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Research Article

New Results on Zagreb Energy of Graphs

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Let G be a graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$, and let d_i be the degree of v_i. The Zagreb matrix of G is the square matrix of order n whose (i, j)-entry is equal to $d_i + d_j$ if the vertices v_i and v_j are adjacent, and zero otherwise. The Zagreb energy $\mathrm{ZE}(G)$ of G is the sum of the absolute values of the eigenvalues of the Zagreb matrix. In this paper, we determine some classes of Zagreb hyperenergetic, Zagreb borderenergetic, and Zagreb equienergetic graphs.

1. Introduction

In this paper, G is a simple undirected graph, with vertex set $V = V(G)$ and edge set $E = E(G)$. The integers $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$ are the *order* and the *size* of the graph G, respectively. For a vertex $v \in V$, the *open neighborhood* of v is the set $N(v) = \{u \in V | uv \in E\}$ and the *degree* of v is $d(v) = |N(v)|$. We write P_n, C_n, and K_n for the path, cycle, and complete graph of order n, respectively. A *bipartite* graph is a graph such that its vertex set can be partitioned into two sets X and Y (called the partite sets) such that every edge meets both X and Y. A *complete bipartite graph* is a bipartite graph such that any vertex of a partite set is adjacent to all vertices of the other partite set. A complete bipartite graph with partite set of cardinalities p and q is denoted by $K_{p,q}$. The complement $\overline{G}$ of G is the simple graph whose vertex set is V and whose edges are the pairs of nonadjacent vertices of G. The line graph of a graph G, written $L(G)$, is the graph whose vertices are the edges of G, with $ef \in E(L(G))$ when $e = uv$ and $f = vw$ in G. The line graph $L(G)$ of a r-regular graph G with n vertices is $(2r-2)$-regular with $nr/2$ vertices.

For each vertex v of a graph G, take a new vertex v' and join v' to all vertices of G adjacent to v. The graph $S'(G)$ thus obtained is called the splitting graph of G. The *cocktail party graph* $\mathrm{CP}(a)$ (for $a \geq 3$) is a graph obtained from the complete graph K_{2a} by deleting a perfect matching.

Any graph on n vertices, with $n \geq 2$, has at least two vertices with the same degree. The graphs with at most two vertices with the same degree are called *antiregular*; for more information, see [1, 17]. For any positive integer n, there exists only one connected antiregular graph on n vertices, denoted by A_n (see Figure 1).

The adjacency matrix $A(G)$ of G is defined by its entries as $a_{ij} = 1$ if $v_i v_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ denote the eigenvalues of $A(G)$. The energy of the graph G is defined as

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

where λ_i, $i = 1, 2, \ldots, n$, are the eigenvalues of graph G.

This concept was introduced by Gutman and is intensively studied in chemistry, since it can be used to approximate the total π-electron energy of a molecule (see, e.g., [8, 9]). Since then, numerous other bounds for $\mathscr{E}$ were found (see, e.g., [11–14]).

The Zagreb indices are widely studied degree-based topological indices and were introduced by Gutman and Trinajstić [7] in 1972. The *Zagreb matrix* of a graph G is a

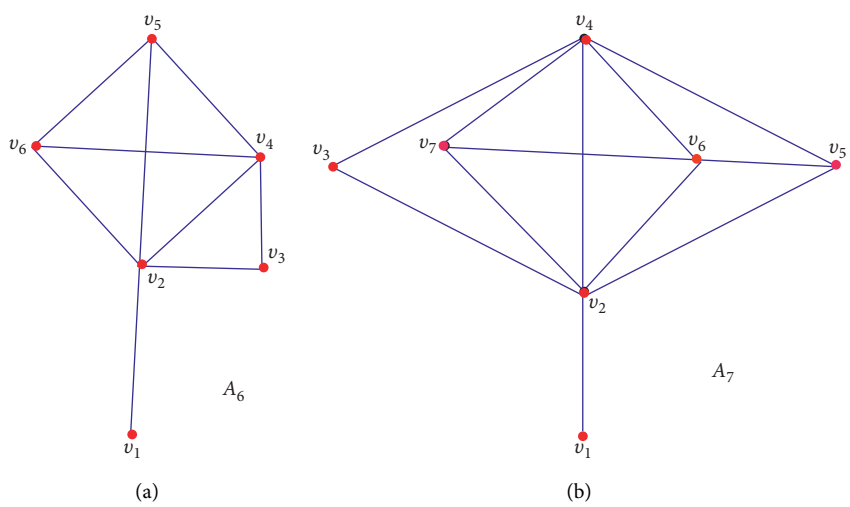

Figure 1: Two antiregular graph with vertices $n = 6$ and $n = 7$.

square matrix $A_z(G) = [m_{ij}]$ of order n, defined in [10], as follows:

$$m_{ij} = \begin{cases} d_i + d_j, & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

The eigenvalues of $A_z(G)$ labeled as $z_1 \geqslant z_2 \geqslant \ldots \geqslant z_n$ are said to be the Zagreb eigenvalues or A_z-eigenvalues of G and their collection is called Zagreb spectrum or A_z-spectrum of G.

If $z_1, z_2, \ldots, z_s$ are the distinct Zagreb eigenvalues of G having the multiplicities $m_1, m_2, \ldots, m_s$, then the Zagreb spectrum of G is denoted as

$$\operatorname{Spec}(A_z) = \begin{pmatrix} z_1 & z_2 & \ldots & z_s \\ m_1 & m_2 & \ldots & m_s \end{pmatrix}, \tag{3}$$

where $m_1 + m_2 + \cdots + m_s = n$.

The sum of all absolute Zagreb eigenvalues is the Zagreb energy denoted by $\mathrm{ZE}(G)$ and defined in [10] as follows:

$$\mathrm{ZE} = \mathrm{ZE}(G) = \sum_{i=1}^{n} |z_i|. \tag{4}$$

Now, we prove the next lemma that will be needed to obtain our results.

Lemma 1. *For a complete graph K_n, the Zagreb eigenvalues are $-2(n-1)$ and $2(n-1)^2$ with multiplicities $(n-1)$ and 1, respectively, and $ZE(K_n) = 4(n-1)^2$.*

Proof. Let G be a graph with vertices $v_1, v_2, v_3, \ldots, v_n$. Then, the Zagreb matrix is as follows:

$$A_z(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_p \end{array} \begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & \ldots & v_p \end{array} \\ \begin{pmatrix} 0 & d_1+d_2 & d_1+d_3 & \ldots & d_1+d_n \\ d_2+d_1 & 0 & d_2+d_3 & \ldots & d_2+d_n \\ d_3+d_1 & d_3+d_2 & 0 & \ldots & d_3+d_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d_n+d_1 & d_n+d_2 & d_n+d_3 & \ldots & 0 \end{pmatrix} \end{array}. \tag{5}$$

Since, K_n is a regular graph of degree $n-1$, we have

$$A_z(K_n) = \begin{bmatrix} 0 & 2n-2 & 2n-2 & \ldots & 2n-2 \\ 2n-2 & 0 & 2n-2 & \ldots & 2n-2 \\ 2n-2 & 2n-2 & 0 & \ldots & 2n-2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 2n-2 & 2n-2 & 2n-2 & \ldots & 0 \end{bmatrix}. \tag{6}$$

It can be easily seen that the Zagreb spectrum of K_n is as follows:

$$\operatorname{Spec} A_z(K_n) = \begin{pmatrix} 2(n-1)^2 & -2(n-1) \\ 1 & n-1 \end{pmatrix}. \tag{7}$$

Therefore, by the definition of the Zagreb energy, we have

$$\mathrm{ZE}(K_n) = 4(n-1)^2. \tag{8}$$

Gutman [5] introduced energy in 1978 and conjectured that the complete graph K_n possesses the maximum energy among all graphs with n vertices. Gutman [6] also proved this to be false leading to the new concept of hyperenergetic graphs.

A graph is *hyperenergetic* [6] if $\mathscr{E}(G) > 2n-2$, *non-hyperenergetic* if $\mathscr{E}(G) < 2n-2$, and *broderenergetic* [4] (other than K_n) if $\mathscr{E}(G) = 2n-2$. If $\mathscr{E}(G) = \mathscr{E}(H)$, then graphs G and H are *equienergetic* [2].

Following the above ideas, a graph G of order n is said to be *Zagreb hyperenergetic* if $\mathrm{ZE}(G) > 4(n-1)^2$, *Zagreb non-hyperenergetic* if $\mathrm{ZE}(G) < 4(n-1)^2$, and *Zagreb broderenergetic* (other than K_n) if $\mathrm{ZE}(G) = 4(n-1)^2$. If $\mathrm{ZE}(G) = \mathrm{ZE}(H)$, then two graphs G and H are called *Zagreb equienergetic*.

In [10], the authors obtained some lower and upper bounds for Zagreb energy, Das [3] presented some new bounds for Zagreb energy, Rakshith [16] discussed the new bounds for Zagreb energy, and Jahanbani et al. [15] obtained new bounds for Zagreb energy.

In this paper, we study the Zagreb energy of line graphs, Zagreb energy of complement graphs, and Zagreb hyperenergetic, Zagreb borderenergetic, and Zagreb equienergetic graphs. □

2. Main Results

In this section, we provide Zagreb energy of complement $\overline{G}$ and Zagreb energy of line graph $L(G)$ of a graph G, and furthermore, we develop results to determine the nature of graphs like complement $\overline{G}$, line graph $L(G)$, and splitting graph $S'(G)$ to be Zagreb hyperenergetic and Zagreb borderenergetic.

We start with the following proposition that helps us to obtain our results.

Proposition 1. *Let G be an r-regular graph ($r \geq 3$) of order n with Zagreb eigenvalues $z_1 \geqslant z_2 \geqslant \ldots \geqslant z_n$. The Zagreb eigenvalues of $A_z(\overline{G})$ are $2(n-r-1)^2$ with multiplicity one and $2(n-r-1)(-z_i/2r-1)$, for $i = 2, 3, \ldots, n$.*

Theorem 1. *Let G be an r-regular graph ($r \geq 3$) of order n with Zagreb eigenvalues $z_1 \geqslant z_2 \geqslant \ldots \geqslant z_n$. The Zagreb energy of complement $\overline{G}$ is*

$$\mathrm{ZE}(\overline{G}) = 2(n-r-1)\left(|(n-r-1)| + \left|\sum_{i=2}^{n}\left(\frac{-z_i}{2r}-1\right)\right|\right). \tag{9}$$

Proof. Since G is r-regular, the complement $\overline{G}$ is $(n-r-1)$-regular. By Equality (4) and Proposition 1, we obtain

$$\begin{aligned}\mathrm{ZE}(\overline{G}) &= 2|(n-r-1)(n-r-1)| \\ &\quad + \left|\sum_{i=2}^{n} 2(n-r-1)\left(\frac{-z_i}{2r}-1\right)\right| \\ &= 2(n-r-1)\left(|(n-r-1)| + \left|\sum_{i=2}^{n}\left(\frac{-z_i}{2r}-1\right)\right|\right).\end{aligned} \tag{10}$$

□

Theorem 2. *For an r-regular graph G of order n, the complement $\overline{G}$ is Zagreb non-hyperenergetic if $r \geq 3$.*

Proof. From Equality (10), we have

$$\mathrm{ZE}(\overline{G}) = 2(n-r-1)\left(|(n-r-1)| + \left|\sum_{i=2}^{n}\left(\frac{-z_i}{2r}-1\right)\right|\right). \tag{11}$$

It is easy to verify that

$$2(n-r-1)\left(|(n-r-1)| + \left|\sum_{i=2}^{n}\left(\frac{-z_i}{2r}-1\right)\right|\right) < 4(n-1)^2. \tag{12}$$

Hence, the complement $\overline{G}$ is a Zagreb non-hyperenergetic graph. □

Proposition 2. *Let G be an r-regular graph ($r \geq 3$) of order n with Zagreb eigenvalues $z_1 \geqslant z_2 \geqslant \ldots \geqslant z_n$. The Zagreb eigenvalues of $A_z(L(G))$ are $(8-8r)$ with multiplicity $n(r-2)/2$ and $4(r-1)(z_i/2r+r-2)$ for $i = 1, 2, \ldots, n$.*

Theorem 3. *Let G be an r-regular graph ($r \geq 3$) of order n with Zagreb eigenvalues $z_1 \geqslant z_2 \geqslant \ldots \geqslant z_n$. The Zagreb energy of line graph $L(G)$ is*

$$\begin{aligned}\mathrm{ZE}(L(G)) &= 4(r-1)\left|\sum_{i=1}^{n}\left(\frac{z_i}{2r}+r-2\right)\right| \\ &\quad + |8-8r|\left(\frac{n(r-2)}{2}\right).\end{aligned} \tag{13}$$

Proof. The line graph $L(G)$ of a r-regular graph G is a $(2r-2)$-regular graph of order $nr/2$. By definition of Zagreb energy and Proposition 2, we have

$$\begin{aligned}\mathrm{ZE}(L(G)) &= \left|\sum_{i=1}^{n} 4(r-1)\left(\frac{z_i}{2r}+r-2\right)\right| \\ &\quad + |(8-8r)|\left(\frac{n(r-2)}{2}\right) \\ &= 4(r-1)\left|\sum_{i=1}^{n}\left(\frac{z_i}{2r}+r-2\right)\right| \\ &\quad + |(8-8r)|\left(\frac{n(r-2)}{2}\right).\end{aligned} \tag{14}$$

□

Theorem 4. *Let G be an r-regular graph ($r \geq 3$) of order n different from K_2 and K_3. Then, $L(G)$ is Zagreb non-hyperenergetic.*

Proof. Applying Theorem 3, we have

$$\mathrm{ZE}(L(G)) = 4(r-1)\left|\sum_{i=1}^{n}\left(\frac{z_i}{2r}+r-2\right)\right| + |(8-8r)|\left(\frac{n(r-2)}{2}\right). \tag{15}$$

It is not hard to see that

$$4(r-1)\left|\sum_{i=1}^{n}\left(\frac{z_i}{2r}+r-2\right)\right| + |(8-8r)|\left(\frac{n(r-2)}{2}\right) < 4\left(\frac{nr}{2}-1\right)^2. \tag{16}$$

Thus, $L(G)$ is a Zagreb non-hyperenergetic graph. □

Remark 1. Note that the graphs K_2 or K_3 are Zagreb borderenergetic.

Example 1. The antiregular graphs A_6 and A_7 illustrated in Figure 1 are non-hyperenergetic.

Let A_6 be a graph with vertices v_1, v_2, v_3, v_4, v_5, and v_6. The Zagreb matrix of A_6 is

$$A_z(A_6) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{array} \begin{array}{c} \begin{array}{cccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \end{array} \\ \begin{pmatrix} 0 & 6 & 0 & 0 & 0 & 0 \\ 6 & 0 & 7 & 9 & 8 & 8 \\ 0 & 7 & 0 & 6 & 0 & 0 \\ 0 & 9 & 6 & 0 & 7 & 7 \\ 0 & 8 & 0 & 7 & 0 & 6 \\ 0 & 8 & 0 & 7 & 6 & 0 \end{pmatrix} \end{array}. \tag{17}$$

Therefore, the Zagreb spectrum of A_6 is as follows:

$$\mathrm{Spec}A_z(A_6)) = \begin{pmatrix} 25.02 & 2.339 & 1.087 & -6 & -13.149 & -9.297 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}. \tag{18}$$

By the definition of the Zagreb energy, we have

$$\mathrm{ZE}(A_6) = 56.892. \tag{19}$$

Analogously, we can see that

$$A_z(A_7) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \end{array} \begin{array}{c} \begin{array}{ccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 \end{array} \\ \begin{pmatrix} 0 & 7 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 9 & 11 & 9 & 19 & 9 \\ 0 & 9 & 0 & 7 & 0 & 0 & 0 \\ 0 & 11 & 7 & 0 & 8 & 9 & 8 \\ 0 & 9 & 0 & 8 & 0 & 7 & 0 \\ 0 & 10 & 0 & 9 & 7 & 0 & 7 \\ 0 & 9 & 0 & 8 & 0 & 7 & 0 \end{pmatrix} \end{array}. \tag{20}$$

Therefore, the Zagreb spectrum of A_7 is as follows:

$$\mathrm{Spec}A_z(A_7)) = \begin{pmatrix} 34.501 & -17.57 & 3.189 & -11.737 & 1.094 & -9.477 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}. \tag{21}$$

Hence, by the definition of the Zagreb energy, we have

$$\mathrm{ZE}(A_7) = 77.568. \tag{22}$$

By definition and Equalities (19) and (22), we deduce that A_6 and A_7 are non-hyperenergetic.

2.1. Some Classes of Zagreb Hyperenergetic and Zagreb Equienergetic Graphs. This section contributes some results towards Zagreb hyperenergetic and Zagreb equienergetic graphs.

Theorem 5. *For a regular graph G, the splitting graph $S'(G)$ is a Zagreb hyperenergetic graph.*

Proof. Let G be a graph with vertices $v_1, v_2, v_3, \ldots, v_p$. Then, the Zagreb matrix is as follows:

$$A_z(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_p \end{array} \begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & \ldots & v_p \end{array} \\ \begin{pmatrix} 0 & d_1+d_2 & d_1+d_3 & \ldots & d_1+d_p \\ d_2+d_1 & 0 & d_2+d_3 & \ldots & d_2+d_p \\ d_3+d_1 & d_3+d_2 & 0 & \ldots & d_3+d_p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d_p+d_1 & d_p+d_2 & d_p+d_3 & \ldots & 0 \end{pmatrix} \end{array}. \tag{23}$$

Let $v_1', v_2', v_3', \ldots, v_p'$ be the vertices added in G corresponding to $v_1, v_2, v_3, \ldots, v_p$ to obtain $S'(G)$ such that $N(v_i) = N(v_i')$. Note that the degree of v_i' is d_i. Then, the

Zagreb matrix of $S'(G)$ can be written as a block matrix as follows:

$$A_z(S'(G)) = \begin{bmatrix} 2A_z(G) & \frac{3}{2}A_z(G) \\ \frac{3}{2}A_z(G) & 0 \end{bmatrix} \tag{24}$$

or

$$A_z(S'(G)) = \begin{bmatrix} 2 & \frac{3}{2} \\ \frac{3}{2} & 0 \end{bmatrix} \otimes A_z(G). \tag{25}$$

Therefore, the Zagreb spectrum of $S'(G)$ is as follows

$$\mathrm{Spec}A_z(S'(G))) = \begin{pmatrix} \left(\frac{2-\sqrt{13}}{2}\right)z_i & \left(\frac{2+\sqrt{13}}{2}\right)z_i \\ p & p \end{pmatrix}, \tag{26}$$

where z_i for $i = 1, 2, 3, \ldots, p$ are the eigenvalues of $A_z(G)$ and $2 \pm \sqrt{13}/2$ are the eigenvalues of $\begin{bmatrix} 2 & 3/2 \\ 3/2 & 0 \end{bmatrix}$. Therefore, by the definition of the Zagreb energy, we can write

$$\begin{aligned} \mathrm{ZE}(S'(G)) &= \sum_{i=1}^{p} \left| \left(\frac{2-\sqrt{13}}{2}\right) z_i \right| \\ &= \sum_{i=1}^{p} |z_i| \left(\frac{2-\sqrt{13}}{2} + \frac{2+\sqrt{13}}{2}\right) \\ &= 2\mathrm{ZE}(G). \end{aligned} \tag{27}$$

Hence, we have

$$\mathrm{ZE}(S'(G)) = 2\mathrm{ZE}(G). \tag{28}$$

Equality (28) gives the desired result. □

Theorem 6. *For $n \geq 3$, $ZE(K_n) = ZE(K_{n-1,n-1})$.*

Proof. Consider the complete graph K_n and the complete bipartite graph $K_{n-1,n-1}$ for $n \geq 3$. The Zagreb spectrum of K_n is

$$\mathrm{Spec}A_z(K_n) = \begin{pmatrix} 2(n-1)^2 & -2(n-1) \\ 1 & n-1 \end{pmatrix}. \tag{29}$$

Therefore, by the definition of Zagreb energy, we have

$$\mathrm{ZE}(K_n) = 2(n-1)^2 + |-2(n-1)|(n-1) = 4(n-1)^2. \tag{30}$$

On the other hand, the Zagreb spectrum of $K_{n-1,n-1}$ is

$$\mathrm{Spec}A_z(K_{n-1,n-1}) = \begin{pmatrix} 0 & 2(n-1)^2 & 2(n-1)(1-n) \\ 2n-4 & 1 & 1 \end{pmatrix}. \tag{31}$$

By the definition of Zagreb energy, we can write

$$\mathrm{ZE}(K_{n-1,n-1}) = 2(n-1)^2 + |2(1-n)|(n-1) = 4(n-1)^2. \tag{32}$$

Thus, from Equalities (30) and (32), the required result follows. □

Theorem 7. *For $a \geq 3$, $ZE(K_{2a-1}) = ZE(CP(a))$.*

Proof. The Zagreb spectrum of the complete graph K_{2a-1} is

$$\mathrm{Spec}A_z(K_{2a-1}) = \begin{pmatrix} 8(a-1)^2 & -4(a-1) \\ 1 & 2(a-1) \end{pmatrix}. \tag{33}$$

Also, the Zagreb spectrum of the cocktail party graph $\mathrm{CP}(a)$ is

$$\mathrm{Spec}A_z(\mathrm{CP}(a)) = \begin{pmatrix} -8(a-1) & 8(a-1)^2 \\ (a-1) & 1 \end{pmatrix}. \tag{34}$$

Therefore,

$$\mathrm{ZE}(K_{2a-1}) = 8(a-1)^2 + |8(1-a)|(a-1) = 16(a-1)^2, \tag{35}$$

$$\mathrm{ZE}(\mathrm{CP}(a)) = 8(a-1)^2 + |-8(a-1)|(a-1) = 16(a-1)^2. \tag{36}$$

Now, Equalities (35) and (36) lead to the result. □

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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