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Heat kernel and $D_{n,r}$ decomposition of some families of weakly semi-regular bipartite graphs



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Abstract

This paper studies the characteristic polynomial of distance matrices and adjacency matrices of some families of weakly semi-regular bipartite graphs. The $D_{n,r}$ decomposition is a decomposition of distance matrices and adjacency matrices of some families of graphs. The general distance matrices and adjacency matrices of these graphs are decomposed into a further simpler form. The spectra of these graphs are also analysed. The $D_{n,r}$ decomposition of these graphs is done so that analysis of eigenvalues and related parameters are possible with this decomposition. The heat kernel of these graphs is analysed.

Keywords: Distance matrix, adjacency matrix, nth SM balancing graphs, nth SM sum graphs, energy and spectrum, heat Kernel of graphs, bipartite Kneser graphs.

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1. Introduction

Characterising the topological structure of graphs is a major problem in graph theory. Graph clustering is also an issue in pattern recognition and computer vision. These issues are addressed by finding the spectrum of the Laplacian matrix or adjacency matrix. The concept of distance and distance matrices play an important role in these studies. Let G = (V, E) be the graph with vertex set V and edge set E. Graph spectral approach is mainly depending on the adjacency matrix $A = [a_{ij}]$ of a graph where

$$a_{ij} = \begin{cases} 1 , & \text{if } v_i v_j \in E, \\ 0, & \text{otherwise.} \end{cases}$$

The heat kernel of a graph is obtained by exponentiating the Laplacian eigen-system with time [1]. The heat kernel of a (q + 1)-regular graph G is given by

$$K_{G}(t, x_{0}, x) = e^{(q+1)t} \sum_{m=0}^{\infty} b_{m}(x)q^{-\frac{m}{2}}l_{m}(2\sqrt{q}t), \qquad (1.1)$$

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where l_m is l-Bessel function of order m, $b_m(x) = c_m(x) - (q-1)(c_{m-2}(x) + c_{m-4}(x) + \cdots)$ and $c_m(x)$ is the number of geodesics from a fixed point x_0 to x of length $m \ge 0$.

Now let us consider the SM family of graphs. Mainly two number systems are used in computer science. They are the binary number systems and the balanced ternary number systems. Two graphs were introduced based on the combinatorial structure of these two number systems. The two families of graphs thus obtained are SM sum graphs and SM Balancing graphs. SM sum graphs are associated with the intrinsic combinatorial relationship between the powers of 2 and the positive integers, which is used in binary number system. These graphs are related to the bipartite Kneser graphs. SM balancing graphs are related with the balanced ternary number system. The ternary number system is used in ternary computers known as SETUN computers (made in Russia). Ternary number system is more convenient for fuzzy logic and thus in artificial intelligence. Let G be a graph and A be its adjacency matrix. The characteristic polynomial det(xI - A), where I is the identity matrix of order same as of A, of the adjacency matrix A is called the characteristic polynomial of G and is denoted by $P_G(x)$. The zeros of det(xI – A) are called the eigenvalues of G. The spectrum of G is the collection of all eigenvalues of G. If λ is an eigenvalue of G, then a non zero vector $x \in \mathbb{R}^n$, satisfying $Ax = \lambda x$, is called an eigenvector of A for λ . The eigenvectors give you the direction of spread of data, while the eigenvalues give the intensity of spread in particular direction. For example, in a social network, the largest eigenvalue gives an idea of the fastest rate at which a gossip can grow in the social circle. The multiplicity of the eigenvalue 0 of the Laplacian matrix [3] of a graph tells us the number of connected components in a graph. eigenvalues and graph spectra are widely used in technology and science. One of the main applications of graph spectra in Chemistry [2] is in the theory of unsaturated conjugated hydrocarbons known as the Huckel molecular orbital theory. In Physics, it is used in Membrane vibration problem. In computer science, graph spectra are used in internet technologies, pattern recognition etc. The largest eigenvalue (dominant eigenvalue) plays an important role in modelling virus propagation in computer network. The smaller the largest eigenvalue, the larger the robustness of a network against the spread of virus. In database, to protect the privacy of personal data, one method is to randomize the network representing relations between individuals by deleting some actual edges and by adding some false edges in such a way by keeping the structure of its global characteristics. This is achieved by using, especially the largest eigenvalues of the adjacency matrix and of the Laplacian. The aim of this paper is to investigate whether the heat kernel can be established for the weakly semi regular bipartite graphs.

2. Preliminary

Definition 2.1 ([7]). Consider the set $T_n = \{3^m : m \text{ is an integer}, 0 \le m \le n-1\}$ for a fixed positive integer $n \ge 2$. Let $I = \{-1, 0, 1\}$. Let $x \le \frac{1}{2}(3^n - 1)$ be any positive integer which is not a power of 3. Then x can be expressed as

$$x = \sum_{j=1}^{n} \alpha_j y_j, \tag{2.1}$$

where $\alpha_j \in I$, $y_j \in T_n$ and y'_j s are distinct. Each y_j such that $\alpha_j \neq 0$ is called a balancing component of x.

Definition 2.2 ([7]). Consider the simple directed graph G = (V, E), where $V = \{v_1, v_2, ..., v_{\frac{1}{2}(3^n-1)}\}$ and adjacency of vertices is defined by: for any two distinct vertices v_x and v_{y_j} , $(v_x, v_{y_j}) \in E$ if (2.1) holds and $\alpha_j = -1$ and the vertex $(v_{y_j}, v_x) \in E$ if (2.1) holds and $\alpha_j = 1$. This digraph G is called the nthSMD balancing graph, denoted by SMD(B_n). Its underlying undirected graph is called the nth SM Balancing graph, denoted by SM(B_n).

Definition 2.3 ([8]). For a fixed integer $n \ge 2$, consider the positive integers $p < 2^n$, that are not powers of 2, then $p = \sum_{i=1}^{n} x_i$, with $x_i = 0$ or 2^m , m is an integer, $0 \le m \le n-1$ and x'_i s are distinct. The coefficient of each x'_i s is 1. Each $x_i \ne 0$ is called an additive component of p.

Definition 2.4 ([8]). For a fixed integer $n \ge 2$, the simple graph $SM(\sum_n)$, called n^{th} SM sum graph, is the graph with vertex set { $v_1, v_2, ..., v_{2^n-1}$ } and adjacency of vertices defined by: v_i and v_j are adjacent if either i is an additive component of j, or j is an additive component of i.

These SM sum graphs are particular cases of bipartite kneser graphs. For a fixed integer n > 1, let $S = \{1, 2, 3, ..., n\}$ and V be the set of all k-subsets and (n-k) subsets of S. The bipartite Kneser graph H(n,k) has V as its vertex set and two vertices A, B are adjacent if and only if $A \subset B$ or $B \subset A$.

For a fixed integer $n \ge 2$, let $T_n = \{3^m : m \text{ is an integer}, 0 \le m \le n-1\}$, $N = \{1, 2, 3, \dots, t\}$, where $t = \frac{1}{2}(3^n - 1)$. Also let $P_n = \{2^m : m \text{ is an integer}, 0 \le m \le n-1\}$, $M = \{1, 2, 3, \dots, 2^n - 1\}$. Then consider $P_n^c = M - P_n$, $T_n^c = N - T_n$ throughout this paper unless otherwise specified.

3. Weakly semi-regular bipartite graphs

A simple graph G is called bipartite if its vertex set V can be partitioned into two disjoint sets V_1 and V_2 such that every edge in the graph connects a vertex in V_1 and a vertex in V_2 and no edge in G connects either two vertices in V_1 or two vertices in V_2 . We call (V_1, V_2) the bipartition of G; V_1 and V_2 are called the parts of G. We consider only connected bipartite graphs in this work.

Definition 3.1 ([10]). A bipartite graph G with bipartition (V_1, V_2) , $|V_1| > 1$ and $|V_2| > 1$ is weakly semiregular if the vertices in exactly one V_i have same degree. The part of G in which all vertices have the same degree is called a SD-part. The other part of G is called a NSD-part.

Let G = (V, E) be a graph. The neighbourhood of $v \in V$, written $N_G(v)$ or N(v), is the set of vertices adjacent to v.

Definition 3.2 ([10]). A weakly semiregular bipartite graph G is called a WSB_{END} graph if the vertices in the NSD-part do not have all distinct degrees and the neighbourhoods of the vertices in the SD-part have same degree sequence.

For each $k \ge 1$, the set of vertices in the NSD-part of degree k is called a k-NSD subpart.

An automorphism of a graph G is an isomorphism with itself. Let G be a connected WSB_{END} graph. Then G has non trivial automorphism group. The automorphism relationship is an equivalence relation on the vertices of a graph. Two vertices are equivalent if there exists an automorphism taking one to the other. Like all equivalence relations, this also produces a partition of the vertex set into equivalence classes. These classes are usually called automorphism classes or orbits. Here the orbits are the vertices of each k-NSD subpart and SD part. The automorphism group of these WSB_{END} graphs have been studied in one of our other works [10].

Suppose there are 5 computers, 3 servers and the maximum allowed connections to each server is n. So we have a total of $n \times 3 = 3n$ possible connections. In the beginning we need to connect 5 computers. One of the arrangements is as follows: two computers (having only 3 ports) to all the 3 servers and 3 computers (having only 2 ports) to two each server. Only one direct connection to a server can be active at any time in this network. This network connection leads to a graph which is a WSB_{END} graph. Suppose this graph be G₁. The question of interchanging the connections without altering the connection structure leads to the notion of automorphism.

In this connection, if we increase the number of computers by one or more, then the new network graph be G_2 . Clearly G_1 is a sub graph of G_2 . Similarly we can get new graphs G_3 , G_4 etc by adding computers upto the maximum possible connections. The same type network connections or graphs may arise in daily life situations. In many cases, these graphs will form a family of WSB_{END} graphs. In these networks, the degrees of the previously existing nodes will remain same in the NSD part. The reverse process is also possible. It is possible to delete vertices to get the old versions of network. This can be used in many real life problems connected with Information technology especially in file retrieving algorithm, isomorphism algorithms etc.

Definition 3.3. Let G_1 be a connected WSB_{END} graph. Let G_2 be the new bipartite graph by adding nodes to the SD part or NSD part or both of G_1 by keeping the degrees of the previously existing nodes unaltered in the NSD part. Here G_1 is a sub graph of G_2 . For each $n \ge 2$, G_n is obtained by adding nodes to the SD part or NSD part or both of G_{n-1} by keeping the degrees of the previously existing nodes unaltered in the NSD part. The family of graphs thus obtained are called \mathscr{TR} -family of graphs if each G_i , i = 1, 2, ..., n is a WSB_{END} graph. It is denoted by $\mathscr{TR}(G_i)_1^n$.

The graphs $SM(\sum_{n})$ and $SM(B_{n})$ are WSB_{END} graphs.

Proposition 3.4. The graphs $SM(\sum_n)$ and $SM(B_n)$ form a \mathcal{TR} -family of graphs for all n > 2.

Proof. Consider the graph G = SM(\sum_n), n > 2. The graph SM(\sum_n) is a bipartite graph with parts $V_1 = \{v_i : i \in \mathscr{P}_n\}$ and $V_2 = \{v_j : j \in \mathscr{P}_n^c\}$ where $\mathscr{P}_n = \{2^m : m \text{ is an integer, } 0 \leq m \leq n-1\}$. As n increases by 1, in each case the graph satisfies the conditions given in the Definition 3.3. G has $2^n - 1$ vertices and $n(2^{n-1} - 1)$ edges. All the vertices of V_1 are of same degree $2^{n-1} - 1$ and the vertices of V_2 are not of same degree and has a degree sequence $\{2_{\binom{n}{2}}, 3_{\binom{n}{3}}, \dots, n_{\binom{n}{3}}, 1\}$ for n > 2. There are $\binom{n}{2}$ vertices of degree 2 and $\binom{n}{3}$ vertices of degree 3 and so on. Also each vertices in V_1 has a neighbourhood with degree sequence $\{2_{\binom{n-1}{2}}, 3_{\binom{n-1}{2-1}}, \dots, n_{\binom{n-1}{n-1}}\}$. This implies that the family of graphs SM(\sum_n) forms a \mathscr{T} -family of graphs for each n. Similarly the family of graphs SM(B_n), is a bipartite graph with partitions $V_3 = \{v_i : i \in T_n\}$ and $V_4 = \{v_j : j \in T_n^c\}$. The vertices in V_3 are of same degree $3^{n-1} - 1$ and each vertex is having a neighbourhood with same degree sequence $\{2_{\binom{n}{2}}, 3_{\binom{n}{2}}, \dots, n_{\binom{2^{n-1}{n-1}}{\binom{n-1}{2}}, 3_{\binom{n-2}{2}}, \dots, n_{\binom{2^{n-1}{n-1}}{\binom{n-1}{n-1}}}$. The vertices in V_4 are of different degree and has a degree and has a degree sequence $\{2_{\binom{2^{n-1}{2}}, 3_{\binom{2^{n-1}{2}}{\binom{n-1}{2}}, 3_{\binom{2^{n-1}{2}}{\binom{n-1}{\binom{n-1}{n-1}}}\}$. It satisfies the conditions for the \mathscr{T} -family of graphs. The vertices in V_4 are of different degree and has a degree sequence $\{2_{\binom{2^{n-1}{2}}, 3_{\binom{2^{n-1}{2}}{\binom{n-1}{\binom{n-1}{n-1}}}}\}$. Therefore the graphs SM(B_n) also forms a \mathscr{T} -family of graphs for each n. Hence proved. □

4. Distance related results of some families of graphs

It is very clear from the SM sum graph that any two odd prime numbers are at distance 2 in the graph $SM(\sum_{n})$. The distance between 1 and any odd number is 1. Some of the distance related results from the previous work is given below.

Lemma 4.1 ([9]). If $G = SM(\sum_n)$, $P_n = \{2^m : m \text{ is an integer, } 0 \leq m \leq n-1\}$, $n \geq 2$, then

 $d(v_i, v_j) = \begin{cases} 1, & \text{if } i \text{ is an additive component of } j \text{ or } j \text{ is an additive component of } i, \\ 2, & \text{if } i, j \in P_n \text{ or } i, j \notin P_n, i \text{ and } j \text{ have at least one common additive component,} \\ 3, & \text{neither } i \text{ nor } j \text{ is an additive component but exactly one of them belongs to } P_n, \\ 4, & i, j \notin P_n, i \text{ and } j \text{ have no common additive component.} \end{cases}$

Proposition 4.2 ([8]). Let $G = SM(\sum_n)$ be an nth SM sum graph. Let $d_r(v_i, v_j)$ denote the number of unordered pairs of vertices for which $d(v_i, v_j) = r$. Then

$$d_{r}(v_{i},v_{j}) = \begin{cases} n.(2^{n-1}-1), & \text{if } r = 1, \\ \frac{n(n-1)}{2} + \left[\frac{(2^{n}-n-2)(2^{n}-n-1)}{2} - \delta\right], & \text{if } r = 2, \\ (n+1).2^{n} - (n+2)2^{n-1} - n^{2}, & \text{if } r = 3, \\ \delta, & \text{if } r = 4, \end{cases}$$

where $\delta = \frac{1}{2} \sum_{r=2}^{n-2} \left[\binom{n}{r} \sum_{k=2}^{n-2} \binom{n-r}{k} \right].$

Remark 4.3. $\delta = 0$ for n = 2 or 3.

The value of δ is the number of pairs of pairwise disjoint subsets of P_n excluding the empty set and singleton sets. Here the diameter of the graph $SM(\sum_n)$ is given as follows.

diam(G) =
$$\begin{cases} 2, & \text{if } n = 2, \\ 3, & \text{if } n = 3, \\ 4, & \text{if } n \ge 4. \end{cases}$$

4.1. Distance matrices of SM families of graphs

Consider the graph $G = SM(\sum_n)$, for $n \ge 2$ with vertex set $V = \{v_i : 1 \le i \le 2^n - 1\}$. The distance matrix of the graph G having $2^n - 1$ vertices is a symmetric matrix $D_n = [d_{ij}]$ of order $p = 2^n - 1$, whose entries d_{ij} are defined as

$$d_{ij} = \begin{cases} d(\nu_i, \nu_j), & \text{if } i \neq j, \\ 0, & \text{if } i = j, \end{cases}$$

where $d(v_i, v_j)$ is given in Lemma 4.1.

Example 4.4. Consider the graph $G = SM(\sum_{n})$. When n = 3, the distance matrix is

	Γ0	2	1	2	1	3	1	
	2	0	1	2	3	1	1	
	1	1	0	3	2	2	2	
$D_3 =$	2	2	3	0	1	1	1	
	1	3	2	1	0	2	2	
	3	1	2	1	2	0	2	
	1	1	2	1	2	2	0	

The characteristic polynomial of this matrix is $x^7 - 72x^5 - 320x^4 - 384x^3$ and the eigenvalues are $4 \pm 2\sqrt{10}$, -4, 0. The determinant of the matrix D_n is zero for all $n \ge 3$.

Proposition 4.5. Let D_i , i = 1, 2, 3, ... n be the distance matrices of a \mathscr{TR} -family of graphs G_i , i = 1, 2, 3, ... n, respectively. Let V_i , i = 1, 2, 3, ... n be the corresponding vertex sets of G_i and $r_{n,m} = |V_n| - |V_m|$, m < n. Then D_n decomposes as follows.

$$D_{n} = \begin{bmatrix} D_{m} & R_{d_{m} \times r_{n,m}} \\ R_{r_{n,m} \times d_{m}}^{\mathsf{T}} & S_{r_{n,m} \times r_{n,m}} \end{bmatrix},$$

where d_m is the number of vertices of G_m . R^T is the transpose of the matrix R, and S is a square matrix.

Proof. Given that graphs G_i , i = 1, 2, 3, ... n having V_i , i = 1, 2, 3, ... n as the corresponding vertex sets of G_i . Given that these graphs form a \mathscr{TR} -family of graphs. Also $r_{n,m} = |V_n| - |V_m|$, m < n and d_m is number of vertices of G_m . Consider two graphs G_n and G_m from this family with G_m is a sub graph of G_n . Therefore $r_{n,m} + d_m$ is the number of vertices of G_m . With a proper labeling we can get the distance matrices of these graphs. Then we get

$$D_{n} = \begin{bmatrix} D_{m} & R_{d_{m} \times r_{n,m}} \\ R_{r_{n,m} \times d_{m}}^{\mathsf{T}} & S_{r_{n,m} \times r_{n,m}} \end{bmatrix}$$

The characteristic polynomial of this matrix is given by

$$det(xI - D_n) = \begin{bmatrix} (xI - D_m) & R_{d_m \times r_{n,m}} \\ -R_{r_{n,m} \times d_m}^T & (xI - S_{r_{n,m} \times r_{n,m}}) \end{bmatrix}.$$

By applying Schur complement formula [5], we get

$$det(xI - D_n) = det(xI - D_m). det[(xI - S_{r_{n,m} \times r_{n,m}}) - R_{r_{n,m} \times d_m}^T.(xI - D_m)^{-1}.R_{d_m \times r_{n,m}}].$$

The computation of eigenvalues depends on the evaluation of determinant matrices which is a very time consuming process for large matrices. These type of decomposition will help in solving the determinant as well as finding the characteristic polynomial of matrices related to graphs.

Definition 4.6. Let D_i , i = 1, 2, 3, ..., n be the distance matrices of some families of graphs G_i , i = 1, 2, 3, ..., n. Let V_i , i = 1, 2, 3, ..., n be the corresponding vertex sets of G_i and $r_{n,m} = |V_n| - |V_m|$, m < n. Then D_n decomposes as follows.

$$D_{n} = \begin{bmatrix} D_{m} & R_{d_{m} \times r_{n,m}} \\ R_{r_{n,m} \times d_{m}}^{\mathsf{T}} & S_{r_{n,m} \times r_{n,m}} \end{bmatrix},$$

where d_m is the number of vertices of G_m . R^T is the transpose of the matrix R, and S is a square matrix. The family of graphs for which the distance matrices satisfying this type of decomposition are called $D_{n,r}$ decomposable family of graphs.

There are many families of graphs that are $D_{n,r}$ decomposable family of graphs.

Theorem 4.7. The following graphs are $D_{n,r}$ decomposable family of graphs.

- 1. The path graph on n vertices.
- 2. The complete bipartite graphs $K_{m,n}$.
- 3. The complete graph K_n .

Proof. From the definition of these graphs, it is obvious that these graphs are $D_{n,r}$ decomposable family of graphs.

Theorem 4.8. Let D_n be the distance matrices of $SM(\sum_n)$ graphs, n > 2. Then in general D_n decomposes as follows.

$$\mathsf{D}_{\mathsf{n}} = \begin{bmatrix} \mathsf{D}_{\mathsf{n}-1} & \mathsf{R}_{\mathsf{p}\times\mathsf{q}} \\ \mathsf{R}_{\mathsf{q}\times\mathsf{p}}^{\mathsf{T}} & \mathsf{S}_{\mathsf{q}\times\mathsf{q}} \end{bmatrix},$$

where $p = 2^{n-1} - 1$ *and* $q = 2^{n-1}$.

Proof. Here the number of vertices in each graph is p + q where $p = 2^{n-1} - 1$ and $q = 2^{n-1}$. Also the graph $SM(\sum_{n})$ is a WSB_{END} graph. Since the SM sum graphs form a \mathscr{TR} -family of graphs and n = |P|, the result follows from the Proposition 4.5.

Observation 4.9. For a weakly semi regular bipartite graphs, the number of different non-zero eigenvalues of the distance matrix is equal to the degree of vertices in SD part.

The distance matrix and related matrices of a graph are the sources of many graph invariants like topological indices etc. So these matrices are used in structure property activity modelling by studying the spectra and related polynomials of these graphs. The reciprocal distance matrices (Harary matrices) of SM family of graphs is obtained from the corresponding distance matrices by replacing all non zero entries by their reciprocals. Therefore the Harary index of the SM sum graphs and SM Balancing graphs are obtained.

4.2. Adjacency matrices of some graphs

Definition 4.10 ([6]). The adjacency matrix of graph G having p vertices is a symmetric matrix $A_n = [a_{ij}]$, of order $p = 2^n - 1$, whose entry a_{ij} is defined as

$$a_{ij} = \begin{cases} 1, & \text{if } v_i \text{ is adjcent to } v_j, \\ 0, & \text{otherwise.} \end{cases}$$

Proposition 4.11. Let A_i , i = 1, 2, 3, ... n be the adjacency matrices of a \mathscr{TR} -family of graphs G_i , i = 1, 2, 3, ... n. Let V_i , i = 1, 2, 3, ... n be the corresponding vertex sets of G_i and $r_{n,m} = |V_n| - |V_m|$, m < n. Then A_n decomposes as follows:

$$A_{n} = \begin{bmatrix} A_{m} & R_{d_{m} \times r_{n,m}} \\ R_{r_{n,m} \times d_{m}}^{\mathsf{T}} & S_{r_{n,m} \times r_{n,m}} \end{bmatrix},$$

where d_m is number of vertices of G_m . R^T is the transpose of the matrix R, and S is a square matrix.

Proof. The proof follows from Proposition 4.5.

Theorem 4.12. Let A_n be the adjacency matrix of $SM(\sum_n)$ graphs. Then A_n decomposes as follows

$$A_{n} = \begin{bmatrix} A_{n-1} & R_{p \times q}^{a} \\ R_{q \times p}^{aT} & S_{q \times q}^{a} \end{bmatrix},$$

where $p = 2^{n-1} - 1$ and $q = 2^{n-1}$.

Proof. Since SM sum graphs form a \mathcal{TR} -family of graphs and here n = p + q, the theorem follows from above proposition.

Theorem 4.13. For a WSB_{END} graph, the number of distinct non-zero eigenvalues is equal to the number of orbits.

Proof. The WSB_{END} graph are non asymmetric. So it has non trivial orbits. The number of non trivial orbits is equal to the number of distinct non-zero eigenvalues. \Box

Usually for finding the eigenvalues, the power method is applied. This above decomposition will make the method faster for matrices of larger order. Also for any bipartite graphs, the adjacency matrix can be written as

$$A_{n} = \begin{bmatrix} 0 & C \\ C^{\mathsf{T}} & 0 \end{bmatrix}.$$

Therefore its characteristic polynomial is

$$det(xI - A_n) = det \begin{bmatrix} xI_p & -C \\ -C^T & xI_{n-p} \end{bmatrix}.$$

The adjacency matrix of the graph $SM(\sum_n)$ with vertex set $V = \{v_i : 1 \le i \le 2^n - 1\}$ is obtained from the corresponding distance matrix of $SM(\sum_n)$ by replacing all entries which are greater than 1 by 0. Similarly we can get the adjacency matrices of $SM(B_n)$.

Example 4.14. Consider the graph $G = SM(\sum_{n})$. When n = 3, the adjacency matrix is

$$A_3 = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}.$$

The eigenvalues of this adjacency matrix are obtained as ± 2.64571 , ± 1 , ± 1 , and 0.

Since $SM(\sum_n)$ and $SM(B_n)$ are bipartite graphs, if λ is an eigenvalue value of this graph with multiplicity m, then $-\lambda$ is also an Eigenvalue with multiplicity m and $\sum \lambda_i = 0$.

5. Energy of graphs

The following theorem is known as the eigenvalue interlacing theorem introduced by Cauchy. The Cauchy interlacing theorem states that the eigenvalues of real symmetric matrix of order n interlace with those of any principal sub matrix of order n - 1.

Theorem 5.1 ([4]). Suppose $A \in \mathbb{R}^{n \times n}$ is a symmetric matrix. Let $B \in \mathbb{R}^{m \times m}$ with m < n be a principal sub matrix (obtained by deleting both i^{th} row and i^{th} column for some values of i). Suppose A has eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n$ and B has eigenvalues $\beta_1 \leq \beta_2 \leq \cdots \leq \beta_m$. Then $\lambda_k \leq \beta_k \leq \lambda_{k+n-m}$ for $k = 1, 2, 3, \ldots, m$ and if m = n - 1, then $\lambda_1 \leq \beta_1 \leq \lambda_2 \leq \beta_2 \leq \cdots \leq \beta_{n-1} \leq \lambda_n$.

Let G be a graph. The energy E(G) of the graph is defined as the sum of absolute values of its eigenvalues. It is one of the most popular graph invariants in chemical graph theory. Gutman introduced this energy of simple graphs. In 2006, Gutman and Zhou introduced concept of Laplacian energy of a graph as the sum of the absolute deviations of the eigenvalues of its Laplacian matrix [4]. The lower and upper bounds of the energy and Laplacian energy of graphs have been introduced by many Mathematicians. Since the building blocks of the WSB_{END} graphs are the regular trees, the Heat Kernel of the these graphs can be found in a same method as given in equation (1.1).

Theorem 5.2. Let G_i , i = 1, 2, 3, ..., n be a \mathcal{TR} -family of $D_{n,r}$ decomposable graphs. Then $E(G_1) < E(G_2) < \cdots < E(G_n)$.

Proof. Given that G_i , i = 1, 2, 3, ..., n are in a \mathscr{TR} family of $D_{n,r}$ decomposable graphs. Let A_i be the corresponding adjacency matrix of the graphs G_i . Let V_i , i = 1, 2, 3, ..., n be the corresponding vertex sets of G_i and $r_{n,m} = |V_n| - |V_m|$, m < n. Then A_n decomposes as follows.

$$A_{n} = \begin{bmatrix} A_{m} & R_{d_{m} \times r_{n,m}} \\ R_{r_{n,m} \times d_{m}}^{\mathsf{T}} & S_{r_{n,m} \times r_{n,m}} \end{bmatrix},$$

where d_m is the number of vertices of G_m . Therefore by using Theorem 5.1, we get that $E(G_1) < E(G_2) < \cdots < E(G_n)$.

Suppose r_A be the rank of the adjacency matrix A of a graph G having p number of vertices and q number of edges. Then there are exactly r_A non-zero eigenvalues. The first Zagreb index $M_1(G)$ is defined as the sum of squares of the vertex degrees of the graph G. Zhou [11] gave the following upper bound for the energy of G in terms of order p > 2, size q and first Zagreb index $M_1(G)$ of a bipartite graph G,

$$\mathsf{E}(\mathsf{G}) \leq 2\sqrt{\frac{\mathsf{M}_1(\mathsf{G})}{\mathsf{p}}} + \sqrt{(\mathsf{p}-2)\left[2\mathsf{q} - \left(2\frac{\mathsf{M}_1(\mathsf{G})}{\mathsf{p}}\right)\right]}$$

For the graph $G = SM(\sum_n)$, the first Zagreb index is

$$M_1(G) = \sum_{r=2}^n \binom{n}{r} r^2 + n(2^{n-1} - 1)^2 = n(n+1)2^{n-2} - n + n(2^{n-1} - 1)^2$$

Therefore

$$\begin{split} \mathsf{E}(\mathsf{G}) &\leqslant 2\sqrt{\frac{n(n+1)2^{n-2} - n + n(2^{n-1} - 1)^2}{2^n - 1}} \\ &+ \sqrt{(2^n - 3)\left[2n(2^{n-1} - 1) - \left(2\frac{n(n+1)2^{n-2} - n + n(2^{n-1} - 1)^2}{2^n - 1}\right)\right]}. \end{split}$$

Theorem 5.3. Let $G = SM(\sum_n)$ be the SM sum graph of order $p = 2^n - 1$ with $q = n(2^{n-1} - 1)$ edges, $\Delta = (2^{n-1} - 1)$ maximum degree and the first Zagreb index $M_1(G)$. Then

$$\mathsf{E}(\mathsf{G}) \leqslant \Delta + \sqrt{\frac{2\mathsf{q}(p^2 - 2\mathsf{q})}{p^2} + \mathsf{H}}$$

where

$$\mathsf{H} = \sqrt{\binom{\binom{r-1}{2}}{\frac{8q^2(p^2 - 2q)^2}{p^4} - 2(n(n+1)2^{n-2} - n + n\Delta^2) - \frac{2(n(n+1)2^{n-2} - n + n\Delta^2 - 2q)^2}{p(p-1)} + 2\Delta^4}}$$

Proof. The proof of this Theorem 5.3 will be completed when we substitute the value of first Zagreb index of G in the result given in Theorem 4.1 from [4]. For the graph $G = SM(\sum_n)$, the first Zagreb index is given by $M_1(G) = \sum_{\nu \in V} d(\nu)^2 = \sum_{r=2}^n {n \choose r} \cdot r^2 + n \cdot (2^{n-1} - 1)^2 = n(n+1)2^{n-2} - n + n(2^{n-1} - 1)^2$. By substituting the value of first Zagreb index, the proof is completed.

5.1. Open problem

Find the general characteristic polynomial of distance matrices and adjacency matrices of SM family of graphs.

6. Conclusion

In this paper we established a new decomposition on the matrices related with some families of weakly semi-regular bipartite graphs. The \mathcal{TR} -family of graphs admits $D_{n,r}$ decomposition which will be useful in many analysis of eigenvalues and related measures. Also the spectra and energy of these types of graphs were analysed. An upper bound is obtained for the energy of SM families of graphs.

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