



Article More on Second Zagreb Energy of Graphs

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Abstract: Let *G* be a graph with *n* vertices. The second Zagreb energy of graph *G* is defined as the sum of the absolute values of the eigenvalues of the second Zagreb matrix of graph *G*. In this paper, we derive the relation between the second Zagreb matrix and the adjacency matrix of graph *G* and derive the new upper bound for the second Zagreb energy in the context of trace. We also derive the second Zagreb energy of *m*-splitting graph and *m*-shadow graph of a graph.

Keywords: Second Zagreb energy; *m*–splitting graph; *m*–shadow graph; regular graph.

MSC: 05C50.

1. Introduction

Let *G* be a simple, connected, and undirected graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$. The number of edges incident with vertex v_i is called the degree of v_i ; denoted by d_i . The adjacency matrix of graph *G* is a square symmetric matrix of order *n* whose (i, j)th entry is defined by

$$a_{ij} = \begin{cases} 1; & v_i v_j \in E(G). \\ 0; & otherwise \end{cases}$$

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are eigenvalues of graph *G*, then the energy of a graph *G* is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The concept of the energy of a graph was first introduced by Gutman[1] in 1978 and he showed the relation between the energy of a graph and the total π -electron energy of organic molecules.

Numerous graph energies like Laplacian energy, Randić energy, Harary energy, Distance energy and many more have created wide scope of research across the world. In [2], we find the survey of Graph Energies by Gutman and Boris Furtula. We refer to Bondy and Murty[3] for the standard terminology and notations related to graph theory and David W. Lewis[4] for Matrix theory.

N. J. Rad, A. Jahanbani and Gutman[5] defined first and second Zagreb energy, which also includes upper and lower bounds for some graph invariant.

Definition 1. [5] Let *G* be a simple graph with *n* vertices $v_1, v_2, ..., v_n$ and let d_i be the degree of $v_i, i = 1, 2, ..., n$. Then the first Zagreb matrix $\mathbf{Z}^{(1)}$ and second Zagreb matrix $\mathbf{Z}^{(2)}$ of a graph *G* are respectively defined as

$$\left(\mathbf{Z}^{(1)} \right)_{ij} = \begin{cases} d_i + d_j; & v_i v_j \in E(G). \\ 0; & otherwise \end{cases}$$
$$\left(\mathbf{Z}^{(2)} \right)_{ij} = \begin{cases} d_i d_j; & v_i v_j \in E(G). \\ 0; & otherwise \end{cases}$$

In this paper, we denote second Zagreb matrix as **Z** instead of $(\mathbf{Z}^{(2)})$ for convenience. If $\rho_1, \rho_2, \ldots, \rho_n$ are eigenvalues of second Zagreb matrix of graph *G*, then the second Zagreb energy of a graph *G* is defined as

$$ZE_{(2)}(G) = \sum_{i=1}^{n} |\rho_i|.$$

In [6], S.M. Sheikholeslami, A. Jahanbani and R. Khoeilar have determined some classes of Zagreb hyperenergetic, Zagreb borderenergetic, and Zagreb equienergetic graphs. Ramanna[7] have deduced the relation between Zagreb energy and edge-Zagreb energy of a graph *G* with minimum degree $\delta \ge 2$, along with some methods to construct (edge) Zagreb equienergetic graphs and proved the existence of (edge) Zagreb equienergetic graphs of order $n \ge 9$.

Definition 2. Let A, $B \in \mathbb{R}^{p \times q}$. Then the Kronecker product of A and B is defined as

$$A \otimes B = \begin{vmatrix} a_{11}B & a_{12}B & a_{13}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & a_{23}B & \dots & a_{2n}B \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & a_{m3}B & \dots & a_{mn}B \end{vmatrix}.$$

Proposition 3. Let $A, B \in \mathbb{R}^{p \times q}$ and λ be an eigenvalue of matrix A and μ be an eigenvalue of B, then $\lambda \mu$ is an eigenvalue of $A \otimes B$.

The remaining part in this paper is divided in two sections. In section 2, we derive properties of Zagreb matrix including the relation between energy of a graph G and its second Zagreb energy. In section 3, we evaluate the second Zagreb energy of *m*-splitting graph and *m*-shadow graph of graph G.

2. Properties of second Zagreb matrix

Theorem 4. Let Z and A(G) be second Zagreb and adjacency matrix of graph G respectively and D be the diagonal matrix of order n with diagonal entries d_i , the degree of vertex v_i of graph G then Z = DA(G)D.

Proof. Let $d_1, d_2, ..., d_n$ be the degrees of *n* vertices $v_1, v_2, ..., v_n$ of graph *G*. So, $n \times n$ diagonal matrix and adjacency matrix of *G* are respectively

$$D = \begin{bmatrix} d_1 & 0 & 0 & \dots & 0 \\ 0 & d_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & d_n \end{bmatrix} and A(G) = \begin{bmatrix} 0 & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & 0 & a_{23} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & 0 \end{bmatrix}$$

where,

$$a_{ij} = \begin{cases} 1 & ; vertices v_i and v_j are adjacent \\ 0 & ; otherwise \end{cases}$$

Now,

$$DA(G)D = \begin{bmatrix} d_1 & 0 & 0 & \dots & 0 \\ 0 & d_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & d_n \end{bmatrix} \begin{bmatrix} 0 & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & 0 & a_{23} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & 0 \end{bmatrix} \begin{bmatrix} d_1 & 0 & 0 & \dots & 0 \\ 0 & d_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & d_n \end{bmatrix}$$
$$= \begin{bmatrix} 0 & d_1 d_2 a_{12} & d_1 d_3 a_{13} & \dots & d_1 d_n a_{1n} \\ d_2 d_1 a_{21} & 0 & d_2 d_3 a_{23} & \dots & d_2 d_n a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d_n d_1 a_{n1} & d_n d_2 a_{n2} & d_n d_3 a_{n3} & \dots & 0 \end{bmatrix} = \begin{bmatrix} 0 & z_{12} & z_{13} & \dots & z_{1n} \\ z_{21} & 0 & z_{23} & \dots & z_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & z_{n3} & \dots & 0 \end{bmatrix} = \mathbf{Z}$$

where,

$$z_{ij} = \begin{cases} d_i d_j & ; vertices \ v_i \ and \ v_j \ are \ adjacent \\ 0 & ; otherwise \end{cases}.$$

Theorem 5. Let *G* be a graph with *n* vertices and let A(G) and **Z** be its adjacency and second Zagreb matrix respectively. If *G* possesses isolated vertex then $det(\mathbf{Z}) = det(A(G)) = 0$. If *G* does not possess isolated vertices then

$$det(\mathbf{Z}) = \prod_{i=1}^{n} d_i^2 det(A(G)).$$

Proof. If *G* has isolated vertices, then according to Theorem 4, both matrices A(G) and **Z** have at least one zero eigen value, and therefore their determinants are equal to zero.

If G does not possess isolated vertices, then from theorem 4,

$$\mathbf{Z} = DA(G)D.$$

$$det(\mathbf{Z}) = det(DA(G)D) = det(D)det(A(G))det(D) = \prod_{i=1}^{n} d_i^2 det(A(G)).$$

Theorem 6. Let G be the graph with n vertices and Z be second Zagreb metrix of graph G. Then

$$tr(\mathbf{Z}) = 0.$$

$$tr(\mathbf{Z}^{2}) = 2\sum_{i\sim j} d_{i}^{2} d_{j}^{2}.$$

$$tr(\mathbf{Z}^{3}) = 2\sum_{i\sim j} (d_{i}^{2} d_{j}^{2} \sum_{k\sim i, j} d_{k}^{2}).$$

$$tr(\mathbf{Z}^{4}) = \sum_{i=1}^{n} (\sum_{i\sim j} d_{i}^{2} d_{j}^{2})^{2} + \sum_{i\neq j} (d_{i}^{2} d_{j}^{2} \sum_{k\sim i, j} d_{k}^{2})^{2}.$$

Proof. By the definition of Zagreb second matrix, $tr(\mathbf{Z}) = 0$ Now, calculating for \mathbf{Z}^2 For i = j,

$$(\mathbf{Z}^2)_{ii} = \sum_{j=1}^n Z_{ij} Z_{ji} = \sum_{j=1}^n (Z_{ij})^2 = \sum_{i \sim j} (Z_{ij})^2 = \sum_{i \sim j} (d_i^2 d_j^2).$$

For $i \neq j$,

$$(\mathbf{Z}^2)_{ij} = \sum_{k=1}^n Z_{ik} Z_{kj} = Z_{ii} Z_{ij} + Z_{ij} Z_{jj} + \sum_{k \sim i,j} Z_{ik} Z_{kj} = d_i d_j \sum_{k \sim i,j} d_k^2.$$

Hence,

$$tr(\mathbf{Z}^{2}) = \sum_{i=1}^{n} \sum_{i \sim j} d_{i}^{2} d_{j}^{2} = 2 \sum_{i \sim j} d_{i}^{2} d_{j}^{2}.$$

The diagonal entries of \mathbf{Z}^3 are

$$(\mathbf{Z}^3)_{ii} = \sum_{j=1}^n Z_{ij}(\mathbf{Z}^2)_{jk} = \sum_{i \sim j} d_i d_j (\mathbf{Z}^2)_{ij} = \sum_{i \sim j} d_i^2 d_j^2 \Big(\sum_{k \sim i,j} d_k^2\Big).$$

Therefore,

$$tr(\mathbf{Z}^3) = \sum_{i=1}^n \sum_{i \sim j} d_i^2 d_j^2 \Big(\sum_{k \sim i, j} d_k^2 \Big) = 2 \sum_{i \sim j} d_i^2 d_j^2 \Big(\sum_{k \sim i, j} d_k^2 \Big).$$

For $tr(\mathbf{Z}^4)$, Let us define $\|\mathbf{Z}^2\|_F$ be the Frobenius norm of \mathbf{Z}^2 then

$$tr(\mathbf{Z}^4) = ||\mathbf{Z}^2||_F^2.$$

therefore,

$$tr(\mathbf{Z}^{4}) = \sum_{i,j=1}^{n} |(\mathbf{Z}^{2})_{ij}|^{2} = \sum_{i=j}^{n} |(\mathbf{Z}^{2})_{ij}|^{2} + \sum_{i\neq j}^{n} |(\mathbf{Z}^{2})_{ij}|^{2} = \sum_{i,j=1}^{n} \left(\sum_{i\sim j}^{n} d_{i}^{2} d_{j}^{2}\right)^{2} + \sum_{i\neq j}^{n} d_{i}^{2} d_{j}^{2} \left(\sum_{i,j\sim k}^{n} d_{k}^{2}\right)^{2}.$$

Theorem 7. Let G be a graph with n vertices. Then second Zagreb energy,

$$ZE_{(2)}(G) \leq \sqrt{2n\sum_{i\sim j} d_i^2 d_j^2}.$$

Here equality holds if and only if G is a graph having degree of each vertex either 0 or 1.

Proof. The variance of the numbers $|\rho_i|, i = 1, 2, ..., n$ is equal to

$$\frac{1}{n}\sum_{i=1}^{n}|\rho_{i}|^{2}-\left(\frac{1}{n}\sum_{i=1}^{n}|\rho_{i}|\right)^{2}\geq0.$$

where,

$$\sum_{i=1}^{n} |\rho_i|^2 = \sum_{i=1}^{n} \rho_i^2 = tr(\mathbf{Z}^2).$$

Thus,

$$\frac{1}{n}tr(\mathbf{Z}^2) - \left(\frac{1}{n}ZE_{(2)}(G)\right)^2 \ge 0 \iff ZE_{(2)}(G) \le \sqrt{2n\sum_{i \sim j}d_i^2d_j^2}$$

The above inequality follows from Theorem 6.

If *G* has no edges then $\rho_i = 0$, $\forall i = 1, 2, ..., n$ and therefore $ZE_{(2)}(G) = 0$. As there are no adjacent vertices, $\sum_{i \sim j} d_i^2 d_j^2 = 0$.

If *G* is a regular graph of degree one, then $\rho_i = \pm 1$ which implies that the variance of $|\rho_i|$, $\forall i = 1, 2, ..., n$, is zero. Therefore,

$$ZE_{(2)}(G) = \sqrt{2n\sum_{i\sim j}d_i^2d_j^2}$$

For all other graphs, the absolute value of eigenvalues of **Z** are not all equal. Therefore, the variance of $|\rho_i|$, $\forall i = 1, 2, ..., n$, is greater than zero, implying that

$$ZE_{(2)}(G) < \sqrt{2n\sum_{i\sim j}d_i^2d_j^2}.$$

Theorem 8. Let *G* be *r* > 0 regular graph then second Zagreb energy

$$ZE_{(2)}(G) = r^2 E(G).$$

Proof. If r = 0 then graph *G* has no edges and hence $d_i = 0$, where i = 1, 2, ..., n. So, $ZE_{(2)}(G)$ is a null matrix of order $n \times n$. Therefore $\rho_1 = \rho_2 = ... = \rho_n = 0$ and hence $ZE_{(2)}(G) = 0$.

If r > 0, i.e., $d_i = r$, where i = 1, 2, ..., n. Then all non-zero terms in $Z^{(2)}(G)$ are equal to r^2 , which implies $Z^{(2)}(G) = r^2 A(G)$. Therefore $\rho_i = r^2 \lambda_i$, where i = 1, 2, ..., n, which proves the theorem.

3. Second Zagreb energy of *m*-splitting graph and *m*-shadow graph of graph *G*

Definition 9. [8] The splitting graph S'(G) of a graph *G* is obtained by adding to each vertex *v* a new vertex v' such that v' is adjacent to every vertex that is adjacent to *v* in *G*.

Definition 10. [8] The *m*-splitting graph $Spl_m(G)$ of a graph *G* is obtained by adding to each vertex *v* of *G* new *m* vertices, say $v^1, v^2, v^3, \ldots, v^m$ such that $v^i, 1 \le i \le m$ is adjacent to each vertex that is adjacent to *v* in *G*.

The adjacency matrix of m-splitting graph of graph G is

 $\begin{bmatrix} A(G) & A(G) & A(G) & \dots & A(G) \\ A(G) & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A(G) & 0 & 0 & \dots & 0 \end{bmatrix}_{(m+1)p}$

Theorem 11. Let G be a simple graph with p non isolated vertices. Then

$$ZE_{(2)}(Spl_m(G)) = (m+1)\sqrt{m^2 + 6m + 1} ZE_{(2)}(G).$$

Proof. Let *G* be a simple graph with *p* non isolated vertices then from theorem 4, the second Zagreb matrix of *m*-splitting graph of graph *G* with order p(m+1) is $Z_{(2)}(Spl_m(G))$

$$= \begin{bmatrix} (m+1)D & 0 & 0 & \dots & 0 \\ 0 & D & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & D \end{bmatrix} \begin{bmatrix} A(G) & A(G) & A(G) & \dots & A(G) \\ A(G) & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A(G) & 0 & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} (m+1)D & 0 & 0 & \dots & 0 \\ 0 & D & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & D \end{bmatrix}$$
$$= \begin{bmatrix} (m+1)DA(G)(m+1)D & (m+1)DA(G)D & (m+1)DA(G)D & \dots & (m+1)DA(G)D \\ (m+1)DA(G)D & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (m+1)DA(G)D & 0 & 0 & \dots & 0 \end{bmatrix}$$
$$= \begin{bmatrix} (m+1) & 1 & 1 & \dots & 1 \\ 1 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \dots & 0 \end{bmatrix}_{(m+1)}^{(m+1)} \otimes (m+1)DA(G)D$$
$$where B = \begin{bmatrix} (m+1) & 1 & 1 & \dots & 1 \\ 1 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \dots & 0 \end{bmatrix}_{(m+1)}^{(m+1)}$$

Then the distinct eigen values of *B* are

$$\lambda_1 = \frac{1}{2} \Big(\sqrt{(m+1)^2 + 4m} - (m+1) \Big), \ \lambda_2 = \frac{1}{2} \Big(\sqrt{(m+1)^2 + 4m} + (m+1) \Big), \ \lambda_3 = 0.$$

So, Spec(B) =
$$\begin{pmatrix} 0 & \frac{1}{2} \Big(\sqrt{(m+1)^2 + 4m} - (m+1) \Big) & \frac{1}{2} \Big(\sqrt{(m+1)^2 + 4m} + (m+1) \Big) \\ m-1 & 1 & 1 \end{pmatrix}.$$

Thus, the Zagreb second spectrum of the m-splitting graph of G is

$$Z^{(2)}Spec(Spl_m(G)) = \begin{pmatrix} 0 & \frac{\rho_i(m+1)}{2}(\sqrt{(m+1)^2 + 4m} \pm (m+1)) \\ p(m-1) & 2p \end{pmatrix}.$$

Therefore, the Zagreb second energy of m-splitting graph of graph G is

$$ZE_{(2)}(Spl_m(G)) = (m+1)\sqrt{m^2 + 6m + 1} ZE_{(2)}(G).$$

Definition 12. [8] Let *G* be a simple graph with *p* vertices. Then *m*-shadow graph $D_m(G)$ of a connected graph *G* is obtained by taking *m* copies of *G* say $G_1, G_2, ..., G_m$ and joining each vertex *u* in G_i to the neighbours of the corresponding vertex *v* in G_j where $1 \le i, j \le m$.

The adjacency matrix of the *m*-shadow graph of graph *G* is

 $\begin{bmatrix} A(G) & A(G) & A(G) & \dots & A(G) \\ A(G) & A(G) & A(G) & \dots & A(G) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A(G) & A(G) & A(G) & \dots & A(G) \end{bmatrix}_{mp} .$

Theorem 13. Let G be a simple graph with p non isolated vertices. Then

$$ZE_{(2)}(D_m(G)) = m^3 ZE_{(2)}(G)$$

Proof. Let *G* be a simple graph with *p* non isolated vertices then from theorem 4, the second Zagreb matrix of *m*-shadow graph of graph *G* with order *pm* is $Z_{(2)}(D_m(G))$

$$= \begin{bmatrix} mD & 0 & 0 & \dots & 0 \\ 0 & mD & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & mD \end{bmatrix} \begin{bmatrix} A(G) & A(G) & A(G) & \dots & A(G) \\ A(G) & A(G) & A(G) & \dots & A(G) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A(G) & A(G) & A(G) & \dots & A(G) \end{bmatrix} \begin{bmatrix} mD & 0 & 0 & \dots & 0 \\ 0 & mD & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & mD \end{bmatrix}$$
$$= \begin{bmatrix} mDA(G)mD & mDA(G)mD & mDA(G)mD & \dots & mDA(G)mD \\ mDA(G)mD & mDA(G)mD & mDA(G)mD & \dots & mDA(G)mD \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ mDA(G)mD & mDA(G)mD & mDA(G)mD & \dots & mDA(G)mD \end{bmatrix}_{pm}$$
$$= \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix}_{m} \otimes m^{2}DA(G)D$$
$$= J_{m} \otimes m^{2}DA(G)D.$$

The distinct eigen values of J_m are m and 0.

$$So, Spec(J_m) = \begin{pmatrix} 0 & m \\ m-1 & 1 \end{pmatrix}.$$

Thus, the Zagreb second spectrum of the m-shadow graph of G is

$$Z_{(2)}Spec(D_m(G)) = \begin{pmatrix} 0 & m^3\rho_1 & m^3\rho_2 & \dots & m^3\rho_p \\ p(m-1) & p & p & \dots & p \end{pmatrix}.$$

Therefore, the Zagreb second energy of m-shadow graph of graph G is

$$ZE_{(2)}(D_m(G)) = m^3 ZE_{(2)}(G).$$

4. Conclusion

The energy of a graph is one of the emerging concepts in graph theory which serves as a frontier between chemistry and mathematics. The adjacency matrix of any graph *G* has been related to its second Zagreb matrix. Various bounds can be evaluated using the upper bound of the second Zagreb energy which is derived in this paper. We also compute the second Zagreb energy of m-splitting graph and m-shadow graph.

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