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BEHAVIOR OF ENERGY FOR A CLASS OF CLUSTER GRAPHS

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ABSTRACT. The energy of a graph is defined as the sum of absolute eigenvalues of a graph G. In this paper, we introduce a class of cluster graphs obtained from complete graph by deleting some of its edges and we find its spectra and energy. Further, we have classified some of these graphs as hyper energetic graphs. One result of I. Gutman and L. Pavlović becomes a particular case of our result.

1. INTRODUCTION

Let G be a simple, undirected graph with n vertices and m edges. Let $V(G) = \{v_1, v_2, ..., v_n\}$ be the vertex set of G and $\varepsilon(G) = \{e_1, e_2, \ldots, e_m\}$. The graphs with large number of edges are referred as cluster graphs [4]. Such graphs are well studied in chemistry to approximate the total π electron energy of a molecule. The adjacency matrix of G is defined as $A(G) = [a_{ij}]$ in which $a_{ij} = 1$ if v_i is adjacent to v_j and $a_{ij} = 0$, otherwise. The roots of the characteristic polynomial $\phi(G : \lambda) = |\lambda I - A(G)|$ of G are known as the eigenvalues of G denoted by $\lambda_1, \lambda_2, ..., \lambda_n$ [3]. The energy of G is defined by $E(G) = |\lambda_1| + |\lambda_2| + ... + |\lambda_n|$ [5]. Graphs whose energy is more than energy of complete graph i.e $2(n-1)$ are known as hyper energetic graphs [6]. Other works related to computation of energy $E(G)$ and its dependency can be seen in [2, 8].

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In [7] and [9] five classes of graphs have been introduced obtained from the complete graph by deleting some of its edges and their corresponding spectra and energies have been discussed. Here is one of those five definition and the corresponding polynomial which becomes a particular case of our result.

Definition 1.1. *[7] Let v be a vertex of the complete graph K_n, $n \geq 3$, and let e_i, $i = 1, 2, \ldots, k$, $1 \leq k \leq n-1$ be its distinct edges, all being incident to v. The graph $Ka_n(k)$ is obtained by deleting e_i, $i = 1, 2, \ldots, k$, from K_n. In addition $Ka_n(0) \equiv K_n$.*

Theorem 1.1. *[7] For $n \geq 3$ and $0 \leq k \leq n-1$,*
$\phi(Ka_n(k), \lambda) = (\lambda+1)^{n-3}[\lambda^3 - (n-3)\lambda^2 - (2n-k-3)\lambda + (k-1)(n-1-k)]$.

In this paper, we discuss the spectra and energy for a class of graphs that are obtained from a complete graph K_n, by deleting a cluster of graphs having one vertex in common. We discuss the spectra and eigenvalues of these graphs and obtain the bounds for its energy. Later we state the conditions under which the defined graphs are hyperenergetic.
We state a lemma which is necessary for the result.
Let I be the identity matrix and J be the matrix whose all entries are equal to 1.

Lemma 1.1. *[1] The eigenvalues of $n \times n$ matrix $aI + bJ$ are a with multiplicity $n-1$ and $a + nb$ with multiplicity one.*

2. Main Results

Definition 2.1. *Let $(K_p)_i$, $i = 0, 1, 2, \ldots, k$, $1 \leq k \leq \left\lfloor \frac{n-1}{p-1} \right\rfloor$ be the complete sub graphs with p vertices of the complete graph K_n, $n \geq 3$ having one vertex in common. The graph $Ka_n(p, k, 1)$ is obtained from K_n by deleting all the edges of $(K_p)_i$, $i = 0, 1, 2, \ldots, k$. In addition $Ka_n(0, k, 1) \equiv Ka_n(p, 0, 1) \equiv Ka_n(0, 0, 1) \equiv K_n$.*

Theorem 2.1. *For $n \geq 3$, $1 \leq k \leq \left\lfloor \dfrac{n-1}{p-1} \right\rfloor$ and $1 \leq p \leq n$.*

(2.1)
$$\phi(Ka_n(p, k, 1) : \lambda) = \lambda^{k(p-2)}(\lambda+p-1)^{k-1}(\lambda+1)^{n-kp+k-2}\big[\lambda^3 + (p+1-n)\lambda^2 + \\ +(kp^2 + 2p + k - pn - 2pk - 1)\lambda + (n-kp+k-1)(p-1)(k-1)\big].$$

Proof. Without loss of generality, we assume that the vertices of $(K_p)_i$ are $v_{(i-1)(p-1)+2}, v_{(i-1)(p-1)+3} \ldots v_{(i-1)(p-1)+p}$ where $i = 1, 2, \ldots, k$ and let the common vertex of all k copies of K_p be v_1. Then characteristic polynomial of $Ka_n(p, k, 1)$ is

$$\phi(Ka_n(p,k,1):\lambda) = \det(\lambda I - A(Ka_n(p,k,1)))$$
$$= \begin{vmatrix} \lambda I_p & -Q^T_{p-1,p} & -Q^T_{p-1,p} & \cdots & -J_{p,n-k(p-1)-1} \\ -Q_{p-1,p} & \lambda I_{p-1} & -J_{p-1} & \cdots & -J_{p,n-k(p-1)-1} \\ -Q_{p-1,p} & -J_{p-1} & \lambda I_{p-1} & \cdots & -J_{p,n-k(p-1)-1} \\ \vdots & \vdots & \vdots & & \vdots \\ -J_{n-k(p-1)-1} & -J_{n-k(p-1)-1} & -J_{n-k(p-1)-1} & \cdots & (\lambda I - J)_{n-k(p-1)-1} \end{vmatrix}.$$

$Q_{p-1,p}$ is the block matrix of order $(p-1, p)$ whose first column is zero and rest all entries are one. J is a matrix of ones. Subtracting first column from all other columns element wise $(C_2 - C_1, C_3 - C_1, \ldots, C_n - C_1)$ we get the following determinant where L_{p-1} is a unit row matrix of order $p-1$.

$$= \begin{vmatrix} \lambda & -\lambda L_{p-1} & -\lambda L_{p-1} & \cdots & -\lambda L_{p-1} & (-1-\lambda) L_{n-k(p-1)-1} \\ O & \lambda I_{p-1} & -J_{p-1} & \cdots & -J_{p-1} & -J_{p-1\times n-k(p-1)-1} \\ O & -J_{p-1} & \lambda I_{p-1} & \cdots & -J_{p-1} & -J_{p-1\times n-k(p-1)-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ O & -J_{p-1} & -J_{p-1} & \cdots & \lambda I_{p-1} & -J_{p-1\times n-k(p-1)-1} \\ -L'_{n-k(p-1)-1} & O & O & \cdots & O & (\lambda+1) I_{n-k(p-1)-1} \end{vmatrix}.$$

Take $(\lambda + 1)$ common from last row and denote $1/(\lambda + 1) = W$ and $Z = n - k(p-1) - 1$. Adding all the elements row wise in the matrices of the last column and then adding the sum to the first column matrices we get a matrix of order $K(p-1)+1$.

$$= (\lambda+1)^Z \begin{vmatrix} \lambda - Z & -\lambda L_{p-1} & -\lambda L_{p-1} & \cdots & -\lambda L_{p-1} \\ -WZL'_{p-1} & \lambda I_{p-1} & -J_{p-1} & \cdots & -J_{p-1} \\ -WZL'_{p-1} & -J_{p-1} & \lambda I_{p-1} & \cdots & -J_{p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -WZL'_{p-1} & -J_{p-1} & -J_{p-1} & \cdots & \lambda I_{p-1} \end{vmatrix}.$$

Subtracting the second column from the all the succeeding columns and taking $|\lambda I + J|$ common from last $k-1$ columns we get

$$= (\lambda+1)^Z \, |\lambda I + J|_{p-1}^{k-1} \begin{vmatrix} \lambda - Z & -\lambda L_{p-1} & O & \cdots & O \\ -WZL'_{p-1} & \lambda I_{p-1} & -I & \cdots & -I \\ -WZL'_{p-1} & -J_{p-1} & I & \cdots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -WZL'_{p-1} & -J_{p-1} & O & \cdots & I \end{vmatrix}.$$

Adding last $k-2$ rows to the second row reduces the matrix to

$$= (\lambda+1)^Z \, |\lambda I + J|_{p-1}^{k-1} \begin{vmatrix} \lambda - Z & -\lambda L_{p-1} \\ -kWZL'_{p-1} & \lambda I_{p-1} - (k-1)J_{p-1} \end{vmatrix}.$$

Using Lemma 1.1 for $|\lambda I + J|_{p-1}^{k-1}$ and $|\lambda I_{p-1} - (k-1)J_{p-1}|$ and on simplification we get

$$= (\lambda+1)^Z \, |\lambda I + J|_{p-1}^{k-1} \, \lambda^{p-2} \left\{ (\lambda - Z)[\lambda + (k-1)(p-1)] + \lambda(p-1)WZk \right\}.$$

On substitution of values of W as $\dfrac{1}{\lambda+1}$ and Z as $n-kp+k-1$ with simplification leads to the required result (2.1). □

3. Spectra and Energy of $Ka_n(p,k,1)$

From equation (2.1), the spectra of $Ka_n(p,k,1)$ is

$$\begin{pmatrix} -1 & 1-p & 0 & \mu_1 & \mu_2 & \mu_3 \\ n-kp+k-2 & k-1 & pk-2k & 1 & 1 & 1 \end{pmatrix}$$

where μ_1, μ_2 and μ_3 are the roots of the polynomial $P(\lambda)$

$$P(\lambda) = \lambda^3 - (n-p-1)\lambda^2 + (kp^2 + 2p + k - pn - 2pk - 1)\lambda + (n-kp+k-1)(p-1)(k-1).$$

The zeros of $P(\lambda)$ are necessarily real valued, because
$P(0) = (n-kp+k-1)(p-1)(k-1) > 0$,
$P'(0) = -p(n-kp+k-1) - (p-1)(k-1) \leq 0$.
Two of the zeros are positive and other negative.

Let $\mu_1 > \mu_2 > 0 > \mu_3$. As $\mu_1 + \mu_2 + \mu_3 = -(n-p-1)$ and $\mu_1\mu_2\mu_3 = -(n-kp+k-1)(p-1)(k-1)$, hence the values of μ_2 and μ_3 are

(3.1)
$$\mu_2 = \frac{1}{2}\left[(n-p-1-\mu_1) + \sqrt{(n-p-1-\mu_1)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{\mu_1}}\right]$$
(3.2)
$$\mu_3 = \frac{1}{2}\left[(n-p-1-\mu_1) - \sqrt{(n-p-1-\mu_1)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{\mu_1}}\right],$$
so we get

$$|\mu_2| + |\mu_3| = \sqrt{(n-p-1-\mu_1)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{\mu_1}}.$$

Consequently the energy of $Ka_n(p,k,1)$ will be

$$E(Ka_n(p,k,1)) = (n-p-1) + |\mu_1| + |\mu_2| + |\mu_3|$$
$$E(Ka_n(p,k,1)) = n-p-1+\mu_1 + \sqrt{(n-p-1-\mu_1)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{\mu_1}}.$$

Here we introduce an auxiliary function $F_{n,p,k}(x)$

(3.3)
$$F_{n,p,k}(x) = n-p-1+x+\sqrt{(n-p-1-x)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{x}}.$$

Clearly $F_{n,p,k}(\mu_1) \equiv E(Ka_n(p,k,1))$, then

$$\frac{dF}{dx} = 1 - \frac{(n-p-1-x) + \frac{2(k-1)(p-1)(n-kp+k-1)}{x^2}}{\sqrt{(n-p-1-x)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{x}}}.$$

The right hand side of above equation is greater than zero if $(n-p-1-x) + \frac{2(k-1)(p-1)(n-kp+k-1)}{x^2} < \sqrt{(n-p-1-x)^2 + \frac{4(k-1)(p-1)(n-kp+k-1)}{x}}$, on solving $\frac{(k-1)(p-1)(n-kp+k-1)}{x^3} + \frac{(n-p-1)}{x} < 2$.

For $x \geq n-p-1$ and for $n > k(p-1)-1$, $2 \leq k \leq \frac{n-2}{p-1}$ the above inequality is satisfied. This means that in the interval $[n-p-1, \infty)$ the function $F_{n,p,k}(x)$ monotonically increases.

Because $P(n-p)<0$ and $P(n-p+1)>0$ we have the following Lemma.

Lemma 3.1. *For all* $n>k(p-1)-1$, $2\leq k\leq \dfrac{n-2}{p-1}$

$$n-p<\mu_1<n-p+1.$$

Combining Lemma 3.1 with equation (3.1) and equation (3.2) we obtain the bounds for μ_2 and μ_3 as follows
Bound for μ_2

$$\frac{1}{2}[-1+\mu']>\mu_2>[-1+\mu''].$$

Bound for μ_3

$$\frac{1}{2}[-1-\mu']>\mu_3>[-1-\mu''].$$

where
$\mu^{'}=\sqrt{1+\dfrac{4(k-1)(p-1)(n-kp+k-1)}{n-p}}$ and
$\mu^{''}=\sqrt{1+\dfrac{4(k-1)(p-1)(n-kp+k-1)}{n-p+1}}$.

Combining Lemma 3.1 with equation (3.3) and taking into consideration the demonstration of monotony of $F_{n,p,k}$ we obtain the bound for energy.

Corollary 3.1. *For all* $n>k(m-1)-1$, $2\leq k\leq \dfrac{n-2}{m-1}$.

$$F_{n,m,k}(n-m)<E<F_{n,m,k}(n-m+1).$$

Here $F_{n,p,k}(x)$ is given by equation (3.3). We see that
$F_{n,p,k}(n-p)=2n-2p-1+\sqrt{1+\dfrac{4(k-1)(p-1)(n-kp+k-1)}{n-p}}$
and
$F_{n,p,k}(n-p+1)=2(n-p)+2\sqrt{1+\dfrac{4(k-1)(p-1)(n-kp+k-1)}{n-p+1}}$
the result can be improved by taking $\mu^{'}$ and $\mu^{''}$
Hence the bound for energy of cluster graphs $Ka_n(p,k,1)$ is

$$2n-2p-1+\mu^{'}<E(Ka_n(p,k,1))<2n-2p+2\mu^{''}.$$

4. Conditions for hyperenergetic

On direct computation of energy using equation (2.1), we observe that as we delete the edges of k copies of K_p having one vertex in common from K_n, the energy of graph increases, becomes hyperenergetic for a certain range and again decreases. In Figure 1 we have considered $Ka_n(p, k, 1)$ with one particular value n=79, with various combinations of k and p. That is we are deleting k copies of K_p graphs from K_n having one vertex in common. We observe that only for a particular combination of k, p and n the graph becomes hyperenergetic.

Hence we can construct hyperenergetic graphs from K_n by deleting k copies of K_p having one vertex in common satisfying the conditions given in (4.1)

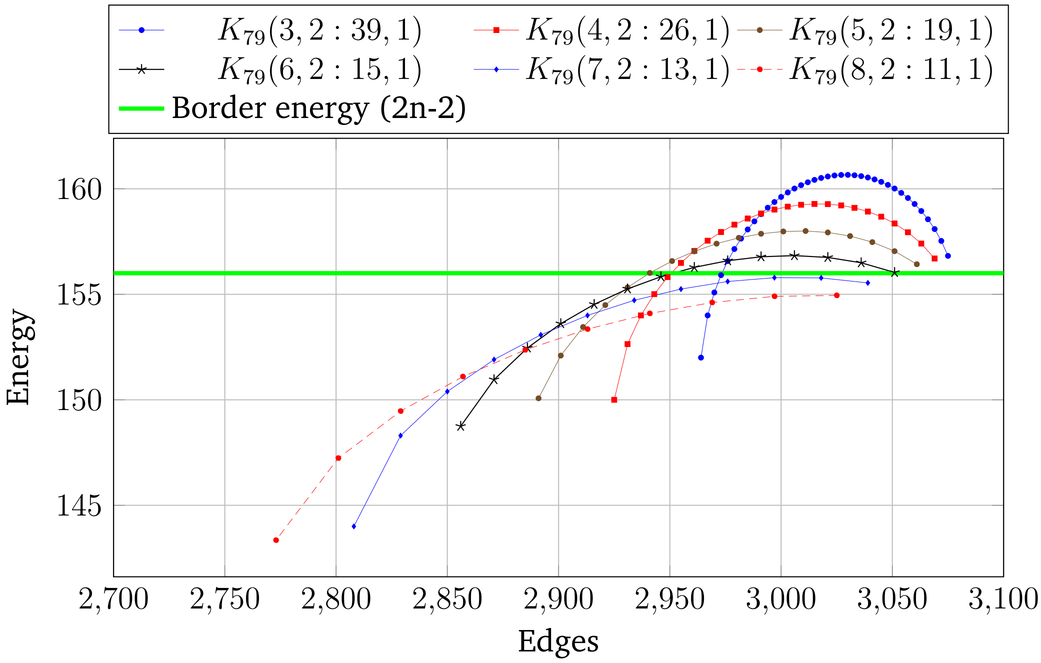

FIGURE 1. Variation in energy of $K_an(p, k, 1)$

4.1. Conditions under which the graph $Ka_n(p, k, 1)$ is hyperenergetic.

The graph $Ka_n(p, k, 1)$ is hyperenergetic when its energy exceeds the energy of complete graph i.e. $2n - 2$. From corollary 3.1 we see that the lower bound of $E[Ka_n(p, k, 1)]$ is $F_{n,p,k}(n - p)$. Thus if

$$F_{n,p,k}(n - p) > 2n - 2$$

we get hyperenergetic class, on further direct simplification we get

$$(k-1)(n-kp+k-1) > p(n-p)$$

which holds true whenever :

$$\left.\begin{aligned} k=6, \quad & p=3, n \geq 28 \\ & p=4, n \geq 79 \\ k=7, \quad & p=3, n \geq 27 \\ & p=4, n \geq 58 \\ & p=5, n \geq 149 \\ \cdots & \\ k=k, \quad & p=3, n \geq \frac{(2k-5)(k+2)}{(k-4)} \\ & p=4, n \geq \frac{3k^2-2k-17}{k-5} \\ & \cdots \\ & p=k-2, n \geq k^3-5k^2+8k-5 \end{aligned}\right\} \tag{4.1}$$

Thus the relation $E[Ka_n(p,k,1)] > E(K_n)$ holds for any choice of n,p,k specified in (4.1). That is by deleting $k\frac{p(p-1)}{2}$ edges from K_n we get a class of hyperenergetic graphs where k,p,n obey the above relations , provided these edges have one vertex in common.

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