On the First Zagreb Energy of Graphs

SANGAM MADABHAVI, K ARATHI BHAT and SHAHISTHA HANIF*

***Abstract*—Researchers have been devoting themselves to the study of extended adjacency matrices, one of the many novel graph matrices that are being proposed as a potential extension of the spectral theory of classical graph matrices. The concept of the Zagreb matrix and Zagreb energy of a graph has been introduced to expand some beneficial molecular topological properties. The (first) Zagreb matrix $Z(G) = (z_{ij})_{n\times n}$ 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. The spectral properties of the Zagreb matrix of some classes of graphs are explored in this article. The main contribution of the article is that the Zagreb energy of a graph, obtained by means of various graph products like the strong product, corona product, Kronecker product etc. are investigated, and well-established relations are derived in terms of their base graphs.**

***Index Terms*—Zagreb matrix, Kronecker product, Cartesian product, coronal, quotient matrix.**

I. INTRODUCTION

Graphs considered here are simple, finite, undirected, and connected with vertex set $V = V(G)$ and edge set $E = E(G)$. The adjacency matrix $A(G)$ of a graph G is the $n \times n$ matrix in which its $(i,j)^{th}$-entry is 1 if $v_iv_j \in E(G)$ and 0 otherwise. By the denotation $u \sim_G v$ (or $u \nsim_G v$) we mean that u is adjacent to v (or u is not adjacent to v) in G. The degree of a vertex u in G is denoted by $d_G(u)$. The suffix G in the notations $\sim_G$, $\nsim_G$ and $d_G(u)$ is conveniently ignored if the graph under discussion is clearly understood. For a subset $S \subseteq V(G)$, the subgraph induced by the vertices in S is denoted by $\langle S \rangle$.

Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{n-1} \geq \lambda_n$ be the eigenvalues of $A(G)$. The largest eigenvalue λ_1 is usually referred to as the spectral radius of the graph G. The energy of the graph G is defined as $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$.

The first and second Zagreb indices are defined as

$$M_1(G) = \sum_{v \epsilon V(G)} d^2(v) = \sum_{uv \epsilon E(G)} [(d(u) + d(v))],$$

$$M_2(G) = \sum_{uv \epsilon E(G)} [(d(u)d(v))].$$

In general convention, we write TI for a topological index that can be represented as $TI = TI(G) = \sum_{u \sim v} \Phi_{d_u d_v}$, where Φ is an appropriately chosen function with the property $\Phi_{d_u d_v} = \Phi_{d_v d_u}$.

A general extended adjacency matrix $A_\Phi(G) = (a_{\Phi_{uv}})$ of G is defined as

$$A_\phi(G) = (a_{\Phi uv})_{n\times n} = \begin{cases} \Phi_{d_u d_v}; & \text{if } u \sim v \\ 0; & \text{otherwise} \end{cases}.$$

If $\Phi_{d_u d_v} = d(u) + d(v)$, i.e., $TI = M_1(G)$ (the first Zagreb index), we get the (first) Zagreb matrix [2]. The (first) Zagreb matrix of a graph G is a square matrix $Z^{(1)}(G) = Z(G)$ of order n, and is defined as

$$Z_{ij} = \begin{cases} d(u) + d(v); & \text{if } uv \in E(G) \\ 0; & \text{otherwise.} \end{cases}$$

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

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

The largest eigenvalue ζ_1 is the the spectral radius of the Zagreb matrix, if its eigenvalues can be expressed as $\zeta_1 \geq \zeta_2 \geq \ldots \geq \zeta_n$. A few articles on the spectral properties of the Zagreb matrix can be found in [2]–[6].

Let A be the matrix of order n described in the block form

$$A = \begin{pmatrix} M_{11} & \ldots. & M_{1t} \\ \vdots & \ddots & \vdots \\ M_{t1} & \ldots. & M_{tt} \end{pmatrix}_{n\times n},$$

where the blocks M_{ij} are $n_i \times n_j$ matrices for any $1 \leq i, j \leq t$ and $n = n_1 + \cdots + n_t$.

A partition D of a square matrix A is said to be equitable if all the blocks of the partitioned matrix have constant row sums and each of the diagonal blocks is of square order. A quotient matrix B of a square matrix A corresponding to an equitable partition is a matrix whose entries are the constant row sums of the corresponding blocks of A. A quotient matrix is a useful tool for finding some eigenvalues of matrix A. In the theory of graph spectra, equitable partitions play an important role, mostly because of the following results.

Theorem I.1. *[7] Let A be a real symmetric matrix with a quotient matrix B. Then the characteristic polynomial of B divides the characteristic polynomial of A.*

Theorem I.2. *[8] Let D be an equitable partition of the connected graph G. Then $A(G)$ and the quotient matrix B of D has the same spectral radius λ_1.*

Definition I.1. *The Kronecker product of a matrix $A =$*

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Sangam Madabhavi is a research scholar in the department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India, 576104 (email:sangammadabhavi340@gmail.com).

K Arathi Bhat is an Associate Professor of Mathematics department, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India, 576104 (email: arathi.bhat@manipal.edu)

Shahistha Hanif is an Assistant Professor of Mathematics department, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, India, 576104 (*Corresponding author to provide email: shahistha.hanif@manipal.edu; Phone: 9972785394).

$(a_{ij})_{p\times q}$ *and* $B_{r\times s}$ *is defined as*

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

Theorem I.3. *[1] 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 $\sigma(A\otimes B)=(\mu_i\lambda_j), 1\le i\le m,\ 1\le j\le n$.*

The rest of the article is organized as follows: Section 2 deals with Zagreb eigenvalues of a few standard classes of graphs. One might be interested to know, how the Zagreb energy of two graphs can be related with the graph obtained from the original graphs by applying some graph operations. The spectral properties of the Zagreb matrix of a graph which is obtained by applying some graph operations like Kronecker product, Corona product, Cartesian product and Strong product on two graphs are discussed in Section 3 along with the Zagreb energy of a shadow graph which is obtained by applying some graph operation on a given graph itself.

II. Some standard classes of graphs

A great deal of knowledge is available in the literature about the energy of standard classes like wheel, complete k-partite graph and friendship graph pertaining to the adjacency matrix. In a similar vein, this section deals with the Zagreb energy of a wheel, a complete k-partite graph and a friendship graph.

A. Wheel Graph

The wheel graph, denoted by W_n, can be obtained by join of K_1 and C_{n-1}. Let the vertices of W_n be labeled as $v_1, v_2,\dots,v_n$. The vertex $v_k\sim v_{k+1}$ for $2\le k\le n-1$, and $v_n\sim v_2$ and v_1 is adjacent to all the other vertices. The following remark gives the determinant of wheel graphs.

Remark II.1. *[9] If $n\ge 4$, then*

$$det\,(A(W_n))=\begin{cases}2(n-1), & \text{if } n \bmod 4 \text{ is } 3\\ 0, & \text{if } n \bmod 4 \text{ is } 1\\ 1-n, & \text{otherwise}\end{cases}.$$

Theorem II.1. *Let $\lambda_k\neq 2$ be the eigenvalues of $A(C_{n-1})$ with the corresponding eigenvector V_k for $k=1,2,\dots,n-2$. Then for each of $1\le k\le n-2$, $6\lambda_k$ are the Zagreb eigenvalues of $Z(W_n)$ with eigenvectors $(0,V_k)^T$. Further, the other two eigenvalues of $Z(W_n)$ are $6\pm\sqrt{n^3+3n^2+32}$ with corresponding eigenvectors $(\frac{n^2+n-2}{6\pm\sqrt{n^3+3n^2+32}},1,1,\dots,1)^T$.*

Proof: The Zagreb matrix of W_n can be viewed as a block matrix as

$$Z(W_n)=\begin{pmatrix}0 & (n+2)J_{1,n-1}\\ (n+2)J_{n-1,1} & 6A(C_{n-1})\end{pmatrix}.$$

Let $X=[0,\ V_k]^T$. Then, $Z(W_n)X=6\lambda_kV_k$, where $1\le k\le n-2$, which proves the first part of the theorem. Further, the quotient matrix of $Z(W_n)$ is given by,

$$B_z(W_n)=\begin{pmatrix}0 & (n+2)\\ (n+2)(n-1) & 12\end{pmatrix}.$$

The characteristic polynomial of the above quotient matrix is,

$$x^2-12x-(n+2)^2(n-1)=0.$$

Hence, $6\pm\sqrt{n^3+3n^2+32}$ are the eigenvalues of $Z(W_n)$. On solving $B_z(W_n)X=\lambda X$, we get the desired eigenvectors. ■

From Theorem I.2 we have the following note.

Note II.1. *The spectral radius of $Z(W_n)$ is given by $6+\sqrt{n^3+3n^2+32}$.*

Corollary II.2. *The determinant of $Z(W_n)$ is given by,*

$$det\,(Z(W_n))=\begin{cases}6^{n-2}\ 2(n+2)^2 2(n-1), & \text{if } n \bmod 4 \text{ is } 3\\ 0, & \text{if } n \bmod 4 \text{ is } 1\\ 6^{n-2}\ 2(n+2)^2(1-n), & \text{otherwise}\end{cases}.$$

Proof: We have,

$$det\,(Z(W_n))=(n+2)^2 det\begin{pmatrix}0&1&1&1&\dots&1&1\\1&0&6&0&\dots&0&6\\1&6&0&6&\dots&0&0\\ \vdots&\vdots&\vdots&\vdots&\ddots&\vdots&\vdots\\1&0&0&0&\dots&0&6\\1&6&0&0&\dots&6&0\end{pmatrix}.$$

By performing $R_i\to R_i-R_{i+1}, 2\le i\le n-1$, we get

$$det\,(Z(W_n))\simeq 6^{n-2}(n+2)^2 det\begin{pmatrix}0&1&1&\dots&1&1\\0&-1&1&\dots&0&1\\0&1&-1&\dots&0&0\\ \vdots&\vdots&\vdots&\ddots&\vdots&\vdots\\0&-1&0&\dots&-1&1\\1&1&0&\dots&1&0\end{pmatrix}.$$

By performing $R_i\to R_i+R_{i+1}+R_{i+2}+\dots+R_n$; $i=2,3,\dots,n-1$ we get,

$$det\,(Z(W_n))=6^{n-2}(n+2)^2 det\,(A(W_n))$$

and by Remark II.1 the proof follows. ■

B. Complete k-partite Graph

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 G 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 $K_{p_1,p_2,\dots,p_k}$.

Theorem II.3. *The Z-spectrum of $K_{p,p,\dots,p}$ is given by*

$$\begin{pmatrix}2p^2(k-1)^2 & -2p^2(k-1)) & 0\\ 1 & k-1 & pk-k\end{pmatrix},$$

where the first and the second rows in the above array represent the eigenvalues and their multiplicities, respectively. The Zagreb energy is given by

$$Z\mathcal{E}(K_{p,p,\dots,p})=4p^2(k-1)^2.$$

Proof: We know that the spectrum of $A(K_{p,p,\dots,p})$ is given by

$$\begin{pmatrix}p(k-1) & -p & 0\\ 1 & k-1 & pk-k\end{pmatrix}.$$

The proof follows by noting that,

$$Z(K_{p,p,\ldots,p}) = 2p(k-1)A(K_{p,p,\ldots,p}).$$

∎

The results for the complete bipartite graphs follow as a special case when $k=2$.

Corollary II.4. *The Z-spectrum of complete bipartite graph $K_{p,q}$ is given by*

$$\begin{pmatrix} (p+q)\sqrt{pq} & -(p+q)\sqrt{pq} & 0 \\ 1 & 1 & p+q-2 \end{pmatrix},$$

and

$$Z\mathcal{E}(K_{p,q}) = 2(p+q)\sqrt{pq}.$$

Proof: Proof follows by noting that, $Z(K_{p,q}) = (p+q)A(K_{p,q})$, and the eigenvalues of $A(K_{p,q})$ are $\pm\sqrt{pq}$ with multiplicity 1 and 0 with multiplicity $p+q-2$. ∎

C. Friendship Graph

A friendship graph denoted by F_n, (for $n \geq 2$) with $2n+1$ vertices is obtained from a wheel graph W_{2n+1} by removing every alternate edge on the outer cycle.

$$A(F_n) = \begin{pmatrix} 0 & J_{1,n} & J_{1,n} \\ J_{n,1} & 0_n & I_n \\ J_{n,1} & I_n & 0_n. \end{pmatrix}.$$

The spectrum ([13]) of $A(F_n)$ is given as follows;

$$spec(A(F_n)) = \begin{pmatrix} \frac{1+\sqrt{1+8n}}{2} & \frac{1-\sqrt{1+8n}}{2} & 1 & -1 \\ 1 & 1 & n-1 & n \end{pmatrix}.$$

Similar to this, we give spectrum of $Z(F_n)$ in the following.

Theorem II.5. *Let $Z(F_n)$ be the Zagreb matrix of the friendship graph F_n with $2n+1$ vertices. Then,*

1) $spec(Z(F_n)) = \begin{pmatrix} 2 \pm 2\sqrt{1+2n(n+1)^2} & 4 & -4 \\ 1 & n-1 & n \end{pmatrix}$
2) $Z\mathcal{E}(F_n) = 4\big((2n-1) + \sqrt{1+2n(n+1)^2}\big)$
3) $det(Z(F_n)) = (-1)^{n+1}(2)^{4n+1}n(n+1)^2$.

Proof: The Zagreb matrix of F_n can be viewed as

$$Z(F_n) = \begin{pmatrix} 0 & (2n+2)J_{1,n} & (2n+2)J_{1,n} \\ (2n+2)J_{n,1} & 0_n & 4I_n \\ (2n+2)J_{n,1} & 4I_n & 0_n \end{pmatrix}.$$

Let the characteristic polynomial be $\Phi_Z(\zeta) = det(Z(F_n) - \zeta I)$. That is,

$$\Phi_Z(\zeta) = det\begin{pmatrix} -\zeta & (2n+2)J_{1,n} & (2n+2)J_{1,n} \\ (2n+2)J_{n,1} & -\zeta I_n & 4I_n \\ (2n+2)J_{n,1} & 4I_n & -\zeta I_n \end{pmatrix}$$

By performing the row operation $R_i \rightarrow R_i - R_{n+i}$; $i = 2,\ldots,n+1$ we get,
$\Phi_Z(\zeta) \simeq$

$$(\zeta+4)^n det\begin{pmatrix} -\zeta & (2n+2)J_{1,n} & (2n+2)J_{1,n} \\ 0_{n,1} & -I_n & I_n \\ (2n+2)J_{n,1} & 4I_n & -\zeta I_n \end{pmatrix}$$

By performing the column operation $C_i \rightarrow C_i + C_{n+i}$; $i = 2,\ldots,n+1$ we get,
$\Phi_Z(\zeta) \simeq$

$$(\zeta+4)^n det\begin{pmatrix} -\zeta & (4n+2)J_{1,n} & (2n+2)J_{1,n} \\ 0_{n,1} & 0_n & I_n \\ (2n+2)J_{n,1} & (4-\zeta)I_n & -\zeta I_n \end{pmatrix}$$

By performing $C_i \rightarrow C_i - C_{i+1}$; $i = 2,\ldots,n$, we get,

$$\Phi_Z(\zeta) = (\zeta+4)^n(\zeta-4)^{n-1}\Psi(\zeta)$$

where $\Psi(\zeta)$ is the remaining factor of $\Phi_Z(\zeta)$.
The remaining two eigenvalues of $Z(F_n)$ can be obtained from the quotient matrix which is shown as below.

$$B_Z(F_n) = \begin{pmatrix} 0 & 4n(n+1) \\ 2(n+1) & 4 \end{pmatrix}.$$

The characteristic polynomial of the above quotient matrix is,

$$\zeta^2 - 4\zeta - 8n(n+1)^2 = 0.$$

Hence, the other two eigenvalues of $Z(F_n)$ are $2 \pm 2\sqrt{1+2n(n+1)^2}$.
Now,
$det(Z(F_n)) = \prod_{i=1}^{2n+1}\zeta_i = (-4)^n(4)^{n-1}(2 + 2\sqrt{1+2n(n+1)^2})(2 - 2\sqrt{1+2n(n+1)^2}).det(Z(F_n)) = (-1)^{n+1}(2)^{4n+1}n(n+1)^2$.
$Z\mathcal{E}(F_n) = \sum_{i=1}^{2n+1} \mid \zeta_i \mid = 4\big((2n-1) + \sqrt{1+2n(n+1)^2}\big)$. ∎

III. Binary Operations of Graphs

In this section we investigate the Zagreb energy of some binary operations. Firstly, the Zagreb energy of a graph obtained by means of some graph operation on a given graph G is considered. We show that the new graph's Zagreb energy is a multiple of Zagreb energy of the original graph, which is referred as a base graph. Next, we derive conditions on G and H such that Zagreb energy of the graph Γ, which is obtained by applying some graph operations on G and H, can be related to the Zagreb energy of G and H.

A. Shadow Graph

The shadow graph $D_2(G)$ of a connected graph G is constructed by taking two copies of G, say G' and G''. Join each vertex u' in G' to the neighbors of the corresponding vertex u'' in G''.

Theorem III.1. $Z\mathcal{E}(D_2(G)) = 4Z\mathcal{E}(G)$.

Proof: The Zagreb matrix of $D_2(G)$ can be written as a block matrix as follows:

$$Z(D_2(G)) = 2\begin{pmatrix} Z(G) & Z(G) \\ Z(G) & Z(G) \end{pmatrix} = J_2 \otimes 2Z(G).$$

Hence, from Theorem I.3, $spec(Z(D_2(G))) = \begin{pmatrix} 0 & 4\zeta_i \\ n & 1 \end{pmatrix}$, where ζ_i, $i = 1,2,\ldots,n$, are the eigenvalues of $Z(G)$. Therefore,

$$Z\mathcal{E}(D_2(G)) = \sum_{i=1}^{n} \mid 4\zeta_i \mid = 4Z\mathcal{E}(G).$$

∎

Corollary III.2. *Let G be a regular graph with regularity r. Then,*

$$Z\mathcal{E}(D_2(G)) = 4r\mathcal{E}(G).$$

Definition III.1. *The m-shadow graph $D_m(G)$ of a connected graph G is constructed by taking m copies of G, say $G_1, G_2, \ldots, G_m$ then join each vertex u in G_i to the neighbors of the corresponding vertex v in G_j, $1 \leq i,j \leq m$.*

Theorem III.3. $Z\mathcal{E}(D_m(G)) = m^2 Z\mathcal{E}(G)$.

Proof: Proof follows by noting that

$$Z(D_m(G)) = J_m \otimes mZ(G).$$

■

B. Kronecker Product

Consider two graphs, G and H, with vertex sets V and W, respectively. Then the Kronecker product of G and H denoted by $G \otimes H$ is the graph with vertex set $V \times W$ and two vertices (v, w) and (v', w') are adjacent to each other whenever $v \sim_G v'$ and $w \sim_H w'$.
Note that, $A(G \otimes H)_{mn\times mn} = A(G) \otimes A(H)$

$$= \begin{pmatrix} a_{11}A(H) & a_{12}A(H) & \cdots & a_{1m}A(H) \\ a_{21}A(H) & a_{22}A(H) & \cdots & a_{2m}A(H) \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}A(H) & a_{m2}A(H) & \cdots & a_{mm}A(H) \end{pmatrix}_{mn\times mn}.$$

Note III.1. *Let G and H be two graphs of order m and n with eigenvalues $\{\lambda_1, \ldots, \lambda_m\}$ and $\{\mu_1, \ldots, \mu_n\}$, respectively. Then, the eigenvalues of $A(G \otimes H)$ will be $\{\lambda_i\mu_j : 1 \le i \le m; 1 \le j \le n\}$ and $\mathcal{E}(G \otimes H) = \mathcal{E}(G)\mathcal{E}(H)$.*

Let the vertices of G and H be $\{v_1, v_2, \ldots, v_m\}$ and $\{u_1, u_2, \ldots, u_n\}$ respectively. Observe that $Z(G \otimes H)$ is a block matrix $B = (B_{ij})$ of order m, with all diagonal blocks B_{ii} being a 0 matrix of order n and other blocks B_{ij} are either a 0 matrix of order n or a non-zero block matrix of order n depending upon whether $v_i \nsim_G v_j$ or $v_i \sim_G v_j$ in G. Suppose $v_r \sim_G v_s$ then the block B_{rs} is a non-zero block given by,

$$B_{rs} = \begin{array}{c} \\ (v_r, u_1) \\ (v_r, u_2) \\ \vdots \\ (v_r, u_n) \end{array} \begin{array}{c} \begin{array}{cccc} (v_s, u_1) & (v_s, u_2) & \ldots & (v_s, u_n) \end{array} \\ \left(\begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \end{array} \right) \end{array}.$$

The entries corresponding to $(v_r, u_b)^{th}$ row and $(v_s, u_d)^{th}$ column of the block B_{rs} is $d_G(v_r)d_H(u_b) + d_G(v_s)d_H(u_d)$ if $u_b \sim_H u_d$, otherwise it is zero.

Theorem III.4. *Let $Z(G)$ and $Z(H)$ be the Zagreb matrices of graphs G and H respectively. Then,*

$$Z(G \otimes H) \neq Z(G) \otimes Z(H).$$

Proof: Suppose $v_i \sim_G v_j$ and $v_r \sim_H v_s$. Then, $(v_i, v_r) \sim_{G\otimes H} (v_j, v_s)$. The entry corresponding to $(i, r)^{th}$ row and $(j, s)^{th}$ column in $Z(G \otimes H)$ is given by $(d_G(v_i) \times d_H(v_r)) + (d_G(v_j) \times d_H(v_s))$, which is not equal to the entry corresponding to $(i, r)^{th}$ row and $(j, s)^{th}$ column i.e., $(d_G(v_i) + (d_G(v_j)) \times (d_H(v_r) + d_H(v_s))$. ■

Next, we have a theorem which guarantees that the Zagreb matrices do not preserve the operation of Kronecker product as in the case of adjacency matrices.

Theorem III.5. *$Z(G \otimes H) = A(G) \otimes B$ for some block matrix B if and only if G is regular.*

Proof: We know that if B_{rs} is a non-zero block, then the entries corresponding to $(v_r, u_b)^{th}$ row and $(v_s, u_d)^{th}$ column of the block B_{rs} is $d_G(v_r)d_H(u_b) + d_G(v_s)d_H(u_d)$ if $u_b \sim_H u_d$, otherwise it is zero. Then, the entry corresponding to $(v_r, u_d)^{th}$ row and $(v_s, u_b)^{th}$ column of the block B_{rs} is $d_G(v_r)d_H(u_d) + d_G(v_s)d_H(u_b)$. In order to write $Z(G \otimes H) = A(G) \otimes B$, every non-zero block B_{ij} of $Z(G \otimes H)$ must be same. By symmetry, $d_G(v_r)d_H(u_b) + d_G(v_s)d_H(u_d) = d_G(v_r)d_H(u_d) + d_G(v_s)d_H(u_b)$. This implies $d_G(v_s) = d_G(v_r)$. Hence, the result follows.
Conversely, let G be a regular graph with regularity r and let $v_r \sim_G v_s$ and $u_b \sim_H u_d$. Then the entry corresponding to $(v_r, u_b)^{th}$ row and $(v_s, u_d)^{th}$ column of the block B_{rs} is $r(d_H(u_b) + d_H(u_d))$ which is also equal to the entry corresponding to $(v_l, u_b)^{th}$ row and $(v_t, u_d)^{th}$ column of the block B_{lt}, if $v_l \sim_G v_t$. Hence, each non zero blocks $B_{rs} = B_{lt} = B$. The diagonal blocks B_{ii} and other blocks B_{ij} are equal to a zero matrix of order n when $v_i \nsim_G v_j$. Hence, the converse part follows. ■

Corollary III.6. *Let G and H be two graphs. Then,*

$$Z(G \otimes H) = \frac{1}{2} Z(G) \otimes Z(H) = kA(G) \otimes Z(H)$$

if and only if G is k-regular.

Proof: Proof follows from Theorem III.5 by noting that $B = kZ(H)$ implies G to be regular with regularity k and $Z(G) = 2kA(G)$. ■

Corollary III.7. *Let G be a regular graph with regularity r. Let λ_i, μ_j and θ_l be the eigenvalues of $A(G)$, $Z(G)$ and $Z(H)$ respectively, $1 \le i, j \le m$ and $1 \le l \le n$. Then, the eigenvalues of $Z(G \otimes H)$ are either $\{r\lambda_i\theta_l \mid i = 1, \ldots, m; l = 1, \ldots, n\}$ or $\{\frac{1}{2}\mu_j\theta_l | j = 1, \ldots, m; 1, \ldots, n\}$. Also,*

$$Z\mathcal{E}(G \otimes H) = \frac{1}{2} Z\mathcal{E}(G)Z\mathcal{E}(H) = k\mathcal{E}(G)Z\mathcal{E}(H).$$

Next, we derive conditions on G and H such that the Zagreb matrix $Z(G \otimes H)$ has exactly two entries '0' and 'k' for some constant k.

Theorem III.8. *$Z(G\otimes H)$ is a $(0, k)$ matrix, where k is any constant, if and only if the graphs G and H satisfies any one of the following conditions.*

i) *both G and H are regular.*
ii) *G is a regular graph and H is bipartite biregular graph with partition $\{V_1, V_2\}$ and $\langle V_1\rangle$ is r_1 regular and $\langle V_2\rangle$ is r_2 regular.*
iii) *G is regular and H is a disconnected graph with k components $c_1, c_2, \ldots, c_t$ such that each components c_i is bipartite biregular graph with partition $\{V_1^i, V_2^i\}$ and $\langle V_1^i\rangle$ is r_i regular and $\langle V_2^i\rangle$ is s_i regular, such that $r_i + s_i = r_j + s_j$ where $i \neq j$ and $1 \le i, j \le t$*

Proof: Let $v_r \sim_G v_s$ and $u_b \sim_H u_d$. Then, $(v_r, u_b) \sim_{G\otimes H} (v_s, u_d)$ and $(v_r, u_d) \sim_{G\otimes H} (v_s, u_b)$ in $G \otimes H$. Then the entries corresponding to $(v_r, u_b)^{th}$ row and $(v_s, u_d)^{th}$ column of the block B_{rs} is $d_G(v_r)d_H(u_b) + d_G(v_s)d_H(u_d)$ and that of $(v_r, u_d)^{th}$ row and $(v_s, u_b)^{th}$ column is $d_G(v_r)d_H(u_d) + d_G(v_s)d_H(u_b)$. Now, in order to get all the non-zero entries of the non-zero blocks of $Z(G \otimes H)$ as same, G must be regular.
Let G be regular with regularity r. Now suppose H is connected, then u_b is adjacent to another vertex say, u_c in H. Then the entries corresponding to $(v_r, u_b)^{th}$ row

and $(v_s, u_c)^{th}$ column of the block is $r(d_H(u_b) + d_H(u_c))$ and that must be equal to $r(d_H(u_b) + d_H(u_d))$ implying $d_H(u_d) = d_H(u_c)$. Hence H must be either regular with regularity s or a bipartite biregular graph with partition $\{V_1, V_2\}$ and $\langle V_1\rangle$ is r_1 regular and $\langle V_2\rangle$ is r_2 regular. In both the cases the non-zero entries of the block matrix be either $k = 2rs$ or $k = r(r_1 + r_2)$ a constant.

Suppose H is disconnected graph with t components say $c_1, c_2, \ldots, c_t$. Let $u_b \sim u_d$ in $c_i, 1 \le i \le t$. Then the component c_i must be biregular bipartite graph with partition $\{V_1^i, V_2^i\}$ and $\langle V_1^i\rangle$ is r_i regular and $\langle V_2^i\rangle$ is s_i regular. Similarly, if $u_a \sim u_c$ in $c_j, i \ne j$, then again we get that the component c_j must be biregular bipartite graph with partition $\{V_1^j, V_2^j\}$ and $\langle V_1^j\rangle$ is r_j regular and $\langle V_2^j\rangle$ is s_j regular. In order to get all the non-zero entries of the blocks B_{ij} as some constant, we get $r_i + s_i = r_j + s_j$ for every $1 \le i, j \le t$.

Conversely, if the condition $(i), (ii)$ or (iii) is true then it is easy to observe that $Z(G \otimes H)$ is a $(0, k)$ matrix where k is any constant. ■

Corollary III.9. *Let G be a regular graph with regularity r.*

- *Suppose H is also regular with regularity s, then $Z\mathcal{E}(G \otimes H) = 2rs\mathcal{E}(G)\mathcal{E}(H)$.*
- *Suppose H is bipartite biregular graph with partition $\{V_1, V_2\}$ and $\langle V_1\rangle$ is r_1 regular and $\langle V_2\rangle$ is r_2 regular, then $Z\mathcal{E}(G \otimes H) = r(r_1 + r_2)\mathcal{E}(G)\mathcal{E}(H)$.*

C. Cartesian Product

Let G and H be two graphs with vertex sets V and W respectively. Then the Cartesian product, $G\Box H$ is the graph with vertex set $V \times W$, where $(v, w) \sim_{G\Box H} (v', w')$ when either $v = v'$ and $w \sim_H w'$ or $w = w'$ and $v \sim_G v'$. If $A(G)$ and $A(H)$ are the adjacency matrices of G and H of order m and n respectively, then

$$A(G\Box H) = A(G) \otimes I_n + I_m \otimes A(H).$$

Theorem III.10. *[12] The eigenvalues of $A(G\Box H)$ are $\lambda_i + \mu_j$, where $\lambda_i; i = 1, \ldots, m$ are the eigenvalues of $A(G)$ and $\mu_j; j = 1, \ldots, n$ are the eigenvalues of $A(H)$.*

Lemma III.11. *Let $Z(G)$ and $Z(H)$ be the Zagreb matrices of G and H respectively. Then, $Z(G\Box H)$*

$$= \begin{cases} (d_G(v_i) + d_H(v_r)) + \\ (d_G(v_j) + d_H(v_s)); & (v_i, v_r) \sim_{G\Box H} (v_j, v_s) \\ 0; & \textit{otherwise.} \end{cases}$$

where, $d_G(v_i), d_G(v_j)$ are the degrees of the vertices v_i and v_j in G and $d_H(v_r), d_H(v_s)$ are degrees of the vertices v_r and v_s in H and $v_i \sim_G v_j$ and $v_r \sim_H v_s$.

Theorem III.12. *Let G and H be any two graphs of order m and n respectively. Then,*

$$Z(G\Box H) = A(G)\otimes 2(r + d_H(u_i))I_m + I_m \otimes (Z(H) + 2rA(H))$$

if and only if G is r-regular and $d_H(u_i)$ is the degree of a vertex $u_i, 1 \le i \le n$ in H.

Proof: Let the vertices of G and H be $\{v_1, v_2, \ldots, v_m\}$ and $\{u_1, u_2, \ldots, u_n\}$ respectively. First we try to write $Z(G\Box H) = A(G) \otimes I_n + I_m \otimes D_n$, where D_n is a matrix of order n.

Note that $Z(G\Box H)$ is a block matrix $B = (B_{ij})$ with $B_{rs}, r \ne s$ being a non zero diagonal block, with $(ii)^{th}$ diagonal entry equal to $d_G(v_r) + d_G(v_s) + 2d_H(u_i)$, $1 \le i \le n$, if $v_r \sim_G v_s$ otherwise it is a zero block.

Also, B_{ii} being a non zero block and the entries corresponding to $(v_i, u_r)^{th}$ row and $(v_i, u_s)^{th}$ column is $2d_G(v_i) + d_H(u_r) + d_H(u_s)$ which must be equal to $2d_G(v_j) + d_H(u_r) + d_H(u_s)$. This implies G is regular with regularity r. Hence, the entry corresponding to $(v_i, u_r)^{th}$ row and $(v_i, u_s)^{th}$ column of the block B_{ii} is $2r + d_H(u_r) + d_H(u_s)$. Also, the $(ii)^{th}$ diagonal entry of the block $B_{rs}, r \ne s$ is equal to $2r + 2d_H(u_i)$, $1 \le i \le n$, if $v_r \sim_G v_s$.
Converse is trivial. ■

Theorem III.13. *If G and H are regular with regularity r_1, r_2 and order n, m respectively. Then, $Z(G\Box H)$*

$$= 2(r_1 + r_2)(A(G)\otimes I_n + I_m \otimes A(H)) = 2(r_1 + r_2)A(G\Box H).$$

Proof: Proof follows from Theorem III.10 and III.12. ■

Corollary III.14. *Let G and H be two regular graphs with regularity r_1 and r_2 respectively. If λ_i and μ_j are the eigenvalues of $A(G)$ and $A(H)$ respectively, then the eigenvalues of $Z(G\Box H)$ are $2(r_1 + r_2)(\lambda_i + \mu_j)$ and $Z\mathcal{E}(G\Box H) = 2(r_1 + r_2)(\mathcal{E}(G) + \mathcal{E}(H))$.*

We know that the ladder graph $L_n = P_n\Box K_2$. From Theorem III.12, the following corollary follows.

Corollary III.15. $Z(L_n) = A(K_2) \otimes 2(2 + d_{P_n}(u_i))I_n + I_2 \otimes (Z(P_n) + 2A(P_n))$.

The circular ladder graph $CL_n = C_n\Box K_2$. From Theorem III.13, $Z(C_n\Box K_2) = 6A(C_n\Box K_2)$. Hence using Corollary III.14, we get the eigenvalues of CL_n as given in the corollary below.

Corollary III.16. *The eigenvalues of $Z(CL_n)$ are $12(\cos(\frac{2\pi k}{n}) \pm 1)$ where, $k = 1, \ldots, n$.*

The Hypercube graph $Q_n, n \ge 2$ is defined recursively in terms of the Cartesian product of two graphs as $Q_n = K_2\Box Q_{n-1}$ with $Q_1 = K_2$.

Proposition III.17. *[10] $A(Q_n) = K_2 \otimes I_{2^{n-1}} + I_2 \otimes A(Q_{n-1})$ for $n > 1$ and eigenvalues of $A(Q_n)$ are $\{(n - 2k)^{\binom{n}{k}}; k = 0, \ldots, n\}$.*

The next corollary gives the Zagreb eigenvalues of Q_n using Proposition III.17 and Theorem III.13.

Corollary III.18. *Let $Q_n, n > 1$ be the hypercube graph. Then,*

$$Z(Q_n) = 2n(K_2 \otimes I_{2^{n-1}} + I_2 \otimes A(Q_{n-1}))$$

and eigenvalues of $Z(Q_n)$ are $\{(2n(n - 2k))^{\binom{n}{k}}; k = 0, \ldots, n\}$.

D. Strong Product

Let G and H be two graphs with vertex sets V and W respectively. Then the strong product $G \boxtimes H$ is the graph with vertex set $V \times W$, where two distinct vertices $(u, v) \sim_{G\boxtimes H} (u', v')$ whenever $u = u'$ and $v \sim_H v'$ or

$v = v'$ and $u \sim_G u'$ or $u \sim_G u'$ and $v \sim_H v'$.
If $A(G)$ and $A(H)$ are adjacency matrices of graphs G and H, then,
$A(G \boxtimes H) = (A(G)\Box A(H)) + A(G) \otimes A(H)$

$$= (A(G) + I_G) \otimes (A(H) + I_H) - I_{G\times H}$$

Proposition III.19. *[12] The eigenvalues of $A(G\boxtimes H)$ are $(\lambda+1)(\mu+1)-1$, where λ and μ are the eigenvalues of G and H respectively.*

Lemma III.20. *Let $Z(G)$ and $Z(H)$ be Zagreb matrices of two graphs G and H. Then $Z(G \boxtimes H)$ is expressed as,*
$Z(G\boxtimes H) =$

$$\begin{cases} (d_G(v_i) + d_H(v_r)+ \\ d_G(v_i) \times d_H(v_r))+ \\ (d_G(v_j) + d_H(v_s)+ \\ \quad d_G(v_j) \times d_H(v_s)); & (v_i, v_r) \sim_{G\boxtimes H} (v_j, v_s) \\ \qquad\qquad 0; & otherwise \end{cases}.$$

Theorem III.21. *If G and H are regular with regularity r_1 and r_2, then,*

$$Z(G\boxtimes H) = 2(r_1 + r_2 + r_1r_2)A(G\boxtimes H).$$

Proof: Let the vertices of G and H be $\{v_1, v_2, \ldots, v_m\}$ and $\{u_1, u_2, \ldots, u_n\}$ respectively. Let $v_r \sim_G v_s$ and $u_b \sim_H u_d$. Then, $(v_r, u_b) \sim_{G\boxtimes H} (v_s, u_d), (v_r, u_b) \sim_{G\boxtimes H} (v_r, u_d), (v_r, u_b) \sim_{G\boxtimes H} (v_s, u_b), (v_r, u_d) \sim_{G\boxtimes H} (v_s, u_d)$ and $(v_s, u_b) \sim_{G\boxtimes H} (v_s, u_d)$ in $G \boxtimes H$.

The proof follows from Lemma III.20 and by noting that the entries in $A(G \boxtimes H)$ due to the above adjacencies is 1, where as in $Z(G \boxtimes H)$ is $2(r_1 + r_2 + r_1r_2)$. ■

From Theorem III.21 and Proposition III.19, the following corollary follows.

Corollary III.22. *Let G and H are regular with regularity r_1 and r_2 respectively. If λ_i and μ_j are the eigenvalues of $A(G)$ and $A(H)$ respectively, then eigenvalues of $Z(G\boxtimes H)$ are $2\,(r_1 + r_2 + r_1r_2)\,((\lambda_i + 1)(\mu_j + 1) - 1)$.*

E. Corona Product

Let G and H be two graphs with m and n vertices. The corona product of G and H denoted by $G \circ H$ is obtained by taking one copy of G and m copies of H, and by joining each vertex of the i^{th} copy of H to the i^{th} vertex of G, $i = 1, 2, \ldots, n$.

Consider H to be a regular graph with regularity r_2. Then $Z(H)$ can be viewed as a matrix over the field of rational functions $\mathbb{C}(\lambda)$, and the characteristic equation $det(\lambda I-2(r_2+1)A(H)) = \phi_H(\lambda) \neq 0$, so is invertible. Due to the non-singularity, one can define the coronal of of $A(H)$, denoted by $\chi_H(\lambda) \in \mathbb{C}(\lambda)$. The coronal $\chi_H(\lambda) \in \mathbb{C}(\lambda)$ of $A(H)$ is defined to be the sum of the entries of the matrix $(\lambda I - 2(r_2 + 1)A(H))^{-1}$ [11]. Also,

$$\chi_H(\lambda) = (r_1+r_2+n+1)^2 J_{n,1}(\lambda I_n-2(r_2+1)A(H))^{-1} J_{1,n}.$$

We show that, the Z-spectrum of $G \circ H$ is completely determined by the characteristic polynomials Φ_G and Φ_H and the coronal χ_H of H in the following theorem.

Theorem III.23. *Let G be a r_1-regular graph with m vertices and H be a r_2-regular graph with n vertices, and $\chi_H(\lambda)$ be the coronal of H. Then the characteristic polynomial of $Z(G \circ H)$ is, $\Phi_{Z(G\circ H)}(\lambda) =$*

$$2^m(r_2+1)^m\Phi_H\big(\frac{\lambda}{2(r_2 + 1)}\big)^m 2^m(r_1+n)^m\Phi_G\big(\frac{\lambda - \chi_H(\lambda)}{2(r_1 + n)}\big)$$

Proof: Let $A(G)$ and $A(H)$ be the adjacency matrices of G and H respectively. The Zagreb matrix of corona product two graphs G and H can be expressed as, $Z(G \circ H) = \begin{pmatrix} 2(r_1 + n)A(G) & (r_1 + r_2 + n + 1)J_{1,n} \otimes I_m \\ (r_1 + r_2 + n + 1)J_{n,1} \otimes I_m & 2(r_2 + 1)A(H) \otimes I_m \end{pmatrix}$.
To compute the characteristic polynomial of the matrix $Z(G \circ H)$, we recall the elementary results given below from linear algebra on multiplication of Kronecker products and determinants of block matrices:

i. In cases where each multiplication makes sense, we have
$$M_1M_2 \otimes M_3M_4 = (M_1 \otimes M_3)(M_2 \otimes M_4).$$
ii. If M_4 is invertible, then
$$det\begin{pmatrix} M_1 & M_2 \\ M_3 & M_4\end{pmatrix} = det(M_4)det(M_1 - M_2M_4^{-1}M_3).$$
iii. $(M_1 \otimes M_2)^{-1} = M_2^{-1} \otimes M_1^{-1}$.

Consider, $\Phi_{Z(G\circ H)} =$

$$\begin{aligned}
&= det(\lambda I_{m(n+1)} - Z(G \circ H)) \\
&= det\begin{pmatrix} \lambda I_m - 2(r_1 + n)A(G) & -(r_1 + r_2 + n + 1)J_{1,n} \otimes I_m \\ -(r_1 + r_2 + n + 1)J_{n,1} \otimes I_m & (\lambda I_n - 2(r_2 + 1)A(H)) \otimes I_m)\end{pmatrix} \\
&= det\big((\lambda I_n - 2(r_2 + 1)A(H)) \otimes I_m\big)det\big[(\lambda I_m - 2(r_1 + n)A(G)) \\
&\quad - (r_1 + r_2 + n + 1)^2(J_{1,n} \otimes I_m)\big(\lambda I_n - 2(r_2 + 1)A(H)) \otimes I_m)\big)^{-1}(J_{n,1} \otimes I_m)\big] \\
&= det(\lambda I_n - 2(r_2 + 1)A(H))^m det\big((\lambda - \chi_H(\lambda))I_m - 2(r_1 + n)A(G)\big) \\
&= 2^m(r_2 + 1)^m\Phi_H\big(\frac{\lambda}{2(r_2 + 1)}\big)^m 2^m(r_1 + n)^m\Phi_G\big(\frac{\lambda - \chi_H(\lambda)}{2(r_1 + n)}\big)
\end{aligned}$$

Hence, the proof. ■

Corollary III.24. *Let G be a r_1-regular graph with m vertices and H be a r_2-regular graph with n vertices. Then the coronal of H is given by*

$$\chi_H(\lambda) = (r_1 + r_2 + n + 1)^2\frac{n}{\lambda - 2r_2(r_2 + 1)}.$$

The spectrum of $Z(G \circ H)$ is given by

$$\begin{pmatrix} 2(r_2 + 1)\theta & \frac{(2r_2(r_2+1)+\mu)\pm\sqrt{(2r_2(r_2+1)-\mu)^2+4n(r_1+r_2+n+1)^2}}{2} \\ m & 1\end{pmatrix},$$

where θ is the eigenvalue of H such that $\theta \neq r_2$, and $\mu = 2(r_1 + n)\alpha$, for each eigenvalue α of $A(G)$.

Proof: From Theorem III.23, we can easily note that $2(r_2 + 1)\theta$ is a eigenvalue of $Z(G \circ H)$ with multiplicity m, where θ is an non-maximum eigenvalue of H.
We have $2(r_2 + 1)A(H)J_{n,1} = 2r_2(r_2 + 1)J_{n,1}$.
Hence, $(\lambda I - 2(r_2 + 1)A(H))J_{n,1} = (\lambda - 2r_2(r_2 + 1))J_{n,1}$.

$$\begin{aligned}
\chi_H(\lambda) &= (r_1 + r_2 + n + 1)^2 J_{1,n}(\lambda I_n - 2(r_2 + 1)A(H))^{-1}J_{n,1} \\
&= (r_1 + r_2 + n + 1)^2\big(\frac{J_{1,n}J_{n,1}}{\lambda - 2r_2(r_2 + 1)}\big) \\
&= (r_1 + r_2 + n + 1)^2\big(\frac{n}{\lambda - 2r_2(r_2 + 1)}\big).
\end{aligned}$$

The pole of $\chi_H(\lambda)$ is the $2r_2(r_2 + 1)$, some eigenvalues are root of $\Phi_H(\lambda)$which are not poles of $\chi_H(\lambda)$ and the remaining eigenvalues are obtained by $\lambda - \chi_H(\lambda) = 2(r_1 +$

$n)\alpha = \mu$ for each eigenvalue of α of $A(G)$.

$$\lambda - (r_1 + r_2 + n + 1)^2 \frac{n}{\lambda - 2r_2(r_2 + 1)} = \mu.$$

Solving for λ we get remaining eigenvalues of $G \circ H$. Hence the proof. ■

Corollary III.25. *The spectral radius of $Z(G \circ H)$ is given by,* $(r_1(r_1 + n) + r_2(r_2 + 1)) + \sqrt{(r_1(r_1 + n) - r_2(r_2 + 1))^2 + n(r_1 + r_2 + n + 1)^2}$.

Proof: The quotient matrix of $Z(G \circ H)$ is given by

$$B_z(G \circ H) = \begin{pmatrix} 2(r_1 + n)r_1 & n(r_1 + r_2 + n + 1) \\ (r_1 + r_2 + n + 1) & 2r_2(r_2 + 1) \end{pmatrix}.$$

Simplifying the characteristic polynomial of $B_z(G \circ H)$ we get $\lambda^2 - (r_1(r_1 + n) + r_2(r_2 + 1))\lambda + 4r_1r_2(r_1r_2 + r_1 + nr_2 + n) - n(r_1 + r_2 + n + 1)^2 = 0$. On solving we get two eigenvalues and hence the spectral radius follows from Theorem I.2. ■

IV. Conclusion

As a class of degree-based topological molecular descriptors, the extended adjacency index of a connected graph was proposed. There has been an extensive exploration of spectral properties of the extended adjacency matrix based on a wide range of degree-based topological indices. The extended adjacency matrix associated with the first Zagreb index, known as the Zagreb matrix of some classes of graphs and some derived classes is studied in this article.

The energy of a graph is an emerging concept that serves as a frontier between chemistry and mathematics, introduced in the 1970s. It became a popular topic of research both in mathematical chemistry and in pure spectral graph theory. Eventually, scores of different graph energies have been conceived. The Zagreb energy is one such quantity associated with the Zagreb matrix. Graph products include a wide range of operations that join two or more existing graphs to produce new graphs with distinctive properties and uses. This article explores the Zagreb energy of various products of graphs.

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