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 \( d_v \) be the degree of \( v_i \). The Zagreb matrix \( G \) 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 \( ZE(G) \) 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 \( N(v) = \{u \in V \mid uv \in E\} \) 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 \( CP(a) \) (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 \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \) denote the eigenvalues of \( A(G) \). The energy of the graph \( G \) is defined as

\[
\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|, \tag{1}
\]

where \( \lambda_i, i = 1, 2, \ldots, n, \) 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 \( \pi \)-electron energy of a molecule (see, e.g., [8, 9]). Since then, numerous other bounds for \( \mathcal{E} \) 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
square matrix \( A_z(G) = [m_{ij}] \) of order \( n \), defined in [10], as follows:

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

(2)

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

If \( z_1, z_2, \ldots, z_n \) are the distinct Zagreb eigenvalues of \( G \) having the multiplicities \( m_1, m_2, \ldots, m_n \), then the Zagreb spectrum of \( G \) is denoted as

\[
\text{Spec}(A_z) = \begin{pmatrix} z_1 & z_2 & \ldots & z_n \\
m_1 & m_2 & \ldots & m_n \end{pmatrix},
\]

(3)

where \( m_1 + m_2 + \ldots + m_n = n \).

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

\[
\text{ZE} = \text{ZE}(G) = \sum_{i=1}^{n} |z_i|.
\]

(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 \( \text{ZE}(K_n) = 4(n-1)^2 \).

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

\[
A_z(G) = \begin{pmatrix} 
    v_1 & v_2 & v_3 & \ldots & v_p \\
v_1 & 0 & d_1 + d_2 & d_1 + d_3 & \ldots & d_1 + d_n \\
v_2 & d_2 + d_1 & 0 & d_2 + d_3 & \ldots & d_2 + d_n \\
v_3 & d_3 + d_1 & d_3 + d_2 & 0 & \ldots & d_3 + d_n \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
v_p & d_n + d_1 & d_n + d_2 & d_n + d_3 & \ldots & 0
\end{pmatrix}.
\]

(5)

Since, \( K_n \) is a regular graph of degree \( n-1 \), we have

\[
A_z(K_n) = \begin{pmatrix} 
    0 & 2n-2 & 2n-2 & \ldots & 2n-2 \\
2n-2 & 0 & 2n-2 & \ldots & 2n-2 \\
2n-2 & 2n-2 & 0 & \ldots & 2n-2 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
2n-2 & 2n-2 & 2n-2 & \ldots & 0
\end{pmatrix}.
\]

(6)

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

\[
\text{Spec}_{A_z}(K_n) = \begin{pmatrix} 
    2(n-1)^2 & -2(n-1) & \ldots & \ldots & 1 \\
    \ldots & \ldots & \ldots & \ldots & \ldots \\
    2(n-1)^2 & -2(n-1) & \ldots & \ldots & 1 \\
\end{pmatrix}.
\]

(7)

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

\[
\text{ZE}(K_n) = 4(n-1)^2.
\]

(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 $E(G) > 2n - 2$, non-hyperenergetic if $E(G) < 2n - 2$, and broderenergetic [4] (other than $K_n$) if $E(G) = 2n - 2$. If $E(G) = E(H)$, 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 $ZE(G) > 4(n - 1)^2$, Zagreb non-hyperenergetic if $ZE(G) < 4(n - 1)^2$, and Zagreb broderenergetic (other than $K_n$) if $ZE(G) = 4(n - 1)^2$. If $ZE(G) = ZE(H)$, 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, Rakshit [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 broderenergetic, 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 broderenergetic.

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 $z_1 \geq z_2 \geq \ldots \geq z_n$. 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 $z_1 \geq z_2 \geq \ldots \geq z_n$. The Zagreb energy of complement $\overline{G}$ is

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

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

$$ZE(\overline{G}) = 2(n - r - 1)(n - r - 1)$$

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

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

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 broderenergetic.

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

**Proposition 2.** Let $G$ be an $r$-regular graph $(r \geq 3)$ of order $n$ with Zagreb eigenvalues $z_1 \geq z_2 \geq \ldots \geq z_n$. 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 $z_1 \geq z_2 \geq \ldots \geq z_n$. The Zagreb energy of line graph $L(G)$ is

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

$$+ |(8 - 8r)|\left(\frac{n(r - 2)}{2}\right).$$

**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

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

$$+ |(8 - 8r)|\left(\frac{n(r - 2)}{2}\right).$$

**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
\[ ZE(L(G)) = 4(r - 1) \left| \sum_{i=1}^{n} \left( \frac{z_i}{2r} + r - 2 \right) \right| + \left| (8 - 8r) \left( \frac{n(r - 2)}{2} \right) \right| \quad (15) \]

It is not hard to see that
\[ 4(r - 1) \left| \sum_{i=1}^{n} \left( \frac{z_i}{2r} + r - 2 \right) \right| + \left| (8 - 8r) \left( \frac{n(r - 2)}{2} \right) \right| < 4 \left( \frac{nr}{2} - 1 \right) \cdot \] (16)

Thus, \( L(G) \) is a Zagreb non-hyperenergetic graph. \( \Box \)

**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
\[
A_Z(A_6) = \begin{pmatrix}
v_1 & 0 & 6 & 0 & 0 & 0 \\
v_2 & 6 & 0 & 7 & 9 & 8 \\
v_3 & 0 & 7 & 0 & 6 & 0 \\
v_4 & 0 & 9 & 6 & 0 & 7 \\
v_5 & 0 & 8 & 0 & 7 & 6 \\
v_6 & 0 & 8 & 0 & 7 & 6 \\
\end{pmatrix}
\]
(17)

Therefore, the Zagreb spectrum of \( A_6 \) is as follows:
\[
\text{Spec}A_Z(A_6) = \begin{pmatrix}
34.501 & -17.57 & 3.189 & -11.737 & 1.094 & -9.477 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\end{pmatrix}
\]
(21)

Hence, by the definition of the Zagreb energy, we have
\[ ZE(A_6) = 77.568. \] (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.
Zagreb matrix of $S'(G)$ can be written as a block matrix as follows:

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

or

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

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

$$\text{Spec}_A_z(S'(G)) = \left( \frac{2 - \sqrt{13}}{2}, \frac{2 + \sqrt{13}}{2} \right) \left\{ z_i \right\}.$$  

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 $\frac{2}{3/2}$. Therefore, by the definition of the Zagreb energy, we can write

$$\text{ZE}(S'(G)) = \sum_{i=1}^{p} \left( \frac{2 - \sqrt{13}}{2} \right) z_i = \sum_{i=1}^{p} z_i \left( \frac{2 - \sqrt{13}}{2} + \frac{2 + \sqrt{13}}{2} \right) = 2\text{ZE}(G).$$

Hence, we have

$$\text{ZE}(S'(G)) = 2\text{ZE}(G).$$  \hspace{1cm} (28)

Equality (28) gives the desired result.

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

**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

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

Therefore, by the definition of Zagreb energy, we have

$$\text{ZE}(K_n) = 2(n-1)^2 + |-(n-1)|(n-1) = 4(n-1)^2.$$  \hspace{1cm} (30)

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

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

By the definition of Zagreb energy, we can write

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

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

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

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

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

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

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

Therefore,

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

$$\text{ZE}(\text{CP}(a)) = 8(a-1)^2 + |8(a-1)|(a-1) = 16(a-1)^2.$$  \hspace{1cm} (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.

### References

[1] A. Ali, "A survey of antiregular graphs," *Contributions to Discrete Mathematics*, vol. 1, pp. 67–79, 2020.

[2] V. Brankov, D. Stevanovic, and I. Gutman, "Equienergetic chemical trees," *Journal of the Serbian Chemical Society*, vol. 69, no. 7, pp. 549–554, 2004.

[3] K. C. Das, “On the Zagreb energy and Zagreb Estrada index of graphs,” *MATCH Communications in Mathematical and in Computer Science*, vol. 69, no. 7, pp. 549–554, 2004.

[4] S. Gong, X. Li, G. Xu, I. Gutman, and B. Furtula, "Border-energetic graphs," *MATCH Communications in Mathematical and in Computer*, vol. 74, pp. 321–332, 2015.

[5] I. Gutman, "The energy of a graph," *Ber. Math. Stat. Sekt. Forschungsz. Graz.*, vol. 103, pp. 1–22, 1978.
[6] I. Gutman, “Hyperenergetic molecular graphs,” *Journal of the Serbian Chemical Society*, vol. 64, pp. 199–205, 1999.

[7] I. Gutman and N. Trinajstić, “Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons,” *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[8] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.

[9] I. Gutman, “The energy of a graph: old and new results,” in *Algebraic Combinatorics and Applications*, A. Betten, A. Kohnert, R. Laue, and A. Wassermann, Eds., Springer-Verlag, Berlin, Germany, pp. 196–211, 2001.

[10] N. J. Rad, A. Jahanbani, and I. Gutman, “Zagreb energy and Zagreb estrada index of graphs,” *MATCH Communications in Mathematical and in Computer*, vol. 79, pp. 371–386, 2018.

[11] A. Jahanbani, “Lower bounds for the energy of graphs,” *AKCE International Journal of Graphs and Combinatorics*, vol. 15, no. 1, pp. 88–96, 2018.

[12] A. Jahanbani, “Upper bounds for the energy of graphs,” *MATCH Communications in Mathematical and in Computer*, vol. 79, pp. 275–286, 2018.

[13] A. Jahanbani, “Some new lower bounds for energy of graphs,” *Applied Mathematics and Computation*, vol. 296, pp. 233–238, 2017.

[14] A. Jahanbani and J. R. Zambrano, “Koolen-Moulton-type upper bounds on the energy of a graph,” *MATCH Communications in Mathematical and in Computer*, vol. 83, pp. 497–518, 2020.

[15] A. Jahanbani, R. Khoeilar, and H. Shooshtari, “On the Zagreb matrix and Zagreb energy,” *Asian-European Journal of Mathematics*, in press.

[16] B. R. Rakshith, “On Zagreb energy and edge-Zagreb energy,” *Communications in Combinatorics and Optimization*, vol. 6, pp. 155–169, 2021.

[17] E. Munarini, “Characteristic, admittance and matching polynomials of an antiregular graph,” *Applicable Analysis and Discrete Mathematics*, vol. 3, no. 1, pp. 157–176, 2009.