

The First General Zagreb Connection Index and its Particular Cases on some Special Graphs

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Abstract

Topological index (TI) is an unaltered numeric number that associates with the graph isomerism. These unaltered numbers mostly appear in the kind of degree based TIs. The first degree based TI was introduced by Gutman and Trinajstić in 1972. Such degree based TIs are further classified in two different ways; degree and connection number based TIs. The number of neighbors at distance 1 and 2 from vertex v of graph G are represented by degree and connection number, respectively. In this paper, we newly define connection number based TI in the general version with the name of the first general Zagreb connection index (ZCI). We also compute exact formulae for the first general ZCI on some special graphs such as wheel, gear, helm, flower and sunflower. Moreover, the various particular cases are discussed with the help of abovementioned general version.

Keywords: Connection number; first general Zagreb index; ; particular Zagreb indices; special graphs.

Mathematics Subject Classification: : 05C09, 05C92

1. Introduction

The quantitative structure property-relationship (QSPR) and quantitative structure activity-relationship (QSAR) are beneficial for expensive experimental drug design, study of molecules and investigate the physical & chemical properties of any graphs with the help of topological indices (TIs), see [1, 2]. A TI is a number which depends on the molecular graphs and mostly helpful to judge the properties of chemical compounds. These descriptors are also oftenly used in the most commonly scientific fields such as analytical chemistry, cheminformatics, toxicology, biology, pharmaceutical, organic and environmental chemistry. For more study, we refer to [3, 4, 5].

A TI based on degree is known as degree based TI. First time, this kind of TI was defined by two mathematicians and chemists Gutman and Trinajstić [6]. They also proved that the entire π -electron energy of a molecular graph depends on its structures and it can be derived from the sum of square of vertice's degrees of any molecular graphs. Now, this relation is known as from the name of first Zagreb index (ZI). The more properties and revolutionary findings about this invariant can be seen in this literatures [7, 8, 9] references therein.

The first general ZI was defined by Li and Zheng [10] (2004) to find a unified approach in the extremal trees on some different invariants. This degree based general version is also known as the general zeroth order Randić index [11]. Jamil et al. [12] identified some bounds for that zeroth order general Randić index. M. Liu and B. Liu [13] shown some properties of that general version. Jia-Bao Liu et al. [14] computed first general ZI of F -sum graphs. Awais et al. [15] extended the concept of Jia-Bao Liu such that first general ZI for generalized F -sum graphs. Chaluvvaraju et al. [16] computed some bounds and exact solutions for the first general ZI of line and jump graphs. TIs have been also applied in the spectral graphs theory to count the flexibility and toughness of complex networks [17]. There are so much literatures can be seen in the list of degree based invariants, see [18, 19, 20, 21].

Gutman and Trinajstić [6](1972) defined the concept of degree of a vertex. In that paper, they also defined the concept of connection number to influence E_π . Now many researches have done their work on this descriptor. For that instance, Tang et al. [22](2019) computed exact solutions for Zagreb connection indices (ZCIs) of subdivision-related operations on graphs. Ali et al. [23] enhanced the concept ZCIs in the shape of modified second and third ZCIs. Javaid et al. [24] introduced new modified version with the name of modified fourth ZCI. They also computed exact formulae for several newly defined ZCIs of wheel-related graphs. Shiladhar et al. [25] and Kulli [26] computed exact formulae for leap ZIs (or ZCIs) and minus leap & square leap indices of some special graphs. Recently, Hussain et al. [27] investigated the zinc based MONs and proved that zinc silicate related MONs are better than zinc oxide related MONs. In addition, a list of papers have been listed in the field of chemical graph theory related to connection based ZIs, see [28, 29, 30, 31, 32, 33, 34].

In this paper, we define the first general ZCI. We compute the exact solutions for this newly defined general version on some special graphs such as wheel, gear, helm, flower and sunflower. We also define the some particular cases which named as third ZCI, fourth ZCI, fifth ZCI, sixth ZCI, seventh ZCI and eighth ZCI of aforesaid graphs. The rest of the paper is presented as follows: Section II presents the preliminary definitions of the classical/novel general version of Zagreb indices and some results which are used in the next section, Section III gives the definitions of some special graphs, their main results of first general ZCI and its particular cases on aforesaid graphs and Section IV covers conclusion.

2. Notations and Preliminaries

The simple and connected graph G has $|V(G)| = n$ vertices and $|E(G)| = p$ edges. The number of vertices which are at distance 1 and 2 from vertex v of G are called degree ($d(v)$) and connection number ($\tau(v)$), respectively. If $p = uv$ is the edge connecting with u and v then degree of edge ($d(p)$) is defined as $d(p) = d(u) + d(v) - 2$. The $V(G)$ and $E(G)$ are also known as elements (or components) of G . For more detail and terminology, we can see [35].

Definition 2.1 (See [10]). Let G be a connected graph. Then $\forall \alpha \in R - \{0\}$, the first general Zagreb index ($Z_\alpha(G)$) is given as

$$Z_\alpha(G) = \sum_{v \in V(G)} [d(v)^\alpha].$$

Corresponding to this degree based ZI, connection number based the first general ZI is as follows:

Definition 2.2. Let G be a connected graph. Then $\forall \alpha, \beta \in R - \{0\}$, the first general Zagreb connection index ($G_{\alpha, \beta}(G)$) is given as

$$G_{\alpha, \beta}(G) = \sum_{v \in V(G)} [d(v)^\alpha \times \tau(v)^\beta].$$

By using Definition 2.2, we make the following particular cases in the Table 1 as follows:

Table 1: Connection number based ZIs.

Name	Symbol	Formula
First ZCI (See [22])	$ZC_1(G) = G_{0,2}(G)$	$\sum_{v \in V(G)} [\tau(v)^2]$
Modified first ZCI (See [22])	$ZC_1^*(G) = G_{1,1}(G)$	$\sum_{v \in V(G)} [d(v) \times \tau(v)]$
Third ZCI	$ZC_3(G) = G_{0,3}(G)$	$\sum_{v \in V(G)} [\tau(v)^3]$
Fourth ZCI	$ZC_4(G) = G_{1,2}(G)$	$\sum_{v \in V(G)} [d(v) \times \tau(v)^2]$
Fifth ZCI	$ZC_5(G) = G_{2,1}(G)$	$\sum_{v \in V(G)} [d(v)^2 \times \tau(v)]$
Sixth ZCI	$ZC_6(G) = G_{2,2}(G)$	$\sum_{v \in V(G)} [d(v)^2 \times \tau(v)^2]$
Seventh ZCI	$ZC_7(G) = G_{3,1}(G)$	$\sum_{v \in V(G)} [d(v)^3 \times \tau(v)]$
Eighth ZCI	$ZC_8(G) = G_{1,3}(G)$	$\sum_{v \in V(G)} [d(v) \times \tau(v)^3]$

Now, we discuss some important results which may apply in the main results.

Lemma 2.1.[36] Let G be a connected graph with n vertices and p edges. Then,
 $\tau(u) + d(u) \leq \sum_{v \in N(u)} d(v)$, where equality holds if and only if G is a $\{C_3, C_4\}$ – free graph.

Lemma 2.2.[22] Let G be a connected and $\{C_3, C_4\}$ – free graph with n vertices and p edges. Then,

$$(i) \sum_{v \in V(G)} d(v) = 2p, \quad (ii) \sum_{v \in V(G)} \tau(v) = M_1(G) - 2p.$$

3. Definitions and Main Results

In this section, we defines some special graphs which are wheel, gear, helm, flower and sunflower graphs, respectively. Then, we compute the first general Zagreb connection index (ZCI) and its particular cases such as third, fourth, fifth, sixth and seventh ZCIs on aforesaid graphs.

1. Wheel Graph W_n :

The wheel graph W_n is defined by joining K_1 and C_n . Where K_1 and C_n are the complete and cycle graphs of orders 1 and n respectively. So, order of wheel graph ($|V(W_n)|$) is $n + 1$ and size of wheel graph ($|E(W_n)|$) is $2n$. Apex is the vertex corresponding to K_1 and rim is the set of those vertices which is corresponding to C_n . The graphical depiction of wheel graph is presented in Figure 1.

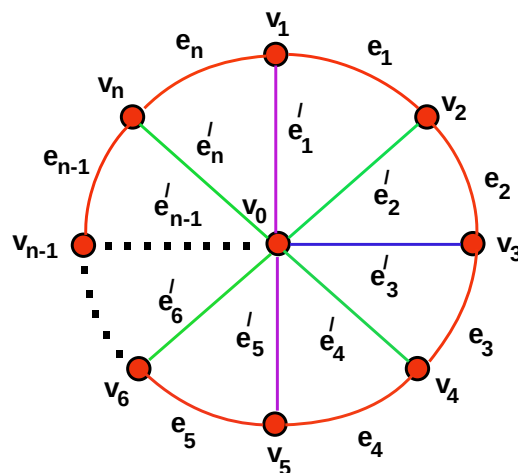


Figure 1. Wheel graph W_n

Table 2: Partition of vertices for W_n .

Degree/Connection number	Apex (v_0)	Rim (v_i)
d_{W_n}	n	3
τ_{W_n}	0	n-3

Theorem 3.1. Let W_n be a wheel graph of order $n + 1$. Then, the first general Zagreb connection index of W_n is

$$G_{\alpha,\beta}(W_n) = 3^\alpha n(n-3)^\beta.$$

Proof. Since W_n is a wheel graph of order $n + 1$, where $n \geq 4$. Also, v_0 is the apex vertex and $\{v_1, v_2, \dots, v_n\}$ is the set of rim vertices for W_n . By definition,

$$\begin{aligned}
 G_{\alpha,\beta}(W_n) &= \sum_{v \in V(W_n)} [d(v)^\alpha \times \tau(v)^\beta] \\
 &= [d(v_0)^\alpha \times \tau(v_0)^\beta] + \sum_{i=1}^n [d(v_i)^\alpha \times \tau(v_i)^\beta] \\
 &= [n^\alpha \times 0^\beta] + n[3^\alpha \times (n-3)^\beta] \\
 &= 3^\alpha n(n-3)^\beta.
 \end{aligned}$$

Now, we find the particular cases for W_n by using Theorem 3.1 as follows:

Corollary 3.1

Case(i) $ZC_1(W_n) = G_{0,2}(W_n) = n(n^2 - 6n + 9)$,

Case(ii) $ZC_1^*(W_n) = G_{1,1}(W_n) = 3n(n-3)$,

These particular cases (i) and (ii) are also derived in [25],

Case(iii) $ZC_3(W_n) = G_{0,3}(W_n) = n(n^3 - 9n^2 + 27n - 27)$,

Case(iv) $ZC_4(W_n) = G_{1,2}(W_n) = 3n(n^2 - 6n + 9)$,

Case(v) $ZC_5(W_n) = G_{2,1}(W_n) = 9n(n-3)$,

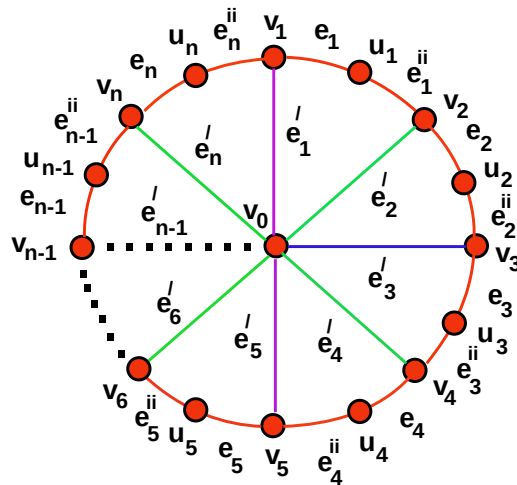
Case(vi) $ZC_6(W_n) = G_{2,2}(W_n) = 9n(n^2 - 6n + 9)$,

Case(vii) $ZC_7(W_n) = G_{3,1}(W_n) = 27n(n-3)$,

Case(viii) $ZC_8(W_n) = G_{1,3}(W_n) = 3n(n^3 - 9n^2 + 27n - 27)$.

2. Gear Graph G_n :

The gear graph G_n is obtained from wheel graph W_n by including a new vertex between each pair of adjacent vertex of rim. So, order of gear graph ($|V(G_n)|$) is $2n + 1$ and size of gear graph ($|E(G_n)|$) is $3n$. Also, the bipartite wheel graph is called gear graph. The graphical depiction of gear graph is presented in Figure 2.

Figure 2. Gear graph G_n Table 3: Partition of vertices for G_n .

Degree/Connection number	Apex (v_0)	Rim (v_i)	Rim (u_i)
d_{G_n}	n	3	2
τ_{G_n}	n	n-1	3

Theorem 3.2. Let G_n be a gear graph of order $2n + 1$. Then, the first general Zagreb connection index of G_n is

$$G_{\alpha,\beta}(G_n) = n^{\alpha+\beta} + 3^{\alpha}n(n-1)^{\beta} + 2^{\alpha}3^{\beta}n.$$

Proof. Since G_n is a gear graph of order $2n + 1$. Also, v_0 is the apex vertex, $\{v_1, v_2, \dots, v_n\}$, $\{u_1, u_2, \dots, u_n\}$ are the sets of rim vertices for G_n . By definition,

$$\begin{aligned}
 G_{\alpha,\beta}(G_n) &= \sum_{v \in V(G_n)} [d(v)^{\alpha} \times \tau(v)^{\beta}] \\
 &= [d(v_0)^{\alpha} \times \tau(v_0)^{\beta}] + \sum_{i=1}^n [d(v_i)^{\alpha} \times \tau(v_i)^{\beta}] + \sum_{i=1}^n [d(u_i)^{\alpha} \times \tau(u_i)^{\beta}] \\
 &= [n^{\alpha} \times n^{\beta}] + n[3^{\alpha} \times (n-1)^{\beta}] + n[2^{\alpha} \times 3^{\beta}] \\
 &= n^{\alpha+\beta} + 3^{\alpha}n(n-1)^{\beta} + 2^{\alpha}3^{\beta}n.
 \end{aligned}$$

Now, we find the particular cases for G_n by using Theorem 3.2 as follows:

Corollary 3.2

Case(i) $ZC_1(G_n) = G_{0,2}(G_n) = n(n^2 - n + 10)$,

Case(ii) $ZC_1^*(G_n) = G_{1,1}(G_n) = n(4n + 3)$,

These particular cases (i) and (ii) are also derived in [25],

Case(iii) $ZC_3(G_n) = G_{0,3}(G_n) = n(n^3 - 2n^2 + 3n + 26)$,

Case(iv) $ZC_4(G_n) = G_{1,2}(G_n) = n(4n^2 - 6n + 21)$,

Case(v) $ZC_5(G_n) = G_{2,1}(G_n) = n(n^2 + 9n + 3)$,

Case(vi) $ZC_6(G_n) = G_{2,2}(G_n) = n(n^3 + 9n^2 - 18n + 45)$,

Case(vii) $ZC_7(G_n) = G_{3,1}(G_n) = n(n^3 + 27n - 3)$,

Case(viii) $ZC_8(G_n) = G_{1,3}(G_n) = n(4n^3 - 9n^2 + 9n + 51)$.

3. Helm Graph H_n :

The helm graph H_n is obtained from wheel graph W_n by joining a pendant edge to the every vertex of the rim. So, order of helm graph ($|V(H_n)|$) is $2n + 1$ and size of helm graph ($|E(H_n)|$) is $3n$. The graphical depiction of helm graph is presented in Figure 3.

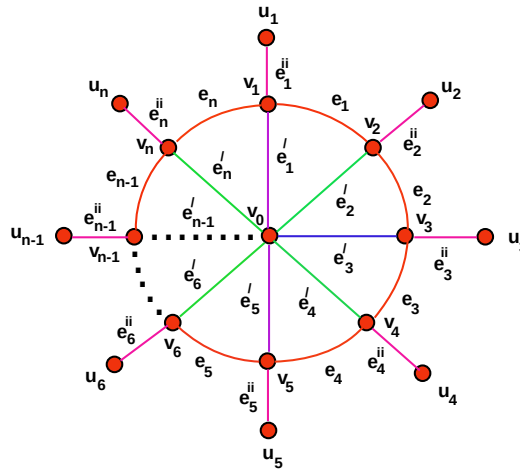


Figure 3. Helm graph H_n

Table 4: Partition of vertices for H_n .

Degree/Connection number	Apex (v_0)	Rim (v_i)	Pendant (u_i)
d_{H_n}	n	4	1
τ_{H_n}	n	n-1	3

Theorem 3.3. Let H_n be a helm graph of order $2n + 1$. Then, the first general Zagreb connection index of H_n is

$$G_{\alpha,\beta}(H_n) = n^{\alpha+\beta} + 4^{\alpha}n(n-1)^{\beta} + 3^{\beta}n.$$

Proof. Since H_n is a helm graph of order $2n + 1$. Also, v_0 is the apex vertex. $\{v_1, v_2, \dots, v_n\}$ and $\{u_1, u_2, \dots, u_n\}$ are the sets of rim and pendant vertices for H_n . By definition,

$$\begin{aligned}
 G_{\alpha,\beta}(H_n) &= \sum_{v \in V(H_n)} [d(v)^{\alpha} \times \tau(v)^{\beta}] \\
 &= [d(v_0)^{\alpha} \times \tau(v_0)^{\beta}] + \sum_{i=1}^n [d(v_i)^{\alpha} \times \tau(v_i)^{\beta}] + \sum_{i=1}^n [d(u_i)^{\alpha} \times \tau(u_i)^{\beta}] \\
 &= [n^{\alpha} \times n^{\beta}] + n[4^{\alpha} \times (n-1)^{\beta}] + n[1^{\alpha} \times 3^{\beta}] \\
 &= n^{\alpha+\beta} + 4^{\alpha}n(n-1)^{\beta} + 3^{\beta}n.
 \end{aligned}$$

Now, we find the particular cases for H_n by using Theorem 3.3 as follows:

Corollary 3.3

Case(i) $ZC_1(H_n) = G_{0,2}(H_n) = n(n^2 - n + 10)$,

Case(ii) $ZC_1^*(H_n) = G_{1,1}(H_n) = n(5n - 1)$,

These particular cases (i) and (ii) are also derived in [25],

Case(iii) $ZC_3(H_n) = G_{0,3}(H_n) = n(n^3 - 2n^2 + 3n + 26)$,

Case(iv) $ZC_4(H_n) = G_{1,2}(H_n) = n(5n^2 - 8n + 13)$,

Case(v) $ZC_5(H_n) = G_{2,1}(H_n) = n(n^2 + 16n - 13)$,

Case(vi) $ZC_6(H_n) = G_{2,2}(H_n) = n(n^3 + 16n^2 - 32n + 25)$,

Case(vii) $ZC_7(H_n) = G_{3,1}(H_n) = n(n^3 + 64n - 61)$,

Case(viii) $ZC_8(H_n) = G_{1,3}(H_n) = n(5n^3 - 12n^2 + 12n + 23)$.

4. Flower Graph Fl_n :

The flower graph Fl_n is obtained from helm graph H_n by joining each pendant vertex to the apex of helm graph. So, order of flower graph ($|V(Fl_n)|$) is $2n + 1$ and size of flower graph ($|E(Fl_n)|$) is $4n$. The graphical depiction of flower graph is presented in Figure 4.

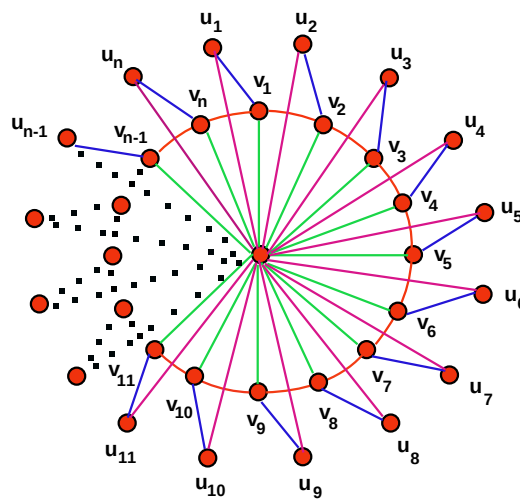


Figure 4. Flower graph Fl_n

Table 5: Partition of vertices for Fl_n .

Degree/Connection number	Apex (v_0)	Rim (v_i)	Extreme (u_i)
d_{Fl_n}	$2n$	4	2
τ_{Fl_n}	0	$2n-4$	$2n-2$

Theorem 3.4. Let Fl_n be a flower graph of order $2n + 1$. Then, the first general Zagreb connection index of Fl_n is

$$G_{\alpha,\beta}(Fl_n) = 2^{\alpha+\beta}n[2^{\alpha}(n-2)^{\beta} + (n-1)^{\beta}].$$

Proof. Since Fl_n is a flower graph of order $2n + 1$. Also, v_0 is the apex vertex. $\{v_1, v_2, \dots, v_n\}$ and $\{u_1, u_2, \dots, u_n\}$ are the sets of rim and extreme vertices for Fl_n . By definition,

$$\begin{aligned}
 G_{\alpha,\beta}(Fl_n) &= \sum_{v \in V(Fl_n)} [d(v)^{\alpha} \times \tau(v)^{\beta}] \\
 &= [d(v_0)^{\alpha} \times \tau(v_0)^{\beta}] + \sum_{i=1}^n [d(v_i)^{\alpha} \times \tau(v_i)^{\beta}] + \sum_{i=1}^n [d(u_i)^{\alpha} \times \tau(u_i)^{\beta}] \\
 &= [(2n)^{\alpha} \times 0^{\beta}] + n[4^{\alpha} \times (2n-4)^{\beta}] + n[2^{\alpha} \times (2n-2)^{\beta}]
 \end{aligned}$$

$$= 2^{\alpha+\beta} n [2^{\alpha} (n-2)^{\beta} + (n-1)^{\beta}].$$

Now, we find the particular cases for Fl_n by using Theorem 3.4 as follows:

Corollary 3.4

Case(i) $ZC_1(Fl_n) = G_{0,2}(Fl_n) = 4n(2n^2 - 6n + 5)$,

Case(ii) $ZC_1^*(Fl_n) = G_{1,1}(Fl_n) = 4n(3n - 5)$,

These particular cases (i) and (ii) are also derived in [25],

Case(iii) $ZC_3(Fl_n) = G_{0,3}(Fl_n) = 8n(2n^3 - 9n^2 + 15n - 9)$,

Case(iv) $ZC_4(Fl_n) = G_{1,2}(Fl_n) = 8n(3n^2 - 10n + 9)$,

Case(v) $ZC_5(Fl_n) = G_{2,1}(Fl_n) = 8n(5n - 9)$,

Case(vi) $ZC_6(Fl_n) = G_{2,2}(Fl_n) = 16n(5n^2 - 18n + 17)$,

Case(vii) $ZC_7(Fl_n) = G_{3,1}(Fl_n) = 16n(9n - 17)$,

Case(viii) $ZC_8(Fl_n) = G_{1,3}(Fl_n) = n(48n^3 - 240n^2 + 432n - 272)$.

5. Sunflower Graph Sf_n :

The sunflower graph Sf_n is obtained from flower graph Fl_n by growing n pendant edges to the apex of flower graph. So, order of sunflower graph ($|V(Sf_n)|$) is $3n + 1$ and size of sunflower graph ($|E(Sf_n)|$) is $5n$. The graphical depiction of sunflower graph is presented in Figure 5.

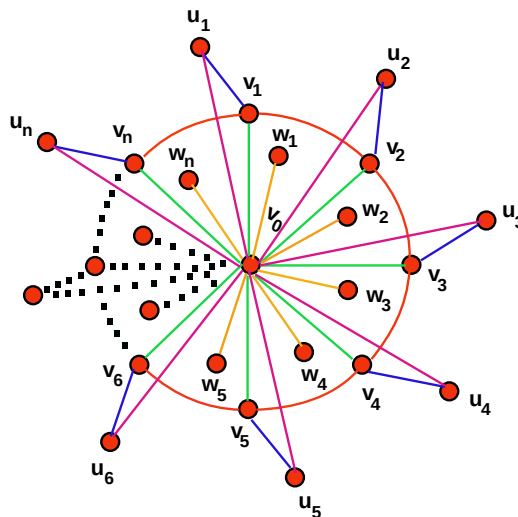


Figure 5. Sunflower graph Sf_n

Table 6: Partition of vertices for Sf_n .

Degree/Connection number	Apex (v_0)	Rim (v_i)	Extreme (u_i)	Pendant (w_i)
d_{Sf_n}	$3n$	4	2	1
τ_{Sf_n}	0	$3n-4$	$3n-2$	$3n-1$

Theorem 3.5. Let Sf_n be a sunflower graph of order $3n + 1$. Then, the first general Zagreb connection index of Sf_n is

$$G_{\alpha,\beta}(Fl_n) = n[4^{\alpha}(3n-4)^{\beta} + 2^{\alpha}(3n-2)^{\beta} + (3n-1)^{\beta}].$$

Proof. Since Sf_n is a sunflower graph of order $3n + 1$. Also, v_0 is the apex vertex. $\{v_1, v_2, \dots, v_n\}$, $\{u_1, u_2, \dots, u_n\}$ and $\{w_1, w_2, \dots, w_n\}$ are the sets of rim, extreme and pendant vertices for Sf_n . By

definition,

$$\begin{aligned}
 G_{\alpha,\beta}(Sf_n) &= \sum_{v \in V(Sf_n)} [d(v)^\alpha \times \tau(v)^\beta] \\
 &= [d(v_0)^\alpha \times \tau(v_0)^\beta] + \sum_{i=1}^n [d(v_i)^\alpha \times \tau(v_i)^\beta] + \sum_{i=1}^n [d(u_i)^\alpha \times \tau(u_i)^\beta] + \sum_{i=1}^n [d(w_i)^\alpha \times \tau(w_i)^\beta] \\
 &= [(3n)^\alpha \times o^\beta] + n[4^\alpha \times (3n-4)^\beta] + n[2^\alpha \times (3n-2)^\beta] + n[1^\alpha \times (3n-1)^\beta] \\
 &= n[4^\alpha(3n-4)^\beta + 2^\alpha(3n-2)^\beta + (3n-1)^\beta].
 \end{aligned}$$

Now, we find the particular cases for Sf_n by using Theorem 3.5 as follows:

Corollary 3.5

Case(i) $ZC_1(Sf_n) = G_{0,2}(Sf_n) = 3n(9n^2 - 14n + 7)$,

Case(ii) $ZC_1^*(Sf_n) = G_{1,1}(Sf_n) = 21n(n-1)$,

These particular cases (i) and (ii) are also derived in [25],

Case(iii) $ZC_3(Sf_n) = G_{0,3}(Sf_n) = n(81n^3 - 189n^2 + 189n - 73)$,

Case(iv) $ZC_4(Sf_n) = G_{1,2}(Sf_n) = n(63n^2 - 216n + 73)$,

Case(v) $ZC_5(Sf_n) = G_{2,1}(Sf_n) = n(63n - 73)$,

Case(vi) $ZC_6(Sf_n) = G_{2,2}(Sf_n) = 3n(63n^2 - 146n + 91)$,

Case(vii) $ZC_7(Sf_n) = G_{3,1}(Sf_n) = 3n(73n - 91)$,

Case(viii) $ZC_8(Sf_n) = G_{1,3}(Sf_n) = n(189n^3 - 567n^2 + 657n - 273)$.

4. Conclusion

In this paper, we computed the first general Zagreb connection index of some special graphs such as wheel, gear, helm, flower and sunflower. We also computed its particular cases which named as third, fourth, fifth, sixth, seventh and eighth ZCIs on aforementioned graphs.

Now, the problem is still open to compute the first general Zagreb connection index on Jahangir related graphs.

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