On the Second Zagreb Matrix of k-half Graphs

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***Abstract*—A bipartite graph in which the neighborhood of the vertices in each partite set forms a chain with respect to set inclusion is known as a chain graph. Recently, extending the concept of nesting from a bipartite graph to a k partite graph, a k-nested graph is defined. A chain graph without any pairs of duplicate vertices is a half graph. Similarly, a 'k-half graph' is a class of k-nested graph with no pairs of duplicate vertices. The second Zagreb matrix or $Z^{(2)}$-matrix denoted by $Z^{(2)}(G) = (z_{ij})_{n\times n}$ of a graph G, whose vertex v_i has degree d_i is defined by $z_{ij} = d_i d_j$ if the vertices v_i and v_j are adjacent and $z_{ij} = 0$ otherwise. Suppose $\zeta_1^{(2)}, \zeta_2^{(2)}, \ldots, \zeta_n^{(2)}$ are the eigenvalues of $Z^2(G)$, then the sum of the absolute values of the eigenvalues of $Z^{(2)}(G)$ is called the second Zagreb energy of G. We obtain the determinant, eigenvalues and inverse of a k-half graph with respect to $Z^{(2)}(G)$. Bounds for the second Zagreb energy and the spectral radius are discussed in this article, along with the main and non-main eigenvalues of a k-half graph with respect to $Z^{(2)}(G)$.**

***Index Terms*—Chain graphs, k-partite graphs, half graphs, main eigenvalues, second Zagreb matrix**

I. INTRODUCTION

WE considered simple, finite, undirected and connected graphs with vertex set $V = V(G)$ and edge set $E = E(G)$. A k-partite graph is a graph whose vertex set can be partitioned into k independent sets and all the edges of the graph are between the partite sets. We denote a k-partite graph with the k-partition of $V = V_1 \cup V_2 \cup \ldots \cup V_k$ by $G(\bigcup_{i=1}^{k} V_i, E)$. If G contains every edge joining the vertices of V_i and $V_j, i \neq j$, then it is a complete k-partite graph. A complete k-partite graph with $|V_i| = p_i, 1 \leqslant i \leqslant k$ is denoted by $K_{p_1,p_2,\ldots,p_k}$. The open neighborhood of a vertex u in G is denoted by $N(u)$ and is given by $N(u) = \{v \in V(G) |\ uv \in E(G)\}$ and the closed neighborhood of u in G is denoted by $N[u]$ and is defined as $N[u] = N(u) \cup \{u\}$. Two vertices u and v in a graph G are duplicate vertices if $N(u) = N(v)$. A vertex $v \in V_i$ $(1 \leqslant i \leqslant k)$ in a k-partite graph $G(\bigcup_{i=1}^{k} V_i, E)$ is said to be a dominating vertex if $N(v) = \bigcup_{j=1}^{k} V_j$, $j \neq i$. In other words, v is of full degree with respect to other partite set.

Readers are referred to [5], [19] for all the elementary notations and definitions not described but used in this paper. A collection $S = \{S_1, S_2, \cdots, S_n\}$ of sets is said to form a chain with respect to set inclusion, if for every $S_i, S_j \in S$ either $S_i \subseteq S_j$ or $S_j \subseteq S_i$.

Definition 1.1: A bipartite chain graph (or simply a chain graph) is a bipartite graph in which the neighborhood of the vertices in each partite set forms a chain with respect to set inclusion.

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Definition 1.2: A graph is a threshold graph if it can be constructed from an empty graph by repeatedly adding either an isolated vertex or a dominating vertex.

Motivated by the nesting property of the extremal graphs (chain and threshold graphs), recently a partial chain graph [13] and a partial threshold graph [14] is defined. Spectral properties of partial chain graphs and partial threshold graphs are discussed in the article [14]. Extending the concept of nesting from a bipartite graph to a k partite graph, the authors of the article [15] defined a k-nested graph as follows.

Definition 1.3: [15] A k-nested graph (KNG) is a k-partite graph in which the neighborhood of the vertices in each partite set forms a chain with respect to set inclusion and each partite set has at least one dominating vertex, i.e., a vertex adjacent to all the vertices of the other partite sets.

In other words, for every two vertices u and v in the same partite set and for their neighborhoods, $N(u)$ and $N(v)$, either $N(u) \subseteq N(v)$ or $N(v) \subseteq N(u)$. Due to the existence of at least one dominating vertex in each partite set, a k-nested graph is always connected.

A chain graph is a 2-nested graph which is also known as a double nested graph (DNG in short). Given a chain graph $G(V_1 \cup V_2, E)$, each of V_i $(i = 1, 2)$ can be partitioned into h non-empty cells $V_{11}, V_{12}, \ldots, V_{1h}$ and $V_{21}, V_{22}, \ldots, V_{2h}$ such that $N(u) = V_{21} \cup ... \cup V_{2\ h-i+1}$, for any $u \in V_{1i}$, $1 \leq i \leq h$. If $m_i = |V_{1i}|$ and $n_i = |V_{2i}|$, then we write $G = DNG(m_1, m_2, ..., m_h; n_1, n_2, ..., n_h)$.

In a KNG, each partite set V_i, $1 \leqslant i \leqslant k$ can be further partitioned into h_i non-empty sets $V_{i1}, V_{i2}, \ldots, V_{ih_i}$ such that for any two vertices say u, v in $V_{ij}, 1 \leqslant j \leqslant h_i$, $N(u) = N(v)$. Suppose $|V_{ij}| = m_{ij}$, then we write $G = KNG(m_{11}, m_{12}, \ldots, m_{1h_1}; m_{21}, m_{22}, \ldots, m_{2h_2}; \ldots; m_{k1}, m_{k2}, \ldots, m_{kh_k})$. The authors [15] noted that the graph $G = KNG(m_{11}, m_{12}, ..., m_{1h_1}; m_{21}, m_{22}, ..., m_{2h_2}; \ldots; m_{k1}, \ldots, m_{kh_k})$ does not represent a single graph, but a family of graphs G_f with the nesting property. Note that $KNG(1; 1; \ldots; 1)$ on n vertices is K_n and $KNG(p_1; p_2; \ldots; p_k)$ is $K_{p_1,p_2,\ldots,p_k}$.

A half graph is a chain graph without any duplicate vertices. Analogous to the half graph, the authors of the article [15] defined and redefined [4] a k-half graph as follows.

Definition 1.4: A k-half graph on kn vertices with $k \geq 2$ is a k-nested graph $G(\bigcup_{i=1}^{k} V_i, E)$ with $|V_i| = n$ and the vertices in each partite set V_i are further partitioned into n non-empty cells, i.e., $V_i = V_{i1} \cup V_{i2} \cup \cdots \cup V_{in}$ in such a way that, for any vertex $u \in V_{ir}$, $N(u) = V_{j1} \cup V_{j2} \cup \cdots \cup V_{j\ n-r+1}, 1 \leq j \neq i \leq k$ and $\forall\ i$ and r.

In a half graph (2-half graph) on $2n$ vertices, the degrees of n vertices in any partite set are $n, n-1, \ldots, 1$. Similarly, in a k- half graph on kn vertices the degrees of n vertices in any partite set are $(k-1)n, (k-1)(n-1), \ldots, (k-1)$.

A k-half graph on kn vertices has $\binom{k}{2}\left(\frac{n(n+1)}{2}\right)$ edges. Figure 1 represents a 3-half graph with 12 vertices and 30 edges.

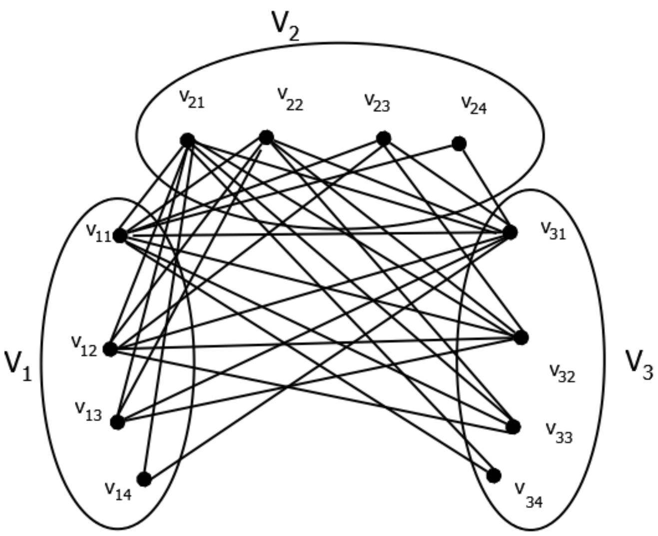

Fig. 1. 3-Half Graph

Here $|V_i| = 4, 1 \le i \le 3$ and $v_{i1}, 1 \le i \le 3$ is the dominating vertex of the set V_i. Observe that
$N(v_{11}) = \{v_{21}, v_{22}, v_{23}, v_{24}, v_{31}, v_{32}, v_{33}, v_{34}\}$, $N(v_{12}) = \{v_{21}, v_{22}, v_{23}, v_{31}, v_{32}, v_{33}\}$, $N(v_{13}) = \{v_{21}, v_{22}, v_{31}, v_{32}\}$ and $N(v_{14}) = \{v_{21}, v_{31}\}$.
Hence, $N(v_{14}) \subseteq N(v_{13}) \subseteq N(v_{12}) \subseteq N(v_{11})$.

The topological indices are numerical graph invariants that characterizes the molecular topology of chemical compounds. Some of the most comprehensively studied degree-based topological indices are the Zagreb indices.

The first and second Zagreb index denoted by $M_1(G) = M_1$ and $M_2(G) = M_2$ of a graph G are defined as

$$M_1 = \sum_{v_i \in V(G)} d_i^2 = \sum_{v_i v_j \in E(G)} d_i + d_j,$$

$$M_2 = \sum_{v_i v_j \in E(G)} d_i d_j.$$

The degree based topological indices have been considered for graphs with self-loops [16] and for hypergraphs [17]. Since the last few years, researchers have focused on exploring the spectral properties of topological indices by appropriate modification of the adjacency matrix $A(G)$. With TI we denote a topological index that can be represented as $TI = TI(G) = \sum_{v_i \sim v_j} F(d_i, d_j)$, where F is an appropriately chosen function with the property $F(x, y) = F(y, x)$. A general extended adjacency matrix $A = (a_{ij})$ of G is defined as $a_{ij} = F(d_i, d_j)$ if the vertices v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. The first extended adjacency matrix corresponding to a degree based topological index defined was the randi´c matrix [3], and the energy of the corresponding matrix was defined in a similar way and termed as the randi´c energy. The concept of an adjacency matrix of simple graphs has been generalized to degree based extended adjacency matrix in [7] and for graphs with self-loops in [18].
If $F(d_i, d_j) = d_i + d_j$, i.e., $TI = M_1(G)$ (the first Zagreb index), we get the first Zagreb matrix [10] and if $F(d_i, d_j) = d_i d_j$, i.e., $TI = M_2(G)$ (the second Zagreb index), we get the second Zagreb matrix [10].

The first Zagreb matrix of a graph G is a square matrix $Z^{(1)}(G)$ of order n, defined as

$$(Z^{(1)})_{ij} = \begin{cases} d_i + d_j, & \text{if } \ v_i v_j \in E(G) \\ 0, & \text{otherwise,} \end{cases}$$

and the second Zagreb matrix of a graph G is a square matrix $Z^{(2)}(G)$ of order n, defined as

$$(Z^{(2)})_{ij} = \begin{cases} d_i . d_j, & \text{if } \ v_i v_j \in E(G) \\ 0, & \text{otherwise.} \end{cases}$$

If the eigenvalues of $Z^{(1)}(G)$ are $\zeta_1^{(1)}, \zeta_2^{(1)}, \ldots, \zeta_n^{(1)}$, then their collection is called the first Zagreb spectrum or $Z^{(1)}$-spectrum of G. The first Zagreb energy of a graph G is denoted by $ZE_1(G)$ and is defined as

$$ZE_1(G) = \sum_{i=1}^{n} |\zeta_i^{(1)}|.$$

Similarly, if the eigenvalues of $Z^{(2)}(G)$ are $\zeta_1^{(2)}, \zeta_2^{(2)}, \ldots, \zeta_n^{(2)}$, then their collection is called the second Zagreb spectrum or $Z^{(2)}$-spectrum of G. The second Zagreb energy of a graph G is denoted by $ZE_2(G)$ and is defined as

$$ZE_2(G) = \sum_{i=1}^{n} |\zeta_i^{(2)}|.$$

The largest eigenvalue $\zeta_1^{(2)}$ is the spectral radius of the second Zagreb matrix if its eigenvalues are possible to be expressed as $\zeta_1^{(2)} \ge \zeta_2^{(2)} \ge \ldots \ge \zeta_n^{(2)}$.

A few bounds on Zagreb energy and the spectral radius of the first Zagreb matrix of the graph G is obtained in [6]. The spectral properties of a k-half graph with respect to the first Zagreb matrix are studied in [4].

In this article, we denote the second Zagreb matrix as $Z(G)$ instead of $Z^{(2)}(G)$ for convenience.

Let $Z(G)$ and $A(G)$ be the 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 the authors of article [11] proved that $Z(G) = DA(G)D$.

In this article, we obtain a few spectral properties of a k-half graph with respect to $Z(G)$.

II. Determinant, Eigenvalues and Inverse

The determinant, eigenvalues and the inverse of a k-half graph with respect to the second Zagreb matrix are discussed in this section using the concept of Kronecker product.

Definition 2.1: The Kronecker product of a matrix $A = (a_{ij})_{p \times q}$ and $B_{r \times s}$ is defined as

$$A \otimes B = \begin{bmatrix} a_{11}B & \ldots & a_{1q}B \\ \vdots & \vdots & \vdots \\ a_{p1}B & \ldots & a_{pq}B \end{bmatrix}.$$

Some of the basic properties of the Kronecker product which are important in obtaining the determinant, eigenvalues and inverse of a k-half graph with respect to $Z(G)$ are listed below.

Theorem 2.1: [9] Let A be a square matrix of order m and let B be a square matrix of order n. Then

$$det(A \otimes B) = det(B \otimes A) = det(A)^n det(B)^m.$$

Theorem 2.2: [9] Let A be a square matrix of order m with spectrum $\sigma(A) = (\mu_i),\ 1 \leq i \leq m$ and B be a square matrix of order n with $\sigma(B) = (\lambda_j),\ 1 \leq j \leq n$. Then $\sigma(A \otimes B) = (\mu_i \lambda_j), 1 \leq i \leq m,\ 1 \leq j \leq n$.
Furthermore, if x_i and y_j are the eigenvectors corresponding to the eigenvalue μ_i and λ_j in A and B respectively then $x_i \otimes y_j$ is an eigenvector corresponding to the eigenvalue $\mu_i \lambda_j$ in $A \otimes B$.

Theorem 2.3: [9] If A ia a square matrix of order m and B is a square matrix of order n and both are non singular then,

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}.$$

By using Theorem 2.1 and Lemma 2.4, one can obtain the determinant of a k-half graph with respect to the second Zagreb matrix.

Lemma 2.4: Let B be a matrix of order n given by

$$\begin{bmatrix} n^2(k-1)^2 & n(n-1)(k-1)^2 & \dots & n(k-1)^2 \\ n(n-1)(k-1)^2 & (n-1)^2(k-1)^2 & \dots & 0 \\ \vdots & \dots & \ddots & 0 \\ 2n(k-1)^2 & 2(n-1)(k-1)^2 & 0 & 0 \\ n(k-1)^2 & 0 & \dots & 0 \end{bmatrix}.$$

Then,

$$det(B) = \begin{cases} (n!)^2(k-1)^{2n}, & \text{if } n \text{ is of the form } 4r \\ & \text{ or } 4r+1, \text{where } \ r \geq 0 \\ -(n!)^2(k-1)^{2n}, & \text{otherwise.} \end{cases}$$

Proof: Proof follows by noting that

$$B = (k-1)^{2n}(n!)^2 \begin{bmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 0 \\ \vdots & \dots & \iddots & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & \dots & 0 \end{bmatrix}.$$

■

Theorem 2.5: Let G be k-half graph on kn vertices. Then, $det(Z(G))$

$$= \begin{cases} [(k-1)^{n(2k+1)}(n!)^{2k}], & \text{if } k \text{ and } n \text{ both are even} \\ & \text{or if } k \text{ is odd then} \\ & n = 4r \text{ or } 4r+1, r \geq 0 \\ -[(k-1)^{n(2k+1)}(n!)^{2k}], & \text{otherwise.} \end{cases}$$

Proof: The second Zagreb matrix of G can be written as block matrix as follows;

$$Z(G) = \begin{bmatrix} 0_n & B_n & \dots & B_n & B_n \\ B_n & 0_n & \dots & B_n & B_n \\ \vdots & \dots & \ddots & & 0_n \\ B_n & B_n & \dots & 0_n & B_n \\ B_n & B_n & \dots & B_n & 0_n \end{bmatrix},$$

where $B_n =$

$$\begin{bmatrix} n^2(k-1)^2 & n(n-1)(k-1)^2 & \dots & n(k-1)^2 \\ n(n-1)(k-1)^2 & (n-1)^2(k-1)^2 & \dots & 0 \\ \vdots & \dots & \iddots & 0 \\ 2n(k-1)^2 & 2(n-1)(k-1)^2 & 0 & 0 \\ n(k-1)^2 & 0 & \dots & 0 \end{bmatrix}$$

and 0_n is a zero matrix of order n.
Note that $Z(G)$ is Kronecker product of the adjacency matrix of the complete graph of order k and the matrix B_n. The proof directly follows from Theorem 2.2. ■

Corollary 2.6: Let G be half graph on $2n$ vertices. Then,

$$det(Z(G)) = \begin{cases} (n!)^4, & \text{if } n \text{ is even} \\ -(n!)^4, & \text{otherwise.} \end{cases}$$

Theorem 2.7: Let B be a matrix of order n given by

$$\begin{bmatrix} n^2(k-1)^2 & n(n-1)(k-1)^2 & \dots & n(k-1)^2 \\ n(n-1)(k-1)^2 & (n-1)^2(k-1)^2 & \dots & 0 \\ \vdots & \dots & \ddots & 0 \\ 2n(k-1)^2 & 2(n-1)(k-1)^2 & 0 & 0 \\ n(k-1)^2 & 0 & \dots & 0 \end{bmatrix}.$$

Let $\lambda_i, 1 \leq i \leq n$ be the eigenvalues of B with the corresponding eigenvectors $Y_i, 1 \leq i \leq n$. Suppose G is a k-half graph on kn vertices, then the Z-spectrum of G is given by
$Spec(Z(G)) =$

$$\begin{pmatrix} -\lambda_1 & -\lambda_2 & \dots & -\lambda_n & (k-1)\lambda_1 & \dots & (k-1)\lambda_n \\ k-1 & k-1 & \dots & k-1 & 1 & \dots & 1 \end{pmatrix},$$

with the eigenvector $X_i = \begin{bmatrix} Y_i \\ Y_i \\ Y_i \\ \vdots \\ Y_i \end{bmatrix}$ corresponding to the Z-eigenvalue $(k-1)\lambda_i, 1 \leq i \leq n$, and

$$X_i = \begin{bmatrix} Y_i \\ -Y_i \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} Y_i \\ 0 \\ -Y_i \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \dots, \begin{bmatrix} Y_i \\ 0 \\ 0 \\ 0 \\ \vdots \\ -Y_i \end{bmatrix}$$

corresponding to the Z-eigenvalue $-\lambda_i$ whose multiplicity is $k-1$.

Proof: The proof follows from Theorem 2.2, by observing the eigenvalues and eigenvectors of the adjacency matrix of the complete graph of order k. ■

Corollary 2.8: If G is a half graph on $2n$ vertices, then $\pm\lambda_i, 1 \leq i \leq n$ are the Z-eigenvalues of G, where $\lambda_i, 1 \leq i \leq n$ are the eigenvalues of B as defined in Lemma 2.4.

Theorem 2.9: Let G be a k-half graph on kn vertices. Then,

$$Z^{-1} = C \otimes D = \begin{bmatrix} c_{11}D & \dots & c_{1k}D \\ \vdots & \vdots & \vdots \\ c_{k1}D & \dots & c_{kk}D \end{bmatrix},$$

where $C = \begin{bmatrix} \frac{2-k}{k-1} & \frac{1}{k-1} & \cdots & \frac{1}{k-1} \\ \frac{1}{k-1} & \frac{2-k}{k-1} & \cdots & \frac{1}{k-1} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{1}{k-1} & \cdots & \cdots & \frac{2-k}{k-1} \end{bmatrix}_{k\times k}$

and

$$D = \begin{bmatrix} 0 & \cdots & 0 & \frac{1}{n(k-1)^2} \\ 0 & \cdots & \frac{1}{2(n-1)(k-1)^2} & \frac{-1}{(n-1)(k-1)^2} \\ 0 & \cdots & \frac{-1}{2(n-2)(k-1)^2} & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & \frac{1}{2(n-1)(k-1)^2} & \cdots & 0 \\ \frac{1}{n(k-1)^2} & \frac{-1}{(n-1)(k-1)^2} & \cdots & 0 \end{bmatrix}_{n\times n}$$

Proof: The Z-matrix of the k-half graph, is the Kronecker product of the adjacency matrix of the complete graph of order k and the matrix B of order n. From Theorem 2.3, the inverse of $Z(G)$ is the Kronecker product of inverse of $A(K_k)$ which is given by the matrix C and inverse of the matrix B which is given by the matrix D. ■

The following corollary follows from Theorem 2.3.

Corollary 2.10: Let G be a half graph on $2n$ vertices. Then,

$$Z^{-1} = \begin{bmatrix} 0_n & D_n \\ D_n & 0_n \end{bmatrix},$$

where $D = \begin{bmatrix} 0 & 0 & \cdots & 0 & \frac{1}{n} \\ 0 & \cdots & 0 & \frac{1}{2(n-1)} & \frac{-1}{n-1} \\ 0 & \cdots & \frac{1}{3(n-2)} & \frac{-1}{2(n-2)} & 0 \\ \vdots & \cdots & \ddots & \cdots & \vdots \\ 0 & \frac{1}{2(n-1)} & \frac{-1}{2(n-2)} & \cdots & 0 \\ \frac{1}{n} & \frac{-1}{n-1} & 0 & \cdots & 0 \end{bmatrix}_{n\times n}$.

III. Bounds

A few bounds on the second Zagreb energy and the spectral radius of a k-half graph are discussed in this section.

Let $a = \{a_1, a_2, \ldots, a_n\}$ be a set of positive real numbers. We define P_k to be the average of products of k-element subsets of a, i.e.,

$P_1 = \frac{1}{n}(a_1 + a_2 + \ldots + a_n)$

$P_2 = \frac{1}{\frac{1}{2}n(n-1)}(a_1a_2 + a_1a_3 + \ldots + a_1a_n + a_2a_3 + \ldots + a_{n-1}a_n)$

$\vdots$

$P_n = a_1a_2\ldots a_n$.

Hence the arithmetic mean is P_1 whereas the geometric mean is $P_n^{\frac{1}{n}}$. The following result is known as the Maclaurin symmetric mean inequality:

Lemma 3.1: [2] For positive real numbers $a_1, a_2, \ldots, a_n$, $P_1 \geq P_2^{\frac{1}{2}} \geq P_3^{\frac{1}{3}} \geq \ldots \geq P_n^{\frac{1}{n}}$.
Equalities hold if and only if $a_1 = a_2 = \ldots = a_n$.

We give a lower bound for $ZE_2(G)$ of a half graph G using the below lemma.

Lemma 3.2: Let G be a k-half graph on kn vertices. Then, $Tr(Z(G)^2) = \frac{k(k-1)^5 n(38n^5 + 114n^4 + 125n^3 + 60n^2 + 17n + 6)}{360}$.

Proof: $Z(G)$ can be viewed as,

$$Z(G) = (k-1)^2 \begin{bmatrix} 0_n & E_n & \ldots & E_n & E_n \\ E_n & 0_n & \ldots & E_n & E_n \\ \vdots & \ldots & \ddots & & 0_n \\ E_n & E_n & \ldots & 0_n & E_n \\ E_n & E_n & \ldots & E_n & 0_n \end{bmatrix},$$

where

$$E_n = \begin{bmatrix} n^2 & n(n-1) & \ldots & 2n & n \\ n(n-1) & (n-1)^2 & \ldots & 2(n-1) & 0 \\ \vdots & \ldots & \ldots & \ddots & 0 \\ 2n & 2(n-1) & \ldots & 0 & 0 \\ n & 0 & \ldots & 0 & 0 \end{bmatrix}$$

and 0_n is a zero matrix of order n.

$$Tr(Z(G)^2) =$$

$$k(k-1)^5(n^2 \sum_{j=1}^{n} j^2 + (n-1)^2 \sum_{j=2}^{n} j^2 + \ldots + n^2)$$

$$= k(k-1)^5 \sum_{i=0}^{n-1} \sum_{j=i+1}^{n} (n-i)^2 j^2$$

$$= \frac{k(k-1)^5 n(38n^5 + 114n^4 + 125n^3 + 60n^2 + 17n + 6)}{360}.$$

■

Theorem 3.3: Let G be a half graph on $2n$ vertices. Then $ZE_2(G) \geq 2\sqrt{\frac{n(38n^5+114n^4+125n^3+60n^2+17n+6)}{360} + n(n-1)(n!)^{\frac{4}{n}}}$ with equality if and only if $G \cong K_{1,1}$.

Proof: Note that $Z(G) = \begin{bmatrix} 0_n & E_n \\ E_n & 0_n \end{bmatrix}$ where

$$E_n = \begin{bmatrix} n^2 & n(n-1) & \ldots & 2n & n \\ n(n-1) & (n-1)^2 & \ldots & 2(n-1) & 0 \\ \vdots & \ldots & \ldots & \ddots & 0 \\ 2n & 2(n-1) & \ldots & 0 & 0 \\ n & 0 & \ldots & 0 & 0 \end{bmatrix}$$

and 0_n is the zero matrix of order n.

Let $\zeta_1, \zeta_2, \ldots, \zeta_{2n}$ be the second Zagreb eigenvalues of $Z(G)$. Since G is bipartite, $ZE_2(G) = 2\sum_{i=1}^{n} \zeta_i$, where ζ_i are the positive eigenvalues of $Z(G)$.

From Lemma 3.2 we have,

$\sum_{i=1}^{2n} \zeta_i^2 = Tr(Z(G))^2 =$

$$\frac{n(38n^5 + 114n^4 + 125n^3 + 60n^2 + 17n + 6)}{180}.$$

Thus,

$$\sum_{i=1}^{n} \zeta_i^2 = \frac{n(38n^5 + 114n^4 + 125n^3 + 60n^2 + 17n + 6)}{360}.$$

We know that

$$\prod_{i=1}^{2n} \zeta_i = det(Z(G)) = (-1)^n (n!)^4.$$

Hence,

$$\prod_{i=1}^{n} \zeta_i = (n!)^2.$$

By Lemma 3.1, we obtain

$$\frac{1}{\frac{n(n-1)}{2}}\sum_{1\le i<j\le n}\zeta_i\zeta_j \ge (\prod_{i=1}^{n}\zeta_i)^{\frac{2}{n}},$$

i.e., $2\sum_{1\le i\le j\le n}\zeta_i\zeta_j \ge n(n-1)(n!)^{\frac{4}{n}}$
with equality holding if and only if $\zeta_1=\zeta_2=\ldots=\zeta_n$.
We have,

$$(\sum_{i=1}^{n}\zeta_i)^2=\sum_{i=1}^{n}\zeta_i^2+2\sum_{1\le i\le j\le n}\zeta_i\zeta_j.$$

Hence,

$$ZE_2(G)=2\sqrt{\sum_{i=1}^{n}\zeta_i^2+2\sum_{1\le i<j\le n}\zeta_i\zeta_j}$$

$$\ge 2\sqrt{\frac{n(38n^5+114n^4+125n^3+60n^2+17n+6)}{360}+(n^2-n)(n!)^{\frac{4}{n}}}$$

Equality holds if $n=1$, i.e., $G\cong K_{1,1}$. ∎

Theorem 3.4: Let G be a k-half graph on kn vertices. Then $ZE_2(G)\ge 2(k-1)^3$

$$\sqrt{\frac{38n^6+114n^5+125n^4+60n^3+17n^2+6n}{360}+(n^2-n)(n!)^{\frac{4}{n}}}$$

with equality if and only if $G\cong K_{1,1}$.

Proof: From Theorem 2.7,

$$ZE_2(G)=(k-1)\sum_{i=1}^{n}|\lambda_i|+\sum_{i=1}^{n}(k-1)|\lambda_i|,$$

where λ_i are the eigenvalues of the matrix B. Hence,

$$ZE_2(G)=2(k-1)\sum_{i=1}^{n}|\lambda_i|.$$

Note that

$$\prod_{i=1}^{n}|\lambda_i|=(k-1)^{2n}(n!)^2.$$

$$\sum_{i=1}^{n}|\lambda_i|^2=n(k-1)^4\left(\frac{38n^5+114n^4+125n^3+60n^2+17n+6}{360}\right) \quad \text{(III.1)}$$

From the arithmetic–geometric mean inequality, we have

$$2\sum_{1\le i<j\le n}|\lambda_i||\lambda_j|\ge n(n-1)(\prod_{i=1}^{n}|\lambda_i|)^{\frac{2}{n}}$$

Hence,

$$2\sum_{1\le i<j\le n}|\lambda_i||\lambda_j|\ge n(n-1)(k-1)^4(n!)^{\frac{4}{n}}. \quad \text{(III.2)}$$

Now,

$$\begin{aligned}ZE_2(G)&=2(k-1)\sum_{i=1}^{n}|\lambda_i|\\&=2(k-1)\sqrt{\left(\sum_{i=1}^{n}|\lambda_i|\right)^2}\\&=2(k-1)\sqrt{\sum_{i=1}^{n}|\lambda_i|^2+2\sum_{1\le i<j\le n}|\lambda_i||\lambda_j|}\end{aligned}$$

Substituting Equation III.1, III.2 in the above expression and simplifying we get
$ZE_2(G)\ge 2(k-1)^3$

$$\sqrt{\frac{n(38n^5+114n^4+125n^3+60n^2+17n+6)}{360}+n(n-1)(n!)^{\frac{4}{n}}}.$$ ∎

Theorem 3.5: Let G be a k-half graph on $2k$ vertices. Then, $ZE_2(G)=8\sqrt{2}(k-1)^3$.

Proof: From Theorem 2.7, we have,

$$Spec(G)=\begin{pmatrix}-\lambda_1 & -\lambda_2 & (k-1)\lambda_1 & (k-1)\lambda_2\\ k-1 & k-1 & 1 & 1\end{pmatrix},$$

where $\lambda_1=(k-1)^2(2+\sqrt{2}),\lambda_2=(k-1)^2(2-\sqrt{2})$ are the Z-eigenvalues of

$$B=\begin{pmatrix}4(k-1)^2 & 2(k-1)^2\\ 2(k-1)^2 & 0\end{pmatrix}.$$

Hence, $ZE_2(G)=8\sqrt{2}(k-1)^3$. ∎

Theorem 3.6: Let G be a k-half graph on $3k$ vertices. Then, the Z-eigenvalues of G are $(k-1)^3\lambda_i$ with multiplicity 1 and $-(k-1)^2\lambda_i$ with multiplicity $k-1$, where $\lambda_i, 1\le i\le 3$ are the roots of the equation $x^3-13x^2-9x+36=0$.

Proof: From Theorem 2.7, we have, $Spec(G)=$

$$\begin{pmatrix}-\lambda_1 & -\lambda_2 & -\lambda_3 & (k-1)\lambda_1 & (k-1)\lambda_2 & (k-1)\lambda_3\\ k-1 & k-1 & k-1 & 1 & 1 & 1\end{pmatrix},$$

where $\lambda_i's$ are the eigenvalues of

$$B=\begin{pmatrix}9(k-1)^2 & 6(k-1)^2 & 3(k-1)^2\\ 6(k-1)^2 & 4(k-1)^2 & 0\\ 3(k-1)^2 & 0 & 0\end{pmatrix}.$$

Solving we get

$$B=(k-1)^2\begin{pmatrix}9 & 6 & 3\\ 6 & 4 & 0\\ 3 & 0 & 0\end{pmatrix}$$

Hence, the result follows. ∎

Using Theorems 3.7, 3.8 and 3.9 from article [12], we obtain few bounds on the spectral radius of a k-half graph.

Theorem 3.7: [12] For a graph G with maximum and minimum degrees Δ and δ, respectively, and the spectral radius $\zeta_1^{(2)}$, we have

$$\delta^3\le\zeta_1^{(2)}\le\Delta^3$$

where both equalities occur if and only if G is regular.

Theorem 3.8: [12] Let G be a graph with n vertices, m edges, the maximum degree Δ and the minimum degree δ. Then the spectral radius $\zeta_1^{(2)}$ satisfies,

$$\frac{2m\delta^2}{n}\le\zeta_1^{(2)}\le\Delta^2\sqrt{2m-n+1},$$

where left hand equality occurs if and only if G is regular, and right hand equality appears if and only $G\cong S_n$ or $G\cong K_n$.

Theorem 3.9: [12] For a graph G of n vertices with maximum degree Δ and second Zagreb index M_2,

$$\zeta_1^{(2)}\le\sqrt{\frac{2(n-1)\Delta^2M_2}{n}}.$$

Theorem 3.10: Let G be a k-half graph on kn vertices. Then,

$$(k-1)^3 \leq \zeta_1^{(2)} \leq n^3(k-1)^3.$$

Theorem 3.11: Let G be a k-half graph on kn vertices. Then,

$$\frac{(k-1)^3(n+1)}{3} \leq \zeta_1^{(2)} \leq n^2(k-1)^2\sqrt{\frac{kn(k-1)(n+1)}{2} - kn + 1}.$$

Next, we give expressions for first and second Zagreb index of a k-half graph.

Theorem 3.12: Let G be a k-half graph on kn vertices. Then, the first Zagreb index M_1 is given by,

$$M_1 = \frac{k(k-1)^2 n(n+1)(2n+1)}{6}.$$

Proof: Proof follows by noting that the first Zagreb index is given by

$$M_1 = \sum_{v_i \in V(G)} d_i^2 = k(k-1)^2\{1^2 + 2^2 + \ldots + n^2\}.$$

■

Theorem 3.13: Let G be a k-half graph on kn vertices. Then, the second Zagreb index M_2 is given by,

$$M_2 = \frac{k(k-1)^3}{48} n(n+1)(5n^2+5n+2).$$

Proof: We know $M_2 = \sum_{v_i v_j \in E(G)} d_i d_j$.

$$\begin{aligned} M_2 &= \binom{k}{2}(k-1)^2(n\sum_{j=1}^{n} j + (n-1)\sum_{j=2}^{n} j + \ldots + n) \\ &= \binom{k}{2}(k-1)^2)\sum_{i=0}^{n-1}\sum_{j=i+1}^{n}(n-i)j \\ &= \binom{k}{2}(k-1)^2)\frac{1}{24}n(n+1)(5n^2+5n+2). \end{aligned}$$

■

Using Theorems 3.9 and 3.13, we can get the better upper bound on the spectral radius of a k-half graph.

Theorem 3.14: Let G be a k-half graph on kn vertices. Then,

$$\zeta_1^{(2)} \leq \frac{(k-1)^2 n}{2}\sqrt{\frac{(kn-1)(k-1)(n+1)(5n^2+5n+2)}{6}}.$$

IV. Main / non-main Eigenvalues

An eigenvalue $\mu \in Spec(A(G))$ is main if the corresponding eigenspace $E(\mu; G)$ is not orthogonal to all-1 vector J; otherwise, it is non-main. The graph with only one main eigenvalue is necessarily regular. In threshold graph all eigenvalues except 0 and -1 are main. But there exist some chain graphs with all eigenvalues are main and also with all eigenvalues are non-main except 0. In [1], the authors characterize the chain graphs with 2 main eigenvalues. One can refer to [8] for few interesting results on main and non main eigenvalues.

Similarly, an eigenvalue $\mu \in Spec(Z(G))$ is main if the corresponding eigenspace $E(\mu; G)$ is not orthogonal to all-1 vector J; otherwise, it is non-main. In this section we obtain main and non-main eigenvalues of a k-half graph with respect to $Z(G)$. First, we show that in a k-half graph on kn vertices, there are at least $kn - n$ non-main Z-eigenvalues.

Theorem 4.1: Let $\lambda_1, \lambda_2, \ldots, \lambda_n$, be the eigenvalues of B. The Z-eigenvalues $-\lambda_i,\ 1 \leq i \leq n$, repeats $k-1$ times, of a k-half graph are non-main Z-eigenvalues.

Proof: From Theorem 2.7, we know that the eigenvalue $-\lambda_i,\ 1 \leq i \leq n$, with multiplicity $k-1$ are the eigenvalues of a k-half graph with the corresponding eigenvectors

$$\begin{bmatrix} Y_i \\ -Y_i \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} Y_i \\ 0 \\ -Y_i \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} Y_i \\ 0 \\ 0 \\ 0 \\ \vdots \\ -Y_i \end{bmatrix}.$$

All these vectors are orthogonal to J. Hence each $-\lambda_i, 1 \leq i \leq n$ is a non-main Z-eigenvalue. ■

Theorem 4.2: Let G be a k-half graph and let $\lambda_1, \lambda_2, \ldots, \lambda_n$, be the eigenvalues of B. If any $\lambda_i,\ 1 \leq i \leq n$ is a non-main (main) Z-eigenvalue of B, then $(k-1)\lambda_i$, the Z-eigenvalue of G is also non-main (main) Z-eigenvalue.

Proof: From Theorem 2.7, We know that $(k-1)\lambda_i$ is a Z-eigenvalue of G with multiplicity 1 and the corresponding eigenvector is given by

$$X_i = \begin{bmatrix} Y_i \\ Y_i \\ Y_i \\ \vdots \\ Y_i \end{bmatrix}.$$

If λ_i is non-main (main), we have $Y_i J = 0, (Y_i J \neq 0)$. Thus, $X_i J = 0, (X_i J \neq 0)$. Hence the eigenvalue $(k-1)\lambda_i$ is also non-main (main). ■

From Theorems 4.1 and 4.2, we know that for a k-half graph on kn vertices, at least $kn - n$ second Zagreb-eigenvalues are non-main and at most n second Zagreb-eigenvalues are main. So, when $n = 2$ i.e., a k-half graph on $2k$ vertices contains at most 2 main Z-eigenvalues. In the next theorem we show that when G is a k-half graph on $2k$ vertices it has exactly 2 main Z-eigenvalues.

Theorem 4.3: Let G be a k-half graph with $2k$ vertices. Then, $(k-1)^3(2 \pm \sqrt{2})$ are the main Z-eigenvalues and $(k-1)^2(-2 \pm \sqrt{2})$ each with multiplicity $k-1$ are the non-main Z-eigenvalues of G.

Proof: From Theorem 2.7, we have

$$Spec(G) = \begin{pmatrix} -\lambda_1 & -\lambda_2 & (k-1)\lambda_1 & (k-1)\lambda_2 \\ k-1 & k-1 & 1 & 1 \end{pmatrix},$$

where $\lambda_1 = (k-1)^2(2+\sqrt{2}), \lambda_2 = (k-1)^2(2-\sqrt{2})$ are the Z-eigenvalues of

$$B = \begin{pmatrix} 4(k-1)^2 & 2(k-1)^2 \\ 2(k-1)^2 & 0 \end{pmatrix}.$$

From Theorem 4.1, $-\lambda_1 = (k-1)^2(-2-\sqrt{2})$ and $-\lambda_2 = (k-1)^2(\sqrt{2}-2)$ with multiplicity $k-1$ are the non-main Z-eigenvalues of G. It follows from Theorem 4.2, that $(k-1)\lambda_1$ and $(k-1)\lambda_2$ are the main Z- eigenvalues of G if and only if $\lambda_1 = (k-1)^2(2+2\sqrt{2})$ and $\lambda_2 = (k-1)^2(2-2\sqrt{2})$ are the main Z-eigenvalues of B.

It is easy to show that the eigenvectors corresponding to the Z-eigenvalues λ_1, λ_2 of B are given by

$$X_1 = \begin{pmatrix} l \\ \frac{2l}{\sqrt{2}+2} \end{pmatrix}, \quad X_2 = \begin{pmatrix} l \\ \frac{3l}{2-\sqrt{2}} \end{pmatrix}$$

where $l \neq 0$. As $X_1^T J \neq 0$ and $X_2^T J \neq 0$, the eigenvalues $(k-1)^2(2+\sqrt{2}), (k-1)^2(2-\sqrt{2})$ are the main Z^2-eigenvalues of the matrix B.
Hence, the main Z-eigenvalues of G are $(k-1)^3(2 \pm \sqrt{2})$. ■

V. Conclusion

The determinant, eigenvalues and inverse of a k-half graph G with respect to the second Zagreb matrix is obtained along with a few bounds on the second Zagreb energy and the spectral radius. The main and non-main eigenvalues of a k-half graph with respect to $Z(G)$ are also discussed. One can try to obtain spectral properties of a k-half graph with respect to its extended adjacency matrices corresponding to other degree based topological indices.

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