Energy and Spectra of Zagreb Matrix of k-half Graph

K ARATHI BHAT* and SHASHWATH S SHETTY

***Abstract*—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. By extending the concept of nesting from a bipartite graph to a k partite graph, a k-nested graph is defined. A half graph is a chain graph having no pairs of duplicate vertices. Similarly, a 'k-half graph' is a class of k-nested graph with no pairs of duplicate vertices. The (first) Zagreb matrix or Z-matrix denoted by $Z(G) = (z_{ij})_{n\times n}$ 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. Let $\zeta_1, \zeta_2, \ldots, \zeta_n$ be the Zagreb eigenvalues of $Z(G)$ and the Zagreb energy is the sum of the absolute values of the Zagreb eigenvalues. We obtain the determinant, eigenvalues and inverse of a k-half graph with respect to the Z-matrix. Bounds for the Zagreb energy and spectral radius are discussed along with the main and non-main Zagreb eigenvalues of a k-half graph.**

***Index Terms*—Chain graphs, k-partite graphs, half graphs, main eigenvalues, Kronecker product.**

I. Introduction

Graphs considered in this paper are simple, finite, undirected and connected 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 complete k-partite graph. A complete k-partite graph with $|V_i| = p_i, 1 \leqslant i \leqslant k$ is denoted by $K_{p_1,p_2,\ldots,p_k}$. We write $u \sim v$ if the vertices u and v are adjacent in G and $u \nsim v$ if they are not adjacent in G. 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 $N[u] = \{u\} \cup N(u)$. 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 [4], [16] 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 $S_j \subseteq S_i$.

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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.

Definition 1.2: A graph is a threshold graph if it can be constructed from the 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 [10] and a partial threshold graph [11] is defined. Spectral properties of partial chain graphs and partial threshold graphs are discussed in the article [11]. Extending the concept of nesting from bipartite graph to a k partite graph, the authors of the article [12] defined a k-nested graph as follows.

Definition 1.3: [12] 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 have 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 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 [12] 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 $K_{p_1,p_2,\ldots,p_k}$.

Example 1.1: The graphs G_1 and G_2 (Figure 1) are the 4-nested graphs with 12 vertices in the family $G_f = KNG(1, 2, 2; 1, 2; 1, 1, 1; 1)$.
The graph G_1 has 32 edges where as the graph G_2 has 36 edges. The vertices $a \in V_1, f \in V_2, i \in V_3, l \in V_4$ are the 4 dominating vertices of the graphs G_1 and G_2. The vertices $a, b, c, d, e \in V_1$. But, as $N_G(b) = N_G(c), b, c \in V_{12}$. Similarly $d, e \in V_{13}$ as $N_G(d) = N_G(e)$. Hence, $V_1 = V_{11} \cup V_{12} \cup V_{13}$. Similarly, $V_2 = V_{21} \cup V_{22}$, $V_3 = V_{31} \cup V_{32} \cup V_{33}$ and $V_4 = V_{41}$. So, $|V_{11}| = 1, |V_{12}| = |V_{13}| = 2$.

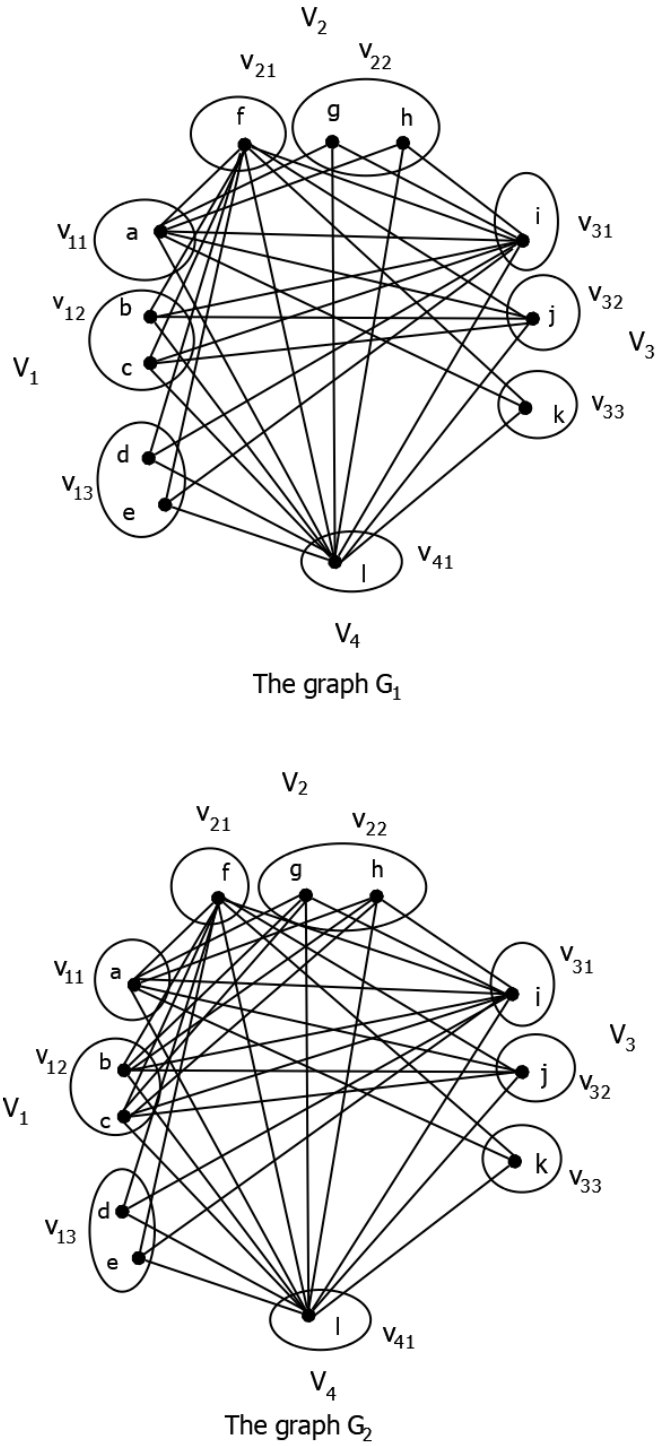

Fig. 1. The graph $G_1, G_2 \in G_f = KNG(1,2,2;1,2;1,1,1;1)$

A half graph is a chain graph without any duplicate vertices. Analogous to half graph the authors of the article [12] defined a k-half graph. We redefine 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 $\binom{k}{2}\left(\dfrac{n(n+1)}{2}\right)$ edges. Figure 2 represents a 4-half graph $G = KNG(1,1,1;1,1,1;1,1,1;1,1,1)$ having 12 vertices and 36 edges.

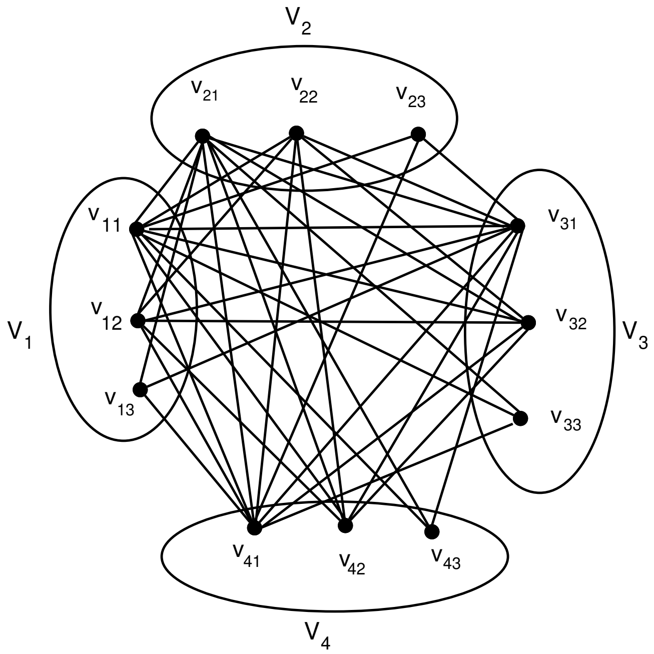

Fig. 2. 4-Half Graph

Here $|V_i| = 3, 1 \leq i \leq 4$ and $v_{i1}, 1 \leq i \leq k$ is the dominating vertex of the set V_i. Observe that $N(v_{11}) = \{v_{21}, v_{22}, v_{23}, v_{31}, v_{32}, v_{33}, v_{41}, v_{42}, v_{43}\}$ and $N(v_{13}) \subseteq N(v_{12}) \subseteq N(v_{11})$. Note that degrees of the three vertices in any partite set are 9,6,3 respectively.

The degree based topological indices have been considered only for simple graphs and very recently for graphs with self-loops [14] and for hypergraphs [15]. 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. Some of the most comprehensively studied degree-based topological indices are the Zagreb indices.

The first Zagreb index, $M_1(G)$ of a graph G is defined as the sum of the squares of the degrees over all the vertices of the graph. 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 [8].

The (first) Zagreb matrix (Z-matrix) of a graph G is a square matrix $Z(G) = (z_{ij})_{n \times n}$ of order n, defined as

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

The eigenvalues of $Z(G)$, labeled as $\zeta_1, \zeta_2, \ldots, \zeta_n$ are known as the Zagreb eigenvalues or $Z-eigenvalues$ of G and their collection is called the Zagreb spectrum or Z-spectrum of G. The Zagreb energy of a graph G is denoted by $ZE(G)$ and is defined as

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

Few bounds on Zagreb energy and the spectral radius of the (first) Zagreb matrix of the graph G is obtained in [5].

In this article we obtain spectral properties of a k-half graph with respect to its Z-matrix.

The rest of the paper is organized as follows; Section II deals with the determinant, eigenvalues and inverse of a k-half graph with respect to the Z-matrix. Bounds on Zagreb energy and spectral radius of a half graph are discussed in Section III and Section IV deals with the main and non-main eigenvalues of a k-half graph.

II. Determinant, Eigenvalues and Inverse

In this section we obtain the determinant, eigenvalues and the inverse of a k-half graph with respect to Z-matrix. The Kronecker product of a matrix $A = (a_{ij})_{p\times q}$ and $B_{r\times s}$ is defined as

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

The following basic properties about the Kronecker product are used to obtain determinant, eigenvalues and inverse of a k-half graph with respect to Z-Matrix.

Theorem 2.1: [7] 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: [7] Let A be a square matrix of order m with spectrum $\sigma(A) = (\mu_i),\ 1 \le i \le m$ and B be a square matrix of order n with $\sigma(B) = (\lambda_j),\ 1 \le j \le n$. Then $\sigma(A \otimes B) = (\mu_i \lambda_j), 1 \le i \le m,\ 1 \le j \le n$.
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: [7] If $A \in M_m$ and $B \in M_n$ 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 Z-matrix.

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

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

Then,

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

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

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

Proof: The 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 $B_n =$

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

and 0_n is a zero matrix of order n.

The Z-matrix of the k-half graph, is a Kronecker product of the adjacency matrix of the complete graph of order k and the matrix B. The proof directly follows from Theorem 2.2. ■

The following corollary follows from Theorem 2.5.

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

$$det(Z(G)) = \begin{cases} (n+1)^{2n}, & \text{if n is even} \\ -(n+1)^{2n}, & \text{otherwise.} \end{cases}$$

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

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

.
Let $\lambda_i, 1 \le i \le n$ be the eigenvalues of B with the corresponding eigenvectors $Y_i, 1 \le i \le n$. 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

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

corresponding to the Z-eigenvalue $-\lambda_i$ of $Z(G)$ 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,

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

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

$$D = \begin{bmatrix} 0 & 0 & \cdots & \frac{1}{(n+1)(k-1)} \\ 0 & \cdots & \frac{1}{(n+1)(k-1)} & \frac{-(n+2)}{(n+1)^2(k-1)} \\ 0 & \cdots & \frac{-(n+2)}{(n+1)^2(k-1)} & \frac{1}{(n+1)^3(k-1)} \\ 0 & \cdots & \ddots & \frac{n}{(n+1)^4(k-1)} \\ \vdots & \cdots & \ddots & \vdots \\ \frac{1}{(n+1)(k-1)} & \frac{-(n+2)}{(n+1)^2(k-1)} & \cdots & \frac{n^{n-3}}{(n+1)^n(k-1)} \end{bmatrix}_{n\times n}$$

Proof: The Z-matrix of the k-half graph, is a Kronecker product of the adjacency matrix of the complete graph of order k and the matrix B of order n. From Theorem 2.9, 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 2.9.

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

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

$$\text{where } D = \begin{bmatrix} 0 & 0 & \cdots & \frac{1}{(n+1)} \\ 0 & \cdots & \frac{1}{(n+1)} & \frac{-(n+2)}{(n+1)^2} \\ 0 & \cdots & \frac{-(n+2)}{(n+1)^2} & \frac{1}{(n+1)^3)} \\ 0 & \cdots & \ddots & \frac{n}{(n+1)^4} \\ \vdots & \cdots & \ddots & \vdots \\ \frac{1}{(n+1)} & \frac{-(n+2)}{(n+1)^2} & \cdots & \frac{n^{n-3}}{(n+1)^n} \end{bmatrix}_{n\times n}.$$

III. BOUNDS

Few bounds on Zagreb energy and 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 $ZE(G)$ of a half graph G using the below lemma.

Lemma 3.2: Let G be a k-half graph on kn vertices. Then,

$$Tr(Z(G)^2) = \frac{k(k-1)^3 n(n+1)(11n^2+11n+2)}{12}.$$

Proof:

$$\begin{aligned} Tr(Z(G)^2) &= k(k-1)\sum_{i=1}^{n} i(2(k-1)n - (k-1)(i-1))^2 \\ &= k(k-1)^3 \sum_{i=1}^{n} i(2n+1-i)^2 \\ &= k(k-1)^3\{(2n+1)^2 \sum_{i=1}^{n} i + \\ &\quad \sum_{i=1}^{n} i^3 - 2(2n+1)\sum_{i=1}^{n} i^2\} \\ &= \frac{k(k-1)^3 n(n+1)(11n^2+11n+2)}{12}. \end{aligned}$$

■

Theorem 3.3: Let G be a half graph on $2n$ vertices. Then

$$ZE(G) \geq \sqrt{\frac{(23n^2+11n-10)n(n+1)}{3}}$$

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

$$E_n = \begin{bmatrix} 2n & 2n-1 & \ldots & n+2 & n+1 \\ 2n-1 & 2n-2 & \ldots & n+1 & 0 \\ \vdots & \ldots & \iddots & \iddots & 0 \\ n+2 & n+1 & 0 & \ldots & 0 \\ n+1 & 0 & 0 & \ldots & 0 \end{bmatrix}$$

and 0_n is the zero matrix of order n.

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

From Lemma 3.2 we have,

$\sum_{i=1}^{2n} \zeta_i^2 = Tr(Z(G))^2 = \dfrac{n(n+1)(11n^2+11n+2)}{6}$.

Thus,

$$\sum_{i=1}^{n} \zeta_i^2 = \frac{n(n+1)(11n^2+11n+2)}{12}.$$

It is well known that

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

Hence,

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

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

$$\begin{aligned} ZE(G) &= 2\sqrt{\sum_{i=1}^{n} \zeta_i^2 + 2 \sum_{1\le i<j\le n} \zeta_i\zeta_j} \\ &\ge 2\sqrt{\frac{(n^2+n)(11n^2+11n+2)}{12} + (n^2-n)(n+1)^2} \\ &\ge \sqrt{\frac{(23n^2+11n-10)n(n+1)}{3}}. \end{aligned}$$

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

$$ZE(G) \ge (k-1)^2 \sqrt{\frac{(23n^2+11n-10)n(n+1)}{3}}$$

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

Proof: From Theorem 2.7,

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

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

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

We note that $\prod_{i=1}^{n} |\lambda_i| = (k-1)^n (n+1)^n$
and
$\sum_{i=1}^{n} |\lambda_i|^2 = (k-1)^2 \left(\frac{n(n+1)(11n^2+11n+2)}{12}\right)$.

Applying the arithmetic–geometric mean inequality, we get

$$\begin{aligned} 2\sum_{1\le i<j\le n} |\lambda_i||\lambda_j| &\ge n(n-1)(\prod_{i=1}^{n} |\lambda_i|)^{\frac{2}{n}} \\ &= n(n-1)(k-1)^2(n+1)^2. \end{aligned}$$

Now,

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

Substituting
$\sum_{i=1}^{n} |\lambda_i|^2 = \dfrac{(k-1)^2 n(n+1)(11n^2+11n+2)}{12}$, and simplifying we get

$$ZE(G) \ge (k-1)^2 \sqrt{\frac{(23n^2+11n-10)n(n+1)}{3}}.$$

■

Using Lemma 3.5, we give another lower bound in terms of determinant of the Z-matrix.

Lemma 3.5: [5] Let G be a graph with n vertices. Then

$$ZE(G) \ge n\sqrt[n]{|detZ(G)|}.$$

Theorem 3.6: Let G be a k-half graph on kn vertices. Then,

$$ZE(G) \ge kn(n+1)(k-1)\sqrt[k]{k-1}$$

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

Proof: From Lemma 3.5 we have,

$$ZE(G) \ge N\sqrt[N]{|detZ(G)|},$$

where N is order of the graph G. Therefore,

$$\begin{aligned} ZE(G) &\ge kn\sqrt[kn]{|detZ(G)|} \\ &= kn\sqrt[kn]{((n+1)^k (k-1)^{k+1})^n} \\ &= kn\sqrt[kn]{(n+1)^{kn}(k-1)^{(k+1)n}} \\ &= kn(n+1)(k-1)\sqrt[k]{k-1}. \end{aligned}$$

■

The following theorem gives the relation between energy of a k-half graph G with respect to the adjacency matrix and the Zagreb matrix.

Theorem 3.7: Let G be a k-half on kn vertices. Let $E(G)$ denote the energy of G with respect to its adjacency matrix $A(G)$. Then,

$$ZE(G) \le k(n-1)E(G),$$

with equality only if $n = 1$, i.e., G is a complete graph on k vertices.

Proof: We have, $ZE(G) \le \Delta(G)E(G)$ and the equality if and only if G is a regular graph, where $\Delta(G)$ is the maximum degree of the graph G. Hence, the proof follows directly. ■

Lemma 3.8: [9] Let G be a graph on n vertices, then

$$ZE(G) \le \sum_{i=1}^{n} \sqrt{\sum_{v_iv_j \in E} (d_i + d_j)^2}$$

Theorem 3.9: Let G be a k-half on kn vertices. Then

$$ZE(G) \le k(k-1) \sum_{j=0}^{n-1} \sqrt{(k-1) \sum_{i=j}^{n-1} (2n-i)^2}$$

Proof: For every dominating vertex v_i of the k-half graph G we have,

$$\sum_{v_iv_j \in E} (d_i + d_j)^2 = (k-1)[(2n(k-1))^2 + \cdots + ((n+1)(k-1))^2]$$
$$= (k-1)^3 \sum_{i=0}^{n-1} (2n-i)^2.$$

Also, for every vertex v_i of degree $(n-1)(k-1)$ of G,

$$\sum_{v_iv_j \in E} (d_i + d_j)^2 = (k-1)^3 \sum_{i=1}^{n-1} (2n-i)^2.$$

Similarly, for every vertex v_j of degree $(n-i+1)(k-1)$ in G, we have

$$\sum_{v_jv_h \in E} (d_j + d_h)^2 = (k-1)^3 \sum_{i=j}^{n-1} (2n-i)^2$$

Now by using Lemma 3.8,

$$\begin{aligned} ZE(G) &\le k\sqrt{(k-1)^3 \sum_{i=0}^{n-1} (2n-i)^2} \\ &+ k\sqrt{(k-1)^3 \sum_{i=1}^{n-1} (2n-i)^2} \\ &\vdots \\ &+ k\sqrt{(k-1)^3(n+1)^2} \\ &= k(k-1) \sum_{j=0}^{n-1} \sqrt{\sum_{i=j}^{n-1} (2n-i)^2 (k-1)} \end{aligned}$$

■

Theorem 3.10: [5] Let G be a graph with n vertices. Then,

$$\sqrt{Tr(Z(G)^2)} \le ZE(G) \le \sqrt{nTr(Z(G)^2)}.$$

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

$$\frac{k-1}{2}\sqrt{nkA} \le ZE(G) \le \frac{nk(k-1)}{2}\sqrt{A},$$

where $A = \dfrac{(k-1)(n+1)(11n^2+11n+2)}{3}$.

Proof: Proof follows from Theorem 3.10 and Lemma 3.2. ■

Theorem 3.12: Let G be a k-half graph on kn vertices and $\zeta_1(G)$ be the spectral radius of G. Then,

$$\zeta_1(G) \ge \frac{\sum_{i=1}^{n} (n-i+1)(k-1)^3(3n-i+2)}{2kn}.$$

Proof: If $\zeta_1(G)$ denote the spectral radius of G then we have

$$\zeta_1(G) = \sup_x \frac{x^\intercal Z(G)x}{x^\intercal x} \ge \frac{J^\intercal Z(G)J}{J^\intercal J},$$

where J is an all one column vector of appropriate size.

$$J^\intercal Z(G)J = (k-1)c_i = (k-1)^2 s_i,$$

where s_i and c_i respectively denote the i^{th} column sum of the matrix B and $Z(G)$ and also

$$s_i = \frac{(k-1)}{2} \sum_{i=1}^{n} (n-i+1)(3n-i+2).$$

■

Lemma 3.13: [13] Let G be a connected graph of order n, maximum degree Δ and Z-spectral radius ζ_1. If $M_1(G)$ denotes the first Zagreb index of the graph G, then

$$\frac{M_1(G) + \sum_{u \in V} d_{2,u}}{n} \le \zeta_1 \le 2\Delta^2,$$

where $d_{2,u}$ is is the sum of degrees of all the vertices which are adjacent to u in G. Equality holds in both if and only if G is regular.

Theorem 3.14: Let G be a k-half graph on kn vertices and $\zeta_1(G)$ be the spectral radius of G. Then,

$$\zeta_1(G) \le 2n^2(k-1)^2.$$

Equality in the above bound holds if and only if G is a complete k-partite graph.

Proof: The upper bound directly follows from Lemma 3.13, by noting that the maximum degree in a k-half graph on kn vertices is $n(k-1)$. ■

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 being main and also with all eigenvalues being non-main except 0. In [1], the authors characterize the chain graphs with 2 main eigenvalues. One can refer to [6] 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 is 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 $-\lambda_i,\ 1 \le i \le n$, repeats $k-1$ times, of a k-half graph are non-main Z-eigenvalues.

Proof: From Theorem 2.7, we know that the eigenvalue $-\lambda_i,\ 1 \le i \le n$, 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 $Y_iJ = 0, (Y_iJ \neq 0)$. Thus, $X_iJ = 0, (X_iJ \neq 0)$.Hence the eigenvalue $(k-1)\lambda_i$ is also non-main (main). ■

From Theorems 4.1 and 4.2, for a k-half graph on kn vertices, at least $kn - n$ Zagreb-eigenvalues are non-main and at most n 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, $(k-1)^2(2 \pm \sqrt{13})$ are the main Z-eigenvalues and $(1-k)(2 \pm \sqrt{13})$ 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 $\lambda_1 = (k-1)(2+\sqrt{13}), \lambda_2 = (k-1)(2-\sqrt{13})$ are the Z-eigenvalues of

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

From Theorem 4.1, $-\lambda_1 = (1-k)(2+\sqrt{13})$ and $-\lambda_2 = (1-k)(2-\sqrt{13})$ 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 $\lambda_1 = (k-1)(2+\sqrt{13})$ and $\lambda_2 = (k-1)(2-\sqrt{13})$ 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

$$X_1 = \begin{pmatrix} l \\ \frac{3l}{\sqrt{13}+2} \end{pmatrix} \ and \ X_2 = \begin{pmatrix} l \\ \frac{3l}{2-\sqrt{13}} \end{pmatrix}$$

where $l \neq 0$. As $X_1^TJ \neq 0$ and $X_2^TJ \neq 0$, the eigenvalues $(k-1)(2+\sqrt{13}), (k-1)(2-\sqrt{13})$ are the main Z-eigenvalues of the matrix B. Hence, the main Z-eigenvalues of G are $(k-1)^2(2 \pm \sqrt{13})$. ■

V. Conclusion

The determinant, Z-eigenvalues and inverse of a k-half graph with respect to the Z-matrix is obtained along with a few Zagreb energy and spectral radius bounds. The main and non-main eigenvalues of a k-half graph with respect to the Z-matrix are also discussed. One can try to obtain spectral properties of a k-half graph with respect to its adjacency matrix and second Zagreb matrix.

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