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ENERGY OF SOME NEW GRAPH

Iram I. Jadav

ABSTRACT. Let G be a graph the eigenvalues of G are obtained from the adjacency matrix of G. The energy of graph G is denoted by $E(G)$, which is the sum of absolute values of its eigen values. Application of the energy graph is in chemistry to approximate the total $\pi-$ electron energy of molecules. Moreover, we present results on the energy of a triangular book graph $B(3,n)$, quadrilateral book graph B_n^4 and restricted square of $B_{(n,n)}$ graph.

1. INTRODUCTION

In 1905, many intellects came out with some matter to combined theories of matrices graph with chemistry. After some time, in 1978 [2] a very well known mathematician Ivan Gutman, had introduced the method of energy of a graph. The idea of the graph energy started from the study of conjugated hydrocarbons by using a tight-binding concept which is known as Huckel molecular orbital (HMO) in chemistry [3–6]. Many researchers are motivated to do work on the energy graph because of its chemical implications on that quantity.

$$E(M) = 2\sum_{j;\lambda_i>0} \lambda_j = \sum_{j=1}^{n} |\lambda_j|. \tag{1.1}$$

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The energy $E(G)$ of a graph is defined to be the sum of the absolute values of its eigen values. If $A(G)$ is adjacency matrix of G and $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n$ are the eigen values of $A(G)$, then,

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

The set $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n$ is the spectrum of G and denoted by spac(G).

Definition 1.1. *[1] Let G be a simple graph with n vertices and m edges. Adjacency matrix of the graph G is given by*

$$A(G) = (a_{ij}) = \begin{cases} 1, & \text{if } v_i \text{ is adjacency to } v_j. \\ 0, & \text{otherwise}. \end{cases} \tag{1.2}$$

The characteristic polynomial of the adjacency matrix is given by $P_G(X)$. The zeroes of the polynomial are given by $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n$ which are eigen values of graph.

Definition 1.2. *[1] The triangular book with $n-$ pages is defined as n copies of cycle C_3 sharing a common edges. The common edge is called the spine or base of the book. This graph is denoted by $B(3, n)$ or B_n. In other words it is the complete tripartite graph $K_{1,1,n}$.*

Definition 1.3. *[1] The quadrilateral book graph B_n^4 for $n \geq 1$ is a planar undirected graph with $2n + 2$ vertices $u_0, u_1, u_2, \ldots, u_n$ and $v_0, v_1, v_2, \ldots, v_n$. $3n + 1$ edges constructed by n quadrilaterals sharing a common edge u_0v_0. In other words the quadrilateral book graph B_n^4 is cartesian product of a star graph $k_{1,n}$ and k_2.*

Definition 1.4. *The restricted square of $B_{(n,n)}$, is a graph G with vertex set $V(G) = V(B_{(n,n)})$ and edge set $E(G) = E(B_{(n,n)}) \bigcup \{uv - i, vu_i / 1 \leq i \leq n\}$.*

Definition 1.5. ***Laplacian energy: [7]*** *Let G be a graph with n vertices and m edges. Let $\mu_1, \mu_2, \mu_3, \ldots, \mu_n$ be the eigenvalues of the Laplacian matrix of graph G. Laplacian matrix $L = L(G)$ of (n, m) graph is defined as a matrix,*

$$L_{ij} = \begin{cases} -1 & \text{if } v_i \text{ and } v_j \text{ are adjacent where } i \neq j \\ 0 & \text{if } v_i \text{ and } v_j \text{ are not adjacent where } i \neq j \\ d_i & \text{if } i = j \end{cases} . \tag{1.3}$$

Here d_i is the degree of the i^{th} vertex of G. The Laplacian energy of the graph G is defined as,

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|. \tag{1.4}$$

Definition 1.6. *Seidel energy: [8]* *Let G be a graph with n vertices and m edges. Let $\{\lambda_1, \lambda_2, \ldots, \lambda_{n-1}, \lambda_n\}$ be the eigenvalues of the Seidel matrix of graph G. $S(G) = S_{ij}$, Seidel matrix is defined as.*

$$S_{ij} = \begin{cases} \text{-1} & \text{if } v_i \text{ and } v_j \text{ are adjacent where } i \neq j \\ 1 & \text{if } v_i \text{ and } v_j \text{ are not adjacent where } i \neq j \\ 0 & \text{other wise}. \end{cases} \tag{1.5}$$

The Seidel energy of the graph G is defined as,

$$ES(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1.6}$$

2. Main Results

Theorem 2.1. *The energy of a triangular book graph $B(3, n)$ is*

$$E(G) = 1 + \left| \frac{1 \pm \sqrt{(1+8n)}}{2} \right|, \quad \text{for } n \geq 2. \tag{2.1}$$

Proof. Let $G = B(3, n)$ be the triangular book graph. Let $u_1, u_2, u_3, \ldots, u_n$ be the vertices of $n-$ pages of triangular book graph. Let u and v be the spine vertices. It is noted that the number of vertices of the graph is $n + 2$ and the number of edges of the graph is $2n + 1$.

The characteristic polynomial using adjacency matrix of the triangular book graph is $\mid A - \lambda I \mid$ which gives the characteristic equation of $B(3, n)$ is

$$\lambda^{n-1}(\lambda + 1)(\lambda^2 - \lambda - 2\lambda) = 0$$

Hence,

$$\begin{aligned} spec(G) &= \text{the set of root of } det(\mid A - \lambda I \mid) \\ &= \begin{pmatrix} 0 & -1 & \frac{1+\sqrt{(1+8n)}}{2} & \frac{1-\sqrt{(1+8n)}}{2} \\ n-1 & 1 & 1 & 1 \end{pmatrix}. \end{aligned}$$

So,

$$E(G) = 1 + \left| \frac{1 \pm \sqrt{(1+8n)}}{2} \right|.$$

Let $\mu_1, \mu_2, \mu_3, \ldots, \mu_{n+2}$ be its eigen values of Laplacian matrix. Respectively characteristic equation of Laplacian matrix of triangular book graph is

$$\mu(\mu-2)^{n-1}(\mu-(n+2))^2 = 0.$$

Hence,

$$\begin{aligned} spec(G) &= \text{the set of root of } det(\mid A - \mu I \mid) \\ &= \begin{pmatrix} 0 & 2 & n+2 \\ 1 & n-1 & 2 \end{pmatrix} \end{aligned}$$

and

$$EL(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| = (n-2)^2/(n+2).$$

After finding the Laplacian energy we find the characteristic equation of the Seidel matrix of a triangular book graph which is

$$(\lambda+1)^{n-1}(\lambda-1)(\lambda^2-(n-2)\lambda-[3(n-1)+2]) = 0.$$

Hence,

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

So, the Seidel energy of triangular book graph is

$$ES(G) = \sum_{i=1}^{n+2} \mid \lambda_i \mid = n + \frac{(n-2) \pm \sqrt{(n^2+8n)}}{2}.$$

□

Theorem 2.2. *The energy of the quadrilateral book graph* B_n^4 *is* $2(n-1)+ \mid -1 \pm \sqrt{n} \mid + \mid 1 \pm \sqrt{n} \mid$.

Proof. Let $G = B_n^4$ be the quadrilateral book graph and $u_3, u_4, u_5, \ldots, u_{2n+2}$ be the vertices of $n-$ pages of quadrilateral book graph and u_1 and u_2 be the spine vertices. Note that the number of vertices of the graph is $2n+2$ and the number of edges of the graph is $3n+1$.

Respectively, the characteristic equation from adjacency matrix of quadrilateral book graph is

$$(\lambda-1)^{n-1}(\lambda+1)^{n-1}(\lambda^2-2\lambda-n+1)(\lambda^2+2\lambda-n+1)=0 \tag{2.2}$$

Hence,

$$\begin{aligned} spec(G) &= \text{the set of root of } det(\mid A-\lambda I\mid) \\ &= \begin{pmatrix} 1 & -1 & -1+\sqrt{n} & -1-\sqrt{n} & 1+\sqrt{n} & 1-\sqrt{n} \\ n-1 & n-1 & 1 & 1 & 1 & 1 \end{pmatrix} \end{aligned}$$

And the energy of the B_n^4 graph is

$$\sum_{i=1}^{2n+2} \mid \lambda_i \mid = 2(n-1)+\mid -1\pm\sqrt{n}\mid + \mid 1\pm\sqrt{n}\mid . \tag{2.3}$$

Respectively, the characteristic equation of the Laplacian matrix of quadrilateral book graph is

$$\mu(\mu-2)(\mu-1)^{n-1}(\mu-2\lceil\frac{n}{2}\rceil)(\mu-(2(\lceil\frac{n}{2}\rceil+1)))=0. \tag{2.4}$$

Here, n is odd and when n is even, then the characteristic equation is

$$\mu(\mu-2)(\mu-1)^{n-1}(\mu-((2\lceil\frac{n}{2}\rceil+1)+1))(\mu-(2\lceil\frac{n}{2}\rceil+1))=0. \tag{2.5}$$

When n is odd,

$$spec(G) = \begin{pmatrix} 0 & 2 & 1 & 2\lceil\frac{n}{2}\rceil+1 & (2\lceil\frac{n}{2}\rceil+1)+1 \\ 1 & 1 & n-1 & 1 & 1 \end{pmatrix}.$$

When n is even,

$$spec(G) = \begin{pmatrix} 0 & 2 & 1 & 2\lceil\frac{n}{2}\rceil & 2(\lceil\frac{n}{2}\rceil+1) \\ 1 & 1 & n-1 & 1 & 1 \end{pmatrix}.$$

Hence, the Laplacian energy of the quadrilateral book graph B_n^4 is

$$\sum_{i=1}^{2n+2} \mid \mu_i - \frac{2m}{n} \mid = n+4+4\lceil\frac{n}{2}\rceil, \text{when n is odd,}$$

$$\sum_{i=1}^{2n+2} \mid \mu_i - \frac{2m}{n} \mid = n+3+4\lceil\frac{n}{2}\rceil, \text{when n is even.}$$

The next aim is to find the characteristic equation from the Seidel matrix of the quadrilateral book graph, which is

$$(\lambda+3)^{n-1}(\lambda+1)(\lambda-1)^{n-1}(\lambda^2-2\lambda-(4n-1))=0.$$

Here, $n \geq 2$.

$$spec(G)=\begin{pmatrix} -1 & 1 & -3 & 1\pm 2\sqrt{n} \\ 1 & n-1 & n-1 & 1 \end{pmatrix}.$$

Hence, the Seidel energy of the quadrilateral book graph B_n^4 is

$$\sum_{i=1}^{2n+2} \mid \lambda \mid = 4n-2\pm 2\sqrt{n}.$$

□

Theorem 2.3. *Energy of restricted square of $B_{(n,n)}$ graph is*

$$\sum_{i=1}^{2n+2} \mid \lambda_i \mid = 4\sqrt{n}.$$

Proof. Let G be the restricted square of bistar $B_{(n,n)}$ with vertex set $V(G) = V(B_{(n,n)})$ and edge set $E(G) = E(B_{(n,n)}) \bigcup \{uv - i, vu_i / 1 \leq i \leq n\}$. Here, the number of vertices of the graph is $2n+2$ and the number of edges of the graph is $4n+1$.

The characteristic equation from adjacency matrix of $B_{n,n}$ is $\mid A-\lambda I \mid = \lambda^{2n} * (\lambda^2-4n)=0$. After the simplification of the characteristic equation, we get the spectrum of eigen values is

$$spec(G)=\begin{pmatrix} 0 & 2\sqrt{n} & -2\sqrt{n} \\ 2n & 1 & 1 \end{pmatrix}.$$

Hence, the energy of the restricted square of $B_{(n,n)}$ graph is

$$\sum_{i=1}^{2n+2} \mid \lambda_i \mid = 4\sqrt{n}.$$

The characteristic equation from the Laplacian matrix of $B_{n,n}$ graph is $\mu(\mu-2)^{2(n-1)+1}(\mu-2n)(\mu-2(n+1))=0$. After the simplification of this characteristic equation we get the spectrum of eigen values is

$$spec(G)=\begin{pmatrix} 0 & 2 & 2n & 2(n+1) \\ 1 & 2(n-1)+1 & 1 & 1 \end{pmatrix}.$$

Hence, the Laplacian energy of the restricted square of $B_{(n,n)}$ graph is

$$\sum_{i=1}^{2n+2} | \mu_i - \frac{2m}{n} |= (8n^2 - 2n + 2/n + 1).$$

Characteristic equation from the Seidel matrix of $B_{n,n}$ is $(\lambda+1)^{2n+1}(\lambda-(2n+1))$.

After the simplification of characteristic equation we get the spectrum of eigen values is

$$spec(G) = \begin{pmatrix} 2n+1 & -1 \\ 1 & 2n+1 \end{pmatrix}.$$

Hence the Seidel energy of the restricted square of $B_{(n,n)}$ graph is

$$\sum_{i=1}^{2n+2} | \lambda_i |= 4n + 2.$$

□

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DEPARTMENT OF MATHEMATICS, SCHOOL OF ENGINEERING, RK UNIVERSITY, RAJKOT, GUJARAT, INDIA.

Email address: jadaviram@gmail.com