several journals. Among his more than 100 publications in SCI index journals, ten of them are included in Essential Science Indicators as Highly Cited articles (top 1% citations) and three of them are honored with Hot articles (top 0.1% citations).



**MUHAMMAD ASLAM MALIK** received the Ph.D. degree in mathematics from the University of the Punjab, Pakistan, in 2004. He completed Postdoctorate under the supervision of Dr. R. T. Curtis from the University of Birmingham, U.K. He has been an Associate Professor with the University of the Punjab. He has produced four Ph.D. and 30 M.Phil. students in the field of mathematics and has vast experience of administration as a coordinator of all academic programs at the university level. He has 25 years of regular teaching experience at postgraduate level/research in mathematics in various highly reputed public sector institutions of Pakistan. His areas of research include algebra, graph theory, and number theory. He has published more than 50 research articles in the journals of national and international repute (top 0.1% citations).

• • •