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On Zagreb Energy of Certain Classes of Graphs

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Abstract Energy of the graph G is the sum of absolute values of eigenvalues of its adjacency matrix. Given a simple connected graph G, its first (second) Zagreb matrix is constructed by including the sum (product) of the degrees of each pair of adjacent vertices of G. Computation of sum of absolute eigen values of these matrices yields the corresponding Zagreb energies. In this paper, the first and second Zagreb energies of certain families of graphs have been computed and a criterion to discern the nature of graph G based on their energies is obtained. The paper focuses on the comparative analysis of first and second Zagreb energies in terms of regular graphs such as cycle graphs, bipartite and tripartite graphs. Our findings reveal that the second Zagreb energy is always greater than first Zagreb energy for all complete bipartite graphs of even order greater than or equal to 4. Also we have established that the same is the case for complete tripartite graphs too. Furthermore, we illustrate that the two Zagreb energies coincide exclusively for the complete bipartite graph with equal partite sets if and only if the graph is of order 2. Additionally, we provide a criterion leading to an infinite set of non-isomorphic Zagreb equi-energetic graphs for all $r > 1$ within partite graphs. The computations of two Zagreb energies for graph operations like t-splitting graph and t-shadow graph are also illustrated. The first and second Zagreb energies for some specific graphs along with bounds on Zagreb energies for wheel graphs are also discussed.

Keywords t-Splitting Graph, t-Shadow Graph, First Zagreb Energy, Second Zagreb Energy

1 Introduction

Consider $G = (V, E)$ as a finite, simple connected graph with $|V| = r$ and $|E| = s$. Let $e = ab$ be the edge that connects vertices a and b. A simple graph G is said to be k-regular when each of its vertices has same degree. For a vertex $b \in V$, open neighbourhood of b is the set $N(b) = \{c \in V/bc \in E\}$. Degree of vertex b is number of edges that are attached to b, denoted by δ_b. When each vertex is joined to every other vertex, the graph is said to be complete. The adjacency matrix of the graph G is a square matrix of order r, denoted by $B(G) = [\beta_{ij}]$ such that $\beta_{ij} = 1$ if the corresponding vertices indexed in i^{th}row and j^{th} column are adjacent and 0, otherwise. All the eigenvalues of the matrix B are real owing to its real and symmetric nature. The adjacency matrix $B's$ spectrum is the spectrum of G, and denoted as $Spec(G)$.

Ivan Gutman defined energy $E(G)$ of the graph G in 1978 [1, 3] by summing the absolute values of eigenvalues of its adjacency matrix. Interestingly, this obtained value coincided with the approximation of the total π-electron energy of a conjugated molecule when the graph structure was suitably chosen. Since then, several graph matrix representations and related energies have been developed. These graph energies associate various properties of organic molecules and thus gain their importance.

2 Preliminaries

Ivan Gutman [4] introduced the concept of Zagreb energy. The first Zagreb matrix of G is a square matrix $FZ(G) = [c_{ij}]$, where

$$c_{ij} = \begin{cases} \delta_i + \delta_j, & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0, & \text{otherwise.} \end{cases}$$

Note that δ_i and δ_j are respectively the degrees of the two vertices v_i and v_j.

$\phi(G,x) = \det(xI - FZ(G))$ represents the characteristic polynomial of $FZ(G)$. The corresponding eigenvalues are real numbers, since elements of $FZ(G)$ are real and symmetric. Let $\lambda_i,\ i = 1, 2, \ldots, r$ be the first Zagreb eigenvalues of $FZ(G)$ with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r$. Similar to the concept of energy of adjacency matrix, the first Zagreb energy of G is defined as $\mathscr{E}[FZ(G)] = \sum_{i=1}^{r} |\lambda_i|$.

The second Zagreb matrix of a graph G is also a square matrix $SZ(G) = [d_{ij}]$, where

$$d_{ij} = \begin{cases} \delta_i \cdot \delta_j, & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0, & \text{otherwise.} \end{cases}$$

If $\mu_1, \mu_2, \ldots, \mu_r$ are the second Zagreb eigenvalues of $SZ(G)$, then its corresponding energy is $\mathscr{E}[SZ(G)] = \sum_{i=1}^{r} |\mu_i|$.

Let P be a matrix of order $m \times n$ and Q be a matrix of order $p \times q$. Then the Kronecker product of P and Q is calculated by

$$P \otimes Q = \begin{pmatrix} a_{11}Q & \ldots & a_{1n}Q \\ & \ddots & \\ a_{m1}Q & \ldots & a_{mn}Q \end{pmatrix}$$

$$\text{where } P = \begin{pmatrix} a_{11} & \ldots & a_{1n} \\ & \ddots & \\ a_{m1} & \ldots & a_{mn} \end{pmatrix}.$$

Lemma 1. *[2] Let P and Q be two matrices of order m and n respectively. Let λ be a random eigenvalue of matrix P with corresponding eigenvector X_1 and μ be an arbitary eigenvalue of matrix Q with corresponding eigenvector X_2. Then $\lambda\mu$ is an eigenvalue of the Kronecker product $P \otimes Q$, with corresponding eigenvector $X_1 \otimes X_2$.*

Given a base graph *G*, new graphs of higher order and size are constructed based on various operations like products, union, join and composition. This concept is very crucial to identify relation between huge complex graph and smaller known families of graphs. Few such graph constructions are considered here. For all the operations, the base graph *G* is considered to be simple, undirected and connected. By adding *t* additional vertices say $u_1, u_2, u_3, \ldots, u_t$ to each vertex *u* of *G*, and each u_i in turn made connected to each neighbour of *u* in *G*, the *t*-splitting graph $S^t(G)$ is constructed. The construction of *t*-shadow graph $D^t(G)$ of *G* is a one by considering t copies of G, such as $G_1, G_2, \ldots, G_t$, and joining each vertex *u* in G_i to neighbours of corresponding vertex *v* in G_j, $1 \leq i, j \leq t$. A wheel graph W_r is formed by joining all vertices in cycle graph $C_r, r \geq 3$ to a central vertex. W_r has $r+1$ vertices and $2r$ edges. Dutch windmill graph D_n^r is created by making *r* duplicates of the cycle graph C_n that shares common vertex in the cycle.

Herschel graph is an undirected bipartite graph that has 11 vertices and 18 edges. It is the smallest polyhedral graph that exhibits no Hamiltonian cycle. Two non-isomorphic graphs of same order *r* are said to be equienergetic if their energies are same. A graph of order *r* is said to be border-energetic if its energy is equal to $2(r-1)$, hyper-energetic if its energy is greater than $2(r-1)$ and non hyper-energetic if its energy is less than $2(r-1)$. The bound $2(r-1)$ is the energy of the complete graph of order *r*.

3 Literature Survey

In [4], N.J. Rad, A. Jahanbani and I. Gutman presented some lower and upper bounds for Zagreb energy. K.C. Das [5] obtained lower and upper bounds on spectral radius of Zagreb matrix of graph G. In [6], A. Jahanbani et al. obtained some new bounds for Zagreb energy of graph. Rakshith discussed new bounds for Zagreb energy in [7]. Sheikoleslmi, A. Jahanbani, Koeilar [8] determined some classes of Zagreb hyper-energetic, Zagreb border-energetic and Zagreb equienergetic graphs. Other interesting results related to the topic of interest are found in [9, 10, 11, 12, 13, 14, 15].

In this study, we first determine first and second Zagreb energies for *k*-regular graphs. We also discuss condition for second Zagreb hyper-energetic, second Zagreb non hyper-energetic, second Zagreb border-energetic and second Zagreb equienergetic graphs to exist. We further investigate the first and second Zagreb energies for the above graph operations and the special graphs.

4 Computation of the two Zagreb energies for regular graphs

In this section, the first and second Zagreb energies for regular graph are computed and the obtained values are compared to classify hyper, border and non-hyper energetic graphs.

Theorem 4.1. *Let G be a k-regular graph of order r. Let $A(G)$, $A[FZ(G)]$, $A[SZ(G)]$ denote respectively the adjacency, first Zagreb and second Zagreb matrices of G. If λ is an eigenvalue of $A(G)$, then*

1. *$2k\lambda$ will be an eigenvalue of $A[FZ(G)]$;*
2. *$k^2\lambda$ will be an eigenvalue of $A[SZ(G)]$.*

Proof. As *G* is *k*-regular, in the first Zagreb matrix $A[FZ(G)]$, all non-zero entries will be $2k$. Accounting to *r*-rows, $A[FZ(G)] = (2k)A(G)$. Hence eigenvalues of $A[FZ(G)]$ can be obtained by multiplying the eigenvalues of $A(G)$ by $(2k)$.

All the non-zero entries of the second Zagreb matrix $A[SZ(G)]$ will be k^2. Hence $A[SZ(G)] = k^2\ A(G)$ and the result follows. □

Theorem 4.2. *Given a k-regular graph G of order r, its first Zagreb energy is given by $\mathscr{E}[FZ(G)] = 2k\mathscr{E}(G)$, where $\mathscr{E}(G)$ denotes (adjacency) energy of G.*

Proof. Proof follows from the definition of $\mathscr{E}[FZ(G)]$ where the corresponding eigenvalues are obtained in Theorem 4.1. □

Corollary 4.3. *The first Zagreb energy of the complete graph K_r is given by $\mathscr{E}[FZ(K_r)] = 4(r-1)^2$.*

Proof. Proof is immediate as regularity of K_r is $r-1$ and $\mathscr{E}(K_r) = 2(r-1)$. □

Corollary 4.4. *The first Zagreb energy of the cycle graph C_r is $\mathscr{E}[FZ(C_r)] = 8\sum_{j=0}^{r-1} |\cos \frac{2\pi j}{r}|$.*

Proof. Result follows by taking $k = 2$ since C_r is 2-regular and $\mathscr{E}(C_r) = 2\sum_{j=0}^{r-1} |\cos \frac{2\pi j}{r}|$. □

Corollary 4.5. *The first Zagreb energy of complete bipartite graph $K_{r,r}$ is $\mathscr{E}[FZ(K_{r,r})] = 4r^2$.*

Proof. Since order and degree of $K_{r,r}$ is $2r$ and r respectively and $\mathscr{E}(K_{r,r}) = 2r$ we get

$$\mathscr{E}[FZ(K_{r,r})] = 2r\mathscr{E}(K_{r,r}) = 2r(2r) = 4r^2.$$

□

Corollary 4.6. *The first Zagreb energy of complete tripartite graph $K_{r,r,r}$ is $\mathscr{E}[FZ(K_{r,r,r})] = 16r^2 = 4\mathscr{E}[FZ(K_{r,r})]$.*

Proof. The order and degree of G is $3r$ and $2r$ respectively with $\mathscr{E}(K_{r,r,r}) = 4r$. Therefore the first Zagreb energy is $\mathscr{E}[FZ(K_{r,r,r})] = 4r\mathscr{E}(K_{r,r,r}) = 4r(4r) = 16r^2$. The equivalency follows from Corollary 4.5. □

Definition 1. *A graph G is said to be first Zagreb hyper-energetic if $\mathscr{E}[FZ(G)] > 4(r-1)^2$, first Zagreb non hyper-energetic if $\mathscr{E}[SZ(G)] < 4(r-1)^2$ and first Zagreb border-energetic if $\mathscr{E}[SZ(G] = 4(r-1)^2$. If $\mathscr{E}[FZ(G_1)] = \mathscr{E}[FZ(G_2)]$ for any two non-isomorphic graphs G_1 and G_2, then we say G_1 and G_2 are first Zagreb equienergetic.*

Theorem 4.7. *Given a k-regular graph G of order r, its second Zagreb energy is given by $\mathscr{E}[SZ(G)] = k^2\mathscr{E}(G)$, where $\mathscr{E}(G)$ denotes the (adjacency) energy of G.*

Proof. Proof follows from the definition of $\mathscr{E}[SZ(G)]$ where the corresponding eigenvalues are obtained in Theorem 4.1. □

Corollary 4.8. *The second Zagreb energy of the complete graph K_r is given by $\mathscr{E}[FZ(K_r)] = 2(r-1)^3$.*

Proof. Proof is immediate as regularity of K_r is $r-1$ and $\mathscr{E}(K_r) = 2(r-1)$. □

Corollary 4.9. *The second Zagreb energy of the cycle graph C_r is $\mathscr{E}[SZ(C_r)] = 8\sum_{j=0}^{r-1}|\cos\frac{2\pi j}{r}|$.*

Proof. Result follows by taking $k = 2$ since C_r is 2-regular and $\mathscr{E}(C_r) = 2\sum_{j=0}^{r-1}|\cos\frac{2\pi j}{r}|$. □

Remark 1. $\mathscr{E}[FZ(C_r)] = \mathscr{E}[SZ(C_r)], \forall r \geq 3$. *The equivalency of the two energies follows from Corollary 4.4 and 4.10.*

Corollary 4.10. *The second Zagreb energy of complete bipartite graph $K_{r,r}$ is $\mathscr{E}[SZ(K_{r,r})] = 2r^3$.*

Proof. Order and degree of $K_{r,r}$ is $2r$ and r respectively and $\mathscr{E}(K_{r,r}) = 2r$. Hence we get

$$\mathscr{E}[SZ(K_{r,r})] = (r^2)\mathscr{E}(K_{r,r}) = r^2[(2r)] = 2r^3.$$

□

Corollary 4.11. *The second Zagreb energy of complete tripartite graph $K_{r,r,r}$ is $\mathscr{E}[SZ(K_{r,r,r})] = 16r^3$.*

Proof. The order and degree of G is $3r$ and $2r$ respectively with $\mathscr{E}(K_{r,r,r}) = 4r$. Therefore second Zagreb energy is $\mathscr{E}[SZ(K_{r,r,r})] = (2r)^2\mathscr{E}(K_{r,r,r}) = 4r^2(4r) = 16r^3$. □

Remark 2. *A graph G is said to be second Zagreb hyper-energetic if $\mathscr{E}[SZ(G)] > 2(r-1)^3$; second Zagreb non hyper-energetic if $\mathscr{E}[SZ(G)] < 2(r-1)^3$ and second Zagreb border-energetic if $\mathscr{E}[SZ(G] = 2(r-1)^3$. If $\mathscr{E}[SZ(G_1)] = \mathscr{E}[SZ(G_2)]$ for any two non-isomorphic graphs G_1 and G_2, $\mathscr{E}[SZ(G_1)] = \mathscr{E}[SZ(G_2)]$ then we say G_1 and G_2 are second Zagreb equienergetic.*

Considering a cycle C_r, complete bipartite graph $K_{\frac{r}{2},\frac{r}{2}}$ and complete tripartite graph $K_{\frac{r}{3},\frac{r}{3},\frac{r}{3}}$, we now plot energies in graph to compare with their nature as defined in the above remarks. Note that graphs $K_{\frac{r}{2},\frac{r}{2}}$ and $K_{\frac{r}{3},\frac{r}{3},\frac{r}{3}}$ exist only when $r = 0(\text{mod}2)$ and $r = 0(\text{mod}3)$ respectively. Further $C_r, K_{\frac{r}{2},\frac{r}{2}}$ and $K_{\frac{r}{3},\frac{r}{3},\frac{r}{3}}$ all are of the same order r.

Observations

From Table 1, we observe the following interesting results.

1. Table 1 shows that $\mathscr{E}[FZ(K_{\frac{r}{2},\frac{r}{2}})] \leq \mathscr{E}[SZ(K_{\frac{r}{2},\frac{r}{2}})]$, for all $r \geq 4$, while $\mathscr{E}[FZ(K_{1,1})] > \mathscr{E}[SZ(K_{1,1})]$ i.e. where $r = 2$.

2. The two Zagreb energies will coincide for the graph $K_{\frac{r}{2},\frac{r}{2}}$ if and only if $4r^2 = 2r^3$ which happens only when $r = 2$.

3. From Corollories 4.6 and 4.13, it is observed that $\mathscr{E}[SZ(K_{r,r,r})] = r\mathscr{E}[FZ(K_{r,r,r})], \forall r \geq 1$.

4. From Corollories 4.5 and 4.6, it is observed that $\mathscr{E}[FZ(K_{r,r,r})] = \mathscr{E}[FZ(K_{m,m})]$, where $m = 2r$. This relation gives rise to an infinite number non-isomorphic first Zagreb equi-energetic pairs of graphs for all $r \geq 1$.

5. A similar observation is found true in the second Zagreb energies.

   i.e. $\mathscr{E}[SZ(K_{r,r,r})] = \mathscr{E}[SZ(K_{m,m})]$ when $m = 2r$.

6. From the above table, it is clear that for $r = 2, 3$ the graph is Zagreb border-energetic and for remaining values of r, it is non hyper-energetic graphs.

5 Computation of the two Zagreb energies for some graph operations

In this section, we will compute the two Zagreb energies of t-splitting graph, t-shadow graph and the wheel graph. In addition, we investigate some properties of these graphs corresponding to such energies.

Theorem 5.1. *Consider G to be a k-regular graph of order r. Then the first Zagreb spectrum of t-splitting graph of G are 0 with multiplicity $t-1$, $\frac{(t+1)\pm\sqrt{t^3+5t^2+6t+1}}{2}$ each with multiplicity 1 and the first Zagreb energy of t-splitting graph of G is given by $\sqrt{t^3+5t^2+6t+1}\mathscr{E}[FZ(G)]$.*

Proof. Let G be a graph with vertices $v_1, v_2, \ldots, v_r$. Let $v'_1, v'_2, v'_3, \ldots, v'_r, v''_1, v''_2, v''_3, \ldots, v''_r, \ldots, v^t_1, v^t_2, v^t_3, \ldots, v^t_r$ be the vertices corresponding to $v_1, v_2, v_3, \ldots, v_r$ which are added in G to obtain $S^t(G)$ such that for each vertex v of G, v_i is adjacent to

Table 1. Comparison of various energies for fixed values of r

r	$\mathscr{E}[FZ(K_{\frac{r}{2},\frac{r}{2}})]$	$\mathscr{E}[SZ(K_{\frac{r}{2},\frac{r}{2}})]$	$\mathscr{E}[FZ(K_{\frac{r}{3},\frac{r}{3},\frac{r}{3}})]$	$\mathscr{E}[SZ(K_{\frac{r}{3},\frac{r}{3},\frac{r}{3}})]$	$\mathscr{E}[FZ(C_r)]$	$\mathscr{E}[SZ(C_r)]$
6	36	54	64	128	32	32
12	144	432	256	1024	59.71	59.71
18	324	1458	576	3456	92.14	92.14
24	576	3456	1024	8192	121.53	121.53
30	900	6750	1600	16000	153.068	153.068
36	1296	11664	2304	27648	182.88	182.88
42	1764	18522	3136	43904	214.10	214.10
48	2304	27648	4096	65536	244.11	244.11
54	2916	39366	5184	93312	275.175	275.175
60	3600	54000	6400	128000	305.30	305.30

all neighbours of v in G. Then the first Zagreb matrix of $S^t(G)$, denoted by $FZ[S^t(G)]$ can be written in block matrix as

$$A \otimes FZ(G) \text{ where } A = \begin{pmatrix} t+1 & \frac{t+2}{2} & \frac{t+2}{2} & \dots & \frac{t+2}{2} \\ \frac{t+2}{2} & 0 & 0 & \dots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ \frac{t+2}{2} & 0 & 0 & 0 & 0 \end{pmatrix}_{(t+1)\times(t+1)}$$

The characteristic polynomial of A together with its spectrum is

$$x^{t-1}\left(x^2-(t+1)x-t\left(\frac{t+2}{2}\right)^2\right).$$

Hence 0 will be an eigen value of A with multiplicity $t-1$. The remaining eigenvalues are solutions to the equation.

$$\left(x^2-(t+1)x-t\left(\frac{t+2}{2}\right)^2\right)=0.$$

Hence the spectrum of A is

$$\begin{pmatrix} 0 & \frac{(t+1)+\sqrt{t^3+5t^2+6t+1}}{2} & \frac{(t+1)-\sqrt{t^3+5t^2+6t+1}}{2} \\ t-1 & 1 & 1 \end{pmatrix}.$$

Using Lemma 1, the spectrum of $FZ[S^t(G)]$ is thus computed as

$$\begin{pmatrix} 0\lambda_i & \left(\frac{(t+1)+\sqrt{t^3+5t^2+6t+1}}{2}\right)\lambda_i & \left(\frac{(t+1)-\sqrt{t^3+5t^2+6t+1}}{2}\right)\lambda_i \\ t-1 & 1 & 1 \end{pmatrix},$$

where λ_i, $i=1,2,\dots,r$ are eigenvalues of $FZ(G)$. Hence by first Zagreb energy definition, we have

$$\begin{aligned}\mathscr{E}[FZ(S^t(G))] &= \sum_{i=1}^{r}\left|\left(\frac{(t+1)\pm\sqrt{t^3+5t^2+6t+1}}{2}\right)\lambda_i\right| \\ &= \sum_{i=1}^{r}|\lambda_i|\left|\left(\frac{(t+1)\pm\sqrt{t^3+5t^2+6t+1}}{2}\right)\right| \\ &= \sum_{i=1}^{r}|\lambda_i|\Bigg(\frac{(t+1)+\sqrt{t^3+5t^2+6t+1}}{2} \\ &\quad + \frac{\sqrt{t^3+5t^2+6t+1}-(t+1)}{2}\Bigg) \\ &= \sqrt{t^3+5t^2+6t+1}\,\mathscr{E}[FZ(G)].\end{aligned}$$

□

Corollary 5.2. *If G is the complete graph on r vertices, then*

$$\mathscr{E}[FZ(S^t(K_r))] = 4(r-1)^2\sqrt{t^3+5t^2+6t+1}.$$

Corollary 5.3. *Let G be the cycle graph of order r. Then*

$$\mathscr{E}[FZ(S^t(C_r))] = 8\sqrt{t^3+5t^2+6t+1}\sum_{j=0}^{r-1}\left|\cos\frac{2\pi j}{r}\right|.$$

Corollary 5.4. *If $K_{r,r}$ is a complete bipartite graph,*

$$\mathscr{E}[FZ(S^t(K_{r,r}))] = 4r^2\sqrt{t^3+5t^2+6t+1}.$$

Corollary 5.5. *If $K_{r,r,r}$ is a complete tripartite graph, then*

$$\mathscr{E}[FZ(S^t(K_{r,r,r}))] = 16r^2\sqrt{t^3+5t^2+6t+1}.$$

Theorem 5.6. *Let G be a k-regular graph of order r. Then the second Zagreb eigenvalues of the t-splitting graph of G are 0 with multiplicity $t-1$ and $\frac{(t+1)[(t+1)\pm\sqrt{t^2+6t+1}]}{2}$ with multiplicity 1 respectively and the second Zagreb energy of t- splitting graph of G is given by*

$$\mathscr{E}[SZ(S^t(G))] = [(t+1)\sqrt{t^2+6t+1}]\mathscr{E}[SZ(G)].$$

Proof. Consider a k-regular graph G with r vertices $v_1, v_2, \dots, v_r$. Let $v_i^j, i=1,2,\dots,r$ & $j=1,2,\dots,t$ be vertices corresponding to $v_1, v_2, v_3, \dots, v_r$ which are added in G to obtain $S^t(G)$ such that for every vertex v of G, where $1 \le i \le t$, v_i is adjacent to each vertex that is adjacent to v in G. Then second Zagreb matrix of $S^t(G)$, denoted by $SZ[S^t(G)]$ can be written as block matrix of form

$$\begin{pmatrix} (t+1)^2 & t+1 & t+1 & \dots & t+1 \\ t+1 & 0 & 0 & \dots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ t+1 & 0 & 0 & 0 & 0 \end{pmatrix}_{(t+1)\times(t+1)} \otimes SZ(G)$$

$= B \otimes SZ(G)$ where $B=(b_{ij})$

is the $(t+1)\times(t+1)$ matrix in which

$$(b_{ij}) = \begin{cases} (t+1)^2, & if\ i=j=1, \\ (t+1), & if\ i=1\ and\ j\neq 1, \\ (t+1), & if\ i\neq 1\ and\ j=1, \\ 0, & otherwise. \end{cases}$$

The characteristic polynomial of *B* along with its spectrum is given by

$x^{t-1}(x^2-(t+1)^2x-t(t+1)^2)$ and

$$\begin{pmatrix} 0 & \frac{(t+1)[(t+1)+\sqrt{t^2+6t+1}]}{2} & \frac{(t+1)[(t+1)-\sqrt{t^2+6t+1}]}{2} \\ t-1 & 1 & 1 \end{pmatrix}$$

respectively.

Hence spectrum of $SZ[S^t(G)]$ is

$$\begin{pmatrix} 0\mu_i & \left(\frac{(t+1)[(t+1)+\sqrt{t^2+6t+1}]}{2}\right)\mu_i & \left(\frac{(t+1)[(t+1)-\sqrt{t^2+6t+1}]}{2}\right)\mu_i \\ t-1 & 1 & 1 \end{pmatrix},$$

where $\mu_i, i=1,2,\ldots,r$ are the eigenvalues of $SZ(G)$. Hence by definition of second Zagreb energy, we get

$$\begin{aligned} &\mathscr{E}[SZ[S^t(G)]] \\ &= \sum_{i=1}^{r}\left|\left(\frac{(t+1)[(t+1)\pm\sqrt{t^2+6t+1}]}{2}\right)\mu_i\right| \\ &= \sum_{i=1}^{r}|\mu_i|\left|\frac{(t+1)[(t+1)\pm\sqrt{t^2+6t+1}]}{2}\right| \\ &= \sum_{i=1}^{r}|\mu_i|\Bigg(\frac{(t+1)[(t+1)+\sqrt{t^2+6t+1}]}{2} \\ &\quad + \frac{(t+1)[\sqrt{t^2+6t+1}-(t+1)]}{2}\Bigg) \\ &= (t+1)\sqrt{t^2+6t+1}\mathscr{E}[SZ(G)]. \end{aligned}$$

□

Corollary 5.7. *If G is the complete graph on r vertices, then*

$$\mathscr{E}[SZ(S^t(K_r))] = 2(r-1)^3(t+1)\sqrt{t^2+6t+1}.$$

Corollary 5.8. *Let G be the cycle graph of order r. Then*

$$\mathscr{E}[SZ(S^t(C_r))] = 8(t+1)\sqrt{t^2+6t+1}\sum_{j=0}^{r-1}\left|\cos\frac{2\pi j}{r}\right|.$$

Corollary 5.9. *If G is a complete bipartite graph, then*

$$\mathscr{E}[SZ(S^t(K_{r,r}))] = 2r^3(t+1)\sqrt{t^2+6t+1}.$$

Corollary 5.10. *If $K_{r,r,r}$ is a complete tripartite graph, then*

$$\mathscr{E}[SZ(S^t(K_{r,r,r}))] = 16r^3(t+1)\sqrt{t^2+6t+1}.$$

Theorem 5.11. *For any k-regular graph G, $\mathscr{E}[FZ(D^t(G))] = (t+1)^2\mathscr{E}[FZ(G)]$.*

Proof. The first Zagreb matrix of *t*-shadowgraph of *G*, denoted by $FZ[D^t(G)]$ can be written as a block matrix in the form $FZ[D^t(G)] = (t+1)J \otimes FZ(G)$, where J is the all ones matrix of order $(t+1)\times(t+1)$. The characteristic polynomial of $(t+1)J$ is given by $x^t(x-(t+1)^2)$. Hence, first Zagreb spectrum of *t*-shadow graph is $\begin{pmatrix} (t+1)^2\,\lambda_i & 0\lambda_i \\ 1 & t \end{pmatrix}$ where $\lambda_i,\ i=1,2,\ldots,r$ are eigenvalues of *FZ(G)*. Hence

$$\begin{aligned} \mathscr{E}[FZ(D^t(G))] &= \sum_{i=1}^{r}|(t+1)^2\lambda_i| \\ &= (t+1)^2\sum_{i=1}^{r}|\lambda_i| = (t+1)^2\mathscr{E}[FZ(G)]. \end{aligned}$$

□

Corollary 5.12. *If G is a complete graph on r vertices, then*

$$\mathscr{E}[FZ(D^t(K_r)] = 4(r-1)^2(t+1)^2.$$

Corollary 5.13. *Let G be a cycle graph of order r. Then*

$$\mathscr{E}[FZ(D^t(C_r))] = 8(t+1)^2\sum_{j=0}^{r-1}\left|\cos\frac{2\pi j}{r}\right|.$$

Corollary 5.14. *If $K_{r,r}$ is a complete bipartite graph, then*

$$\mathscr{E}[FZ(D^t(K_{r,r})] = 4r^2(t+1)^2.$$

Corollary 5.15. *If $K_{r,r,r}$ is a complete tripartite graph, then*

$$\mathscr{E}[FZ(S^t(K_{r,r,r})] = 16r^2(t+1)^2.$$

Theorem 5.16. *For any k-regular graph G, $\mathscr{E}[SZ(D^t(G))] = (t+1)^3\mathscr{E}[SZ(G)]$.*

Proof. The second Zagreb matrix of *t*-shadowgraph of *G*, denoted $SZ[D^t(G)]$ can written as block matrix

$$SZ[D^t(G)] = (t+1)^2J\otimes SZ(G).$$

Hence, spectrum of $(t+1)^2J$ is $\begin{pmatrix} (t+1)^3 & 0 \\ 1 & t \end{pmatrix}$. Therefore second Zagreb spectrum of *t*-shadow graph is $\begin{pmatrix} (t+1)^3\lambda_i & 0\lambda_i \\ 1 & t \end{pmatrix}$. Hence $\mathscr{E}[SZ(D^t(G))] = (t+1)^3\mathscr{E}[SZ(G)]$. □

Corollary 5.17. *If G is a complete graph on r vertices, then*

$$\mathscr{E}[SZ(D^t(K_r)] = 2(r-1)^3(t+1).^3$$

Corollary 5.18. *For a cycle graph C_r,*

$$\mathscr{E}[SZ(D^t(C_r))] = 8(t+1)^3\sum_{j=0}^{r-1}\left|\cos\frac{2\pi j}{r}\right|.$$

Corollary 5.19. *If $K_{r,r}$ is a complete bipartite graph, then*

$$\mathscr{E}[SZ(D^t(K_{r,r}))] = 2(t+1)^3r^3.$$

Corollary 5.20. *For the complete tripartite graph $K_{r,r,r}$,*

$$\mathscr{E}[SZ(S^t(K_{r,r,r}))] = 16r^3(t+1)^3 = (t+1)^3\mathscr{E}[SZ(K_{r,r})].$$

Theorem 5.21. *The first Zagreb energy of wheel graph, W_r, is given by*

$$\mathscr{E}[FZ(W_r)] > 2\sqrt{r^3 + 6r^2 + 9r + 36}.$$

Proof. It is known that spectrum of cycle graph C_r is $2\cos\left(\frac{2\pi j}{r}\right)$, $j = 0, 1, 2, \ldots, r-1$.

Consider the wheel graph W_r with vertices $v, v_1, v_2, \ldots, v_r$, v being central vertex, then first Zagreb matrix of W_r takes the form

$$A[FZ(W_r)] = \begin{pmatrix} 0 & (r+3)J_{1,r} \\ (r+3)J_{r,1} & 6A(C_r) \end{pmatrix},$$

where $J_{1,r} = (1\,1\,\ldots\,1\,1)$.

The characteristic equation of wheel graph is given as

$$(\lambda^2 - 12\lambda - r(r+3)^2)(\lambda^{r-1} + \lambda^{r-2} + \cdots + \lambda).$$

Let $\lambda_1, \lambda_2, \ldots, \lambda_{r+1}$ be roots of above characteristic equation. Then $6 \pm \sqrt{r^3 + 6r^2 + 9r + 36}$ be first two roots of the characteristic equation.

Since $|\lambda_1| + |\lambda_2| + \cdots + |\lambda_{r+1}| > |\lambda_1| + |\lambda_2|$, the first Zagreb energy of wheel graph is

$$\mathscr{E}[FZ(W_r)] > 2\sqrt{r^3 + 6r^2 + 9r + 36}.$$

□

Theorem 5.22. *The second Zagreb energy of wheel graph is given by $\mathscr{E}[SZ(W_r)] > 6\sqrt{r^3 + 9}$.*

Proof. The second Zagreb matrix of W_r is given by

$$\mathscr{E}[SZ(W_r)] = \begin{pmatrix} 0 & 3rJ_{1,r} \\ 3rJ_{r,1} & 9A(C_r) \end{pmatrix},$$

where

$J_{1,r} = (1\,1\,\ldots\,1\,1)$ and

$$A[C_r] = \begin{pmatrix} 0 & 1 & 0 & 0 & . & . & 0 & 1 \\ 1 & 0 & 1 & 0 & . & . & 0 & 0 \\ 0 & 1 & 0 & 1 & . & . & 0 & 0 \\ . & . & . & . & . & . & & . \\ . & . & . & . & . & . & & . \\ 0 & 0 & 0 & 0 & . & . & 0 & 1 \\ 1 & 0 & 0 & 0 & . & . & 1 & 0 \end{pmatrix}.$$

The characteristic equation of wheel graph is given as

$$(\lambda^2 - 18\lambda - 9r^3)(\lambda^{r-1} + \lambda^{r-2} + \cdots + \lambda).$$

This is polynomial of degree $r+1$ and $\lambda_1, \lambda_2, \ldots, \lambda_{r+1}$ be its roots. We can see two roots of characteristic equation λ_1 and λ_2 is $9 \pm 3\sqrt{r^3 + 9}$.

Also $|\lambda_1| + |\lambda_2| + \cdots + |\lambda_{r+1}| > |\lambda_1| + |\lambda_2|$

It is clear that second Zagreb energy of wheel graph is $\mathscr{E}[SZ(W_r)] > 6\sqrt{r^3 + 9}$. □

6 Zagreb energies of some non-regular graphs

In this section, we obtain the two Zagreb energies for Dutch windmill graph and Herschel graph.

Theorem 6.1. *Let G be Dutch windmill graph of cycle length 3. Then first Zagreb energy of G is $\mathscr{E}[FZ(G)] = 8r - 4 + 4\sqrt{1 + 2r(r+1)^2}$.*

Proof. Let $v_1, v_2, \ldots, v_{2r+1}$ be vertices of *G*. The first Zagreb adjacency matrix of *G* is

$$A[FZ(G)] = \begin{pmatrix} 0 & 2r+2 & 2r+2 & \ldots & 2r+2 \\ 2r+2 & 0 & 4 & \ldots & 0 \\ 2r+2 & 4 & 0 & \ldots & 0 \\ . & . & . & \ldots & . \\ . & . & . & \ldots & . \\ 2r+2 & . & . & \ldots & 4 \\ 2r+2 & 0 & 0 & \ldots & 0 \end{pmatrix}.$$

The characteristic polynomial of *G* takes the form $(x+4)^r(x-4)^{r-1}(x^2 - 4x - 8r(r+1)^2)$.

We can easily observe that the first Zagreb spectrum of *G* is

$$\begin{pmatrix} -4 & 4 & 2(1 \pm \sqrt{1 + 2r(r+1)^2}) \\ r & r-1 & 1 \end{pmatrix}$$

Hence by the definition of first Zagreb energy, we get

$$\mathscr{E}[FZ(G)] = |(-4)r| + |4(r-1)| + |(2 + 2\sqrt{1 + 2r(r+1)^2}) + (2\sqrt{1$$

$$= 8r - 4 + 4\sqrt{1 + 2r(r+1)^2}.$$

□

Theorem 6.2. *The second Zagreb energy of Dutch windmill graph G of cycle length 3 is*

$$\mathscr{E}[SZ(G)] = 8r - 4 + 4\sqrt{1 + 8r^3}.$$

Proof. The second Zagreb adjacency matrix of *G* with vertices $v_1, v_2, \ldots, v_{2r+1}$ takes the form

$$A[SZ(G)] = \begin{pmatrix} 0 & 4r & 4r & \ldots & 4r \\ 4r & 0 & 4 & \ldots & 0 \\ 4r & 4 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 4r & . & . & \ldots & 4 \\ 4r & 0 & 0 & \ldots & 0 \end{pmatrix}.$$

The characteristic polynomial of *G* is $(x+4)^r(x-4)^{r-1}(x^2 - 4x - 32r^3)$ and second Zagreb spectrum of *G* is

$$\begin{pmatrix} -4 & 4 & 2(1 \pm \sqrt{1 + 8r^3}) \\ r & r-1 & 1 \end{pmatrix}.$$

Therefore,

$$\mathscr{E}[SZ(G)] = |(-4)r| + |4(r-1)| + |(2 + 2\sqrt{1 + 8r^3}) + (2\sqrt{1 + 8r^3} - 2)|$$
$$= 8r - 4 + 4\sqrt{1 + 8r^3}.$$

□

Theorem 6.3. *The first Zagreb energy of Dutch windmill graph D_4^r is $\mathscr{E}[F(G)] > 8(r-1)\sqrt{2}$.*

Proof. The first Zagreb adjacency matrix of D_4^r is given by the following matrix of order $3r+1$.

$$\begin{pmatrix} 0 & 2(r+1) & 0 & 2(r+1) & 2(r+1) & 0 & \dots & 0 & 2(r+1) \\ 2(r+1) & 0 & 4 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 4 & 0 & 4 & 0 & 0 & \dots & 0 & 0 \\ 2(r+1) & 0 & 4 & 0 & 0 & 0 & \dots & 0 & 0 \\ 2(r+1) & 0 & 0 & 0 & 0 & 4 & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 4 \\ 2(r+1) & 0 & 0 & 0 & 0 & 0 & \dots & 4 & 0 \end{pmatrix}$$

.

The characteristic polynomial of above matrix takes the form $(x^2-32)^{r-1}(x^{r+3}+x^{r+1}+\cdots+x)$. Then $\pm 4\sqrt{2}$ is an eigenvalue with multiplicity $r-1$. Clearly all the other eigenvalues will be less than or equal to $4\sqrt{2}$. Hence $\mathscr{E}[FZ(D_4^r)] > 8(r-1)\sqrt{2}$. □

Theorem 6.4. *The second Zagreb energy of Dutch windmill graph D_4^r is*

$$\mathscr{E}[SZ(D_4^r)] = (2r-2)4\sqrt{2} + 2\sqrt{32(r+1)(r^2-r+1)}.$$

Proof. The second Zagreb adjacency matrix of D_4^r is

$$\begin{pmatrix} 0 & 4r & 0 & 4r & 4r & \dots & 4r \\ 4r & 0 & 4 & 0 & 0 & \dots & 0 \\ 0 & 4 & 0 & 4 & 0 & \dots & 0 \\ 4r & 0 & 4 & 0 & 0 & \dots & 0 \\ 4r & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 4r & 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}_{(3r+1)\times(3r+1)}.$$

The characteristic polynomial is

$$x^{r+1}(x^2-32)^{r-1}(x^2-32(r+1)(r^2-r+1)).$$

Therefore

$$\mathscr{E}[SZ(G)] = (2r-2)4\sqrt{2} + 2\sqrt{32(r+1)(r^2-r+1)}.$$

□

Theorem 6.5. *The first Zagreb energy of D_5^r is $\mathscr{E}[FZ(D_5^r)] = 8r\sqrt{5} - 4\sqrt{5} + \lambda$.*

Proof. The first Zagreb adjacency matrix of D_5^r is

$$\begin{pmatrix} 0 & 2(r+1) & 0 & 0 & 2(r+1) & \dots & 2(r+1) \\ 2(r+1) & 0 & 4 & 0 & 0 & \dots & 0 \\ 0 & 4 & 0 & 4 & 0 & \dots & 0 \\ 0 & 0 & 4 & 0 & 4 & \dots & 0 \\ 2(r+1) & 0 & 0 & 4 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2(r+1) & 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}.$$

Note that this matrix is of order $4r+1$. The characteristic polynomial is given by $(x^2-4x-16)^{r-1}(x^2+4x-16)^r(x^3-4x^2-8(r+2)(r^2+1)+32(r+1)(r^2+r))$.

Then, we can see that $2(1\pm\sqrt{5})$ (repeated $(r-1)$ times, $2(-1\pm\sqrt{5})$ (repeated r times). Let $\lambda_1, \lambda_2, \lambda_3$ be the remaining roots. Therefore, $\mathscr{E}[FZ(D_5^r)] = 8r\sqrt{5} - 4\sqrt{5} + |\lambda_1| + |\lambda_2| + |\lambda_3|$.

Hence, $\mathscr{E}[FZ(D_5^r)] = 8r\sqrt{5} - 4\sqrt{5} + \lambda$, where $\lambda = |\lambda_1| + |\lambda_2| + |\lambda_3|$. □

Theorem 6.6. *The second Zagreb energy of D_5^r is $\mathscr{E}[SZ(D_5^r)] = 8r\sqrt{5} - 4\sqrt{5} + \lambda$.*

Proof. The second Zagreb adjacency matrix of D_5^r is

$$\begin{pmatrix} 0 & 4r & 0 & 0 & 4r & \dots & 4r \\ 4r & 0 & 4 & 0 & 0 & \dots & 0 \\ 0 & 4 & 0 & 4 & 0 & \dots & 0 \\ 0 & 0 & 4 & 0 & 4 & \dots & 0 \\ 4r & 0 & 0 & 4 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 4r & 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}_{(4r+1)\times(4r+1)}.$$

The characteristic polynomial is $(x^2-4x-16)^{r-1}(x^2+4x-16)^r(x^3-4x^2-16(2r^3+1)+128r^3)$. Then the spectrum of G is given by $2(1\pm\sqrt{5})$ (recurring (r-1) times), $2(-1\pm\sqrt{5})$ (recurring r times) with the remaining eigenvalues named $\lambda_1, \lambda_2, \lambda_3$ that denote the roots of the cubic poynomial.

Hence, $\mathscr{E}[SZ(D_5^r)] = 8r\sqrt{5} - 4\sqrt{5} + \lambda$, where $\lambda = |\lambda_1| + |\lambda_2| + |\lambda_3|$. □

Theorem 6.7. *The first Zagreb energy of Herschel graph G is $\mathscr{E}[FZ(H(G))] = 20\sqrt{5} + 12\sqrt{3} + 28\sqrt{2}$.*

Proof. Consider Herschel graph with $v_1, v_2, \dots, v_{11}$ as vertices. Then the first Zagreb matrix is given as

$$A[FZ(G)] = \begin{pmatrix} 0 & 7 & 0 & 7 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 7 & 0 & 0 & 7 & 7 & 0 & 0 & 0 & 0 \\ 0 & 7 & 0 & 7 & 0 & 0 & 0 & 6 & 0 & 0 & 0 \\ 7 & 0 & 7 & 0 & 0 & 0 & 0 & 0 & 7 & 7 & 0 \\ 6 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 6 & 0 \\ 0 & 7 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 7 \\ 0 & 7 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 7 \\ 0 & 0 & 6 & 0 & 0 & 0 & 6 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 7 & 0 & 0 & 0 & 6 & 0 & 0 & 7 \\ 0 & 0 & 0 & 7 & 6 & 0 & 0 & 0 & 0 & 0 & 7 \\ 0 & 0 & 0 & 0 & 0 & 7 & 7 & 0 & 7 & 7 & 0 \end{pmatrix}_{(11\times11)}.$$

The first Zagreb spectrum of G along with its multiplicities is

$$\begin{pmatrix} -10\sqrt{5} & 10\sqrt{5} & -6\sqrt{3} & 6\sqrt{3} & -7\sqrt{2} & 7\sqrt{2} & 0 \\ 1 & 1 & 1 & 1 & 2 & 2 & 3 \end{pmatrix}.$$

Hence, first Zagreb Energy of Herschel graph is

$$\begin{aligned} \mathscr{E}[FZ(H(G))] &= |-10\sqrt{5}| + |10\sqrt{5}| \\ &\quad + |-6\sqrt{3}| + |6\sqrt{3}| + |2(-7\sqrt{2})| \\ &\quad + |2(7\sqrt{2})| + |3(0)|. \\ &= 20\sqrt{5} + 12\sqrt{3} + 28\sqrt{2}. \end{aligned}$$

□

Theorem 6.8. *The second Zagreb energy of Herschel graph G is* $\mathscr{E}[SZ(H(G))] = 6\sqrt{155} + 18\sqrt{3} + 48\sqrt{2}$.

Proof. The second Zagreb matrix is given as

$$\begin{pmatrix} 0 & 12 & 0 & 12 & 9 & 0 & 0 & 0 & 0 & 0 & 0 \\ 12 & 0 & 12 & 0 & 0 & 12 & 12 & 0 & 0 & 0 & 0 \\ 0 & 12 & 0 & 12 & 0 & 0 & 0 & 9 & 0 & 0 & 0 \\ 12 & 0 & 12 & 0 & 0 & 0 & 0 & 0 & 12 & 12 & 0 \\ 9 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 9 & 0 \\ 0 & 12 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 12 \\ 0 & 12 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 12 \\ 0 & 0 & 9 & 0 & 0 & 0 & 9 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 12 & 0 & 0 & 0 & 9 & 0 & 0 & 12 \\ 0 & 0 & 0 & 12 & 9 & 0 & 0 & 0 & 0 & 0 & 12 \\ 0 & 0 & 0 & 0 & 0 & 12 & 12 & 0 & 12 & 12 & 0 \end{pmatrix}_{(11\times 11)}.$$

with second Zagreb spectrum

$$\begin{pmatrix} -3\sqrt{155} & 3\sqrt{155} & -9\sqrt{3} & 9\sqrt{3} & -12\sqrt{2} & 12\sqrt{2} & 0 \\ 1 & 1 & 1 & 1 & 2 & 2 & 3 \end{pmatrix}.$$

Hence second Zagreb Energy of Herschel graph is

$$\mathscr{E}[SZ(H(G))] = 6\sqrt{155} + 18\sqrt{3} + 48\sqrt{2}.$$

□

7 Conclusion

Graph energies have been extensively studied in the literature, particularly in the realms of connected graphs, molecular graphs, and diverse graph operations. This paper focuses on a comparative analysis of the first and second Zagreb energies in the context of regular graphs. We establish a relationship between the first and second Zagreb energy specifically for the complete tripartite graph, along with a condition leading to an infinite set of non-isomorphic Zagreb equi-energeric graphs for all $r > 1$ within partite graphs. Our findings reveal that $\mathscr{E}[FZ(K_{r/2,r/2})] \leq \mathscr{E}[SZ(K_{r/2,r/2})]$ holds for all $r \geq 4$, and in the case where $r = 2$, $\mathscr{E}[FZ(K_{1,1})] > \mathscr{E}[SZ(K_{1,1})]$. Additionally, we demonstrate that the two Zagreb energies coincide solely for the graph $K_{r/2,r/2}$ if and only if $r = 2$. The paper also includes computations of the two Zagreb energies for various graph operations and specific graphs, along with establishing bounds on Zagreb energies for wheel graphs.

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