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Energy and its bounds for generalised star graphs

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Abstract

The energy of the graph G is defined as the sum of the absolute values of its eigenvalues. In this paper, we study the energy of the generalised star graphs. The purpose of the paper is to study the bounds of the eigenvalues and energy of the generalised star graphs.

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1 Introduction

Let G be a simple, finite, undirected graph with n vertices. The adjacency matrix $A(G) = [a_{ij}]$ is a square matrix of order n whose (i,j)-entry is 1 if the vertices v_i and v_j are adjacent and 0 otherwise. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix A(G). The spectrum of the graph G is defined as the set of eigenvalues of A(G), together with their multiplicities. The energy of the graph G is defined as $[3, 4, 8, 9, 11]E(G) = \sum_{i=1}^{n} |\lambda_i|$. The energy of a graph G was defined by Ivan Gutman in 1978. During these days the energy of a graph is a much studied quantity in the mathematical literature.

One of the most remarkable chemical application of graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of π - electrons in unsaturated conjugated hydrocarbons (HMO theory). The total π - electron energy is equal to the sum of the energies of all π - electrons in the respective molecule which eventually resulted in the development of graph energy. Some chemical applications of graph theory is discussed in [10].

In this paper we are concerned with the eigenvalues and energy of the generalised star graphs. Throughout this paper, we denote a star graph of order n as $K_{1,n-1}$. Let $G_s = G(K_{1,n_1-1}, K_{1,n_2-1}, \ldots, K_{1,n_k-1})$ be a generalised star graph [6] such that the central vertices of the k star graphs K_{1,n_1-1} , $K_{1,n_2-1}, \ldots, K_{1,n_k-1}$ are completely connected. i.e., any two central vertices of the k star graphs are adjacent.

2 Observation

Result 2.1. [1] If $X = (x_1, x_2, ..., x_n)^T$ is an eigen vector corresponding to the eigen value λ of the adjacency matrix A(G) then $\lambda x_i = \sum_{j=1, j \neq i}^n x_j; i = 1, 2, ..., n.$

Result 2.2. [2, 5, 7] For a symmetric real n by n matrix A and λ a real number, the multiplicity of λ as an eigen value of A is $n - rank(A - \lambda I)$

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3 Spectra of Generalised Star Graphs

Lemma 3.1. Let $G_s = G(K_{1,n_1-1}, K_{1,n_2-1}, \ldots, K_{1,n_k-1})$ be the generalised star graph. Then 0 is an eigenvalue of $A(G_s)$ of multiplicity $n_1 + n_2 + \ldots + n_k - 2k$ and the other eigen values satisfy the following system of equations

$$\lambda x_{2i-1} = (n_i - 1) x_{2i} + \sum_{j=1; j \neq i}^k x_{2j-1} \\ \lambda x_{2i} = x_{2i-1}, i = 1, 2, \dots, k. \end{cases}$$
 (A)

Proof: The adjacency matrix $A(G_s)$ of the generalised star graph G_s has rank 2k. Using Result 2.2, we can observe that the multiplicity of the eigen value 0 is $n_1 + n_2 + \ldots + n_k - 2k$. Let $\lambda \neq 0$ be an eigen value of $A(G_s)$. Since $\lambda \neq 0$, all the eigen components corresponding to the pendant vertices, which are connected to the same vertex with an eigen value λ are equal, we can assume that λ is an eigen value corresponding to the eigenvector

$$X = \left(\underbrace{x_{1}, x_{2}, x_{2}, \dots, x_{2}}_{n_{1}}, \underbrace{x_{3}, x_{4}, x_{4}, \dots, x_{4}}_{n_{2}}, \dots, \underbrace{x_{2k-1}, x_{2k}, x_{2k}, \dots, x_{2k}}_{n_{k}}\right)^{T} \dots (B)$$

Using (B) in Result 2.1 we get the system of equations (A).

Corollary 3.2. Let λ be an eigen value with corresponding eigen vector $X = (x_1, x_2, \dots, x_{2k})^T$ of the system of equations (A) then all x_{2i-1} cannot be zero.

Proof: If possible, let x_{2i-1} be zero for all i. Since $\lambda \neq 0$ and $\lambda x_{2i} = x_{2i-1}$, we get $x_{2i} = 0$ for all i, which is not possible.

Theorem 3.3. Let $G_s = G(K_{1,n_1-1}, K_{1,n_2-1}, \dots, K_{1,n_k-1}), k > 2$, be the generalised star graph. Then the bounds of the 2k non-zero eigen values are as follows. The negative eigen values λ are bounded as $\frac{-1-\sqrt{1+4(n_1-1)}}{2} \leq \lambda \leq \frac{(k-1)-\sqrt{(k-1)^2+4(n_k-1)}}{2}$ and the positive eigen values λ are bounded as $\frac{-1+\sqrt{1+4(n_k-1)}}{2} \leq \lambda \leq \frac{(k-1)+\sqrt{(k-1)^2+4(n_1-1)}}{2}$.

Proof: Among the 2k non-zero eigen values, k eigen values are positive and k eigen values are negative. By (A), $\lambda x_{2i-1} = (n_i - 1) \frac{x_{2i-1}}{\lambda} + \sum_{j=1; j \neq i}^k x_{2j-1}; i = 1, 2, \dots, k.$

Since atleast two eigen components x_{2i-1} 's are of different signs, $n_i \ge n_j$ we get the lower bounds from the equation $\lambda^2 + \lambda + (1-r) = 0$; where $r = \frac{n_i x_{2i-1} - n_j x_{2j-1}}{x_{2i-1} - x_{2j-1}}$. Thus $\lambda = \frac{-1 \pm \sqrt{1 + 4(r-1)}}{2}$. Also upper bounds of the eigen values are given by $\lambda^2 - (k-1)\lambda + (1-n_i) = 0$.

Hence $\lambda = \frac{k-1\pm\sqrt{(k-1)^2+4(n_i-1)}}{2}$. Since $n_1 \ge n_i \ge n_j \ge n_k$, the k negative roots have the bounds as $\frac{-1-\sqrt{1+4(n_1-1)}}{2} \le \lambda \le \frac{(k-1)-\sqrt{(k-1)^2+4(n_k-1)}}{2}$ and the k positive roots are bounded by $\frac{-1+\sqrt{1+4(n_k-1)}}{2} \le \lambda \le \frac{(k-1)+\sqrt{(k-1)^2+4(n_1-1)}}{2}$.

Theorem 3.4. Let $G_s = G(K_{1,m-1}, K_{1,m-1}, \dots, K_{1,m-1})$ be a generalized star graph. Then the spectrum of G_s is

$$\begin{pmatrix} 0 & \frac{-1-\sqrt{1+4(m-1)}}{2} & \frac{-1+\sqrt{1+4(m-1)}}{2} & \frac{(k-1)-\sqrt{(k-1)^2+4(m-1)}}{2} & \frac{(k-1)+\sqrt{(k-1)^2+4(m-1)}}{2} \\ k(m-2) & k-1 & k-1 & 1 & 1 \end{pmatrix}$$

Proof: Here, $n_1 = n_2 = \ldots = n_k = m$. By Lemma 3.1, we have 0 is an eigen value of multiplicity k(m-2). From (A) we get,

$$\lambda x_{2i-1} = (m-1)x_{2i} + \sum_{j=1; j \neq i}^{k} x_{2j-1},$$
$$\lambda x_{2i} = x_{2i-1}, \quad i = 1, 2, \dots, k.$$

Using Theorem 3.3, $\lambda = \frac{-1 \pm \sqrt{1+4(m-1)}}{2}$ of multiplicity k-1 and the remaining two eigenvalues are given by $\lambda^2 - (k-1)\lambda + (1-m) = 0$. Hence we obtain $\lambda = \frac{k-1 \pm \sqrt{(k-1)^2+4(m-1)}}{2}$.

Corollary 3.5. Let $G(K_{1,n_1-1}, K_{1,n_2-1})$ be the generalised star graph such that the central vertices of the stars K_{1,n_1-1} and K_{1,n_2-1} are completely connected. Then 0 is an eigen value of multiplicity $n_1 + n_2 - 4$ and the remaining four non-zero eigen values are $\pm \sqrt{\frac{r \pm \sqrt{r^2 - 4s}}{2}}$ where $r = n_1 + n_2 - 1$ and $s = (n_1 - 1)(n_2 - 1)$.

Proof: The proof follows from Lemma 3.1. Since, k = 2, 0 is an eigen value of multiplicity $n_1 + n_2 - 4$ and the four non-zero eigen values are given by the following equations

$$\lambda x_{2i-1} = (n_i - 1)x_{2i} + x_{2j-1}; \ i = 1, 2; \ j = 1, 2; \ j \neq i,$$
$$\lambda x_{2i} = x_{2i-1}, \ i = 1, 2.$$

Thus we get $\lambda^4 - (n_1 + n_2 - 1)\lambda^2 + (n_1 - 1)(n_2 - 1) = 0$ which gives $\lambda = \pm \sqrt{\frac{r \pm \sqrt{r^2 - 4s}}{2}}$ where $r = n_1 + n_2 - 1$ and $s = (n_1 - 1)(n_2 - 1)$.

4 Energies and their bounds for the generalised star graphs

Theorem 4.1. The lower and the upper bounds of the energy of the generalised star graph $G_s = G(K_{1,n_1-1}, K_{1,n_2-1}, \ldots, K_{1,n_k-1})$ are $\begin{bmatrix} k \\ 2 \end{bmatrix} \begin{bmatrix} \sqrt{4n_k - 3} + \sqrt{(k-1)^2 + 4(n_k - 1)} - k \end{bmatrix}$ and $\begin{bmatrix} k \\ 2 \end{bmatrix} \begin{bmatrix} k + \sqrt{4n_1 - 3} + \sqrt{(k-1)^2 + 4(n_1 - 1)} \end{bmatrix}$ respectively.

Proof: Using the lower and upper bounds of the eigen values in Theorem 3.3, the lower bound of the energy is calculated as

$$E(G_s) \ge k \left| \frac{-1 + \sqrt{1 + 4(n_k - 1)}}{2} \right| + k \left| \frac{(k - 1) - \sqrt{(k - 1)^2 + 4(n_k - 1)}}{2} \right|$$

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$$= \left[\frac{k}{2}\right] \left[\sqrt{4n_k - 3} + \sqrt{(k-1)^2 + 4(n_k - 1)} - k\right].$$

Also we get the upper bound of the energy as

$$\begin{split} E(G_s) &\leq k \left| \frac{-1 - \sqrt{1 + 4(n_1 - 1)}}{2} \right| + k \left| \frac{(k - 1) + \sqrt{(k - 1)^2 + 4(n_1 - 1)}}{2} \right| \\ &= \left[\frac{k}{2} \right] \left[k + \sqrt{4n_1 - 3} + \sqrt{(k - 1)^2 + 4(n_1 - 1)} \right]. \end{split}$$

Thus, the lower bound and the upper bound of the energy of the generalised star graph $G_s = G(K_{1,n_1-1}, K_{1,n_2-1}, \dots, K_{1,n_k-1})$ are $\left[\frac{k}{2}\right] \left[\sqrt{4n_k - 3} + \sqrt{(k-1)^2 + 4(n_k-1)} - k\right]$ and $\left[\frac{k}{2}\right] \left[k + \sqrt{4n_1 - 3} + \sqrt{(k-1)^2 + 4(n_1-1)}\right]$ respectively.

Corollary 4.2. The energy of the generalised star graph $G_s = G(K_{1,m-1}, K_{1,m-1}, \dots, K_{1,m-1})$ is $(k-1)\sqrt{4m-3} + \sqrt{(k-1)^2 + 4(m-1)}$.

Proof: Here, $n_1 = n_2 = \cdots = n_k = m$. From Theorem 3.4, the energy of G is calculated as

$$E(G) = (k-1) \left| \frac{-1 + \sqrt{1 + 4(m-1)}}{2} \right| + (k-1) \left| \frac{-1 - \sqrt{1 + 4(m-1)}}{2} \right|$$
$$+ \left| \frac{(k-1) + \sqrt{(k-1)^2 + 4(m-1)}}{2} \right| + \left| \frac{(k-1) - \sqrt{(k-1)^2 + 4(m-1)}}{2} \right|$$
$$= (k-1)\sqrt{4m-3} + \sqrt{(k-1)^2 + 4(m-1)}.$$

Corollary 4.3. The energy of the generalised star graph $G(K_{1,n_1-1}, K_{1,n_2-1})$ is $E(G) = \sqrt{2} \left[\sqrt{r + \sqrt{r^2 - 4s}} + \sqrt{r - \sqrt{r^2 - 4s}} \right]$ where $r = n_1 + n_2 - 1$ and $s = (n_1 - 1)(n_2 - 1)$.

Proof: From Theorem 3.5, the energy is given by

$$E(G) = \left| \sqrt{\frac{r + \sqrt{r^2 - 4s}}{2}} \right| + \left| \sqrt{\frac{r - \sqrt{r^2 - 4s}}{2}} \right| + \left| -\sqrt{\frac{r + \sqrt{r^2 - 4s}}{2}} \right| + \left| -\sqrt{\frac{r - \sqrt{r^2 - 4s}}{2}} \right| = \sqrt{2} \left[\sqrt{r + \sqrt{r^2 - 4s}} + \sqrt{r - \sqrt{r^2 - 4s}} \right]$$

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