## **ENERGY OF SOME CLUSTER GRAPHS**

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ABSTRACT. The energy of a graph G is defined as the sum of the absolute values of the eigenvalues of G. The graphs with large number of edges are referred as graph representation of inorganic clusters, so-called cluster graphs. I. Gutman and L. Pavlović introduced four classes of graphs obtained from complete graph by deleting edges and obtained their spectra and energies. In this paper we introduce another class of graph obtained from complete graph by deleting edges and find its energy. Some results of I. Gutman and L. Pavlović, become particular cases of our results.

### INTRODUCTION

From chemical point of view, the graphs with large number of edges are referred as graph representations of inorganic clusters, so-called cluster graphs [6]. In this paper we consider the spectra and energy of some cluster graphs obtained from complete graph by deleting edges.

Let G be a simple undirected graph with p vertices and q edges. Let  $V(G) = \{v_1, v_2, \dots, v_p\}$  be the vertex set of G. 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 characteristic polynomial of G is  $\phi(G:\lambda) = \det(\lambda I - A(G))$ , where I is a unit matrix of order p. The roots of the equation  $\phi(G:\lambda) = 0$  denoted by  $\lambda_1, \lambda_2, \dots, \lambda_p$  are the eigenvalues of G and their collection is the spectrum of G [1]. The energy [2] of G is defined as  $E(G) = |\lambda_1| + |\lambda_2| + \dots + |\lambda_p|$ . It represents a proper generalization of a formula valid for the total  $\pi$ -electron energy of a conjugated hydrocarbon as calculated with the Hückel molecular orbital (HMO) method in quantum chemistry [5].  $K_p$  is the complete graph on p vertices. The spectrum of  $K_p$  consists of eigenvalues p-1 and -1 (p-1 times). Consequently  $E(K_p) = 2(p-1)$ . It was conjectured some time ago that, among all graphs with p vertices the complete graph has the greatest energy [2]. But this is not true [7]. There are p-

vertex graphs having energy greater than  $E(K_p)$ . The p-vertex graph G with  $E(G) > E(K_p)$  is referred as hyperenergetic graph [3].

### SOME CLUSTER GRAPHS

I. Gutman and L. Pavlović [4] introduced four classes of graphs obtained from complete graph by deleting edges and analyzed their energies. For completeness we reproduce these here.

<u>DEFINITION 1</u> [4]: Let v be a vertex of the complete graph  $K_p$ ,  $p \ge 3$  and let  $e_i$ , i = 1, 2, ..., k,  $1 \le k \le p$  – 1, be its distinct edges, all being incident to v. The graph  $Ka_p(k)$  is obtained by deleting  $e_i$ , i = 1, 2, ..., k from  $K_p$ . In addition  $Ka_p(0) \cong K_p$ .

<u>DEFINITION 2</u> [4]: Let  $f_i$ ,  $i=1,2,\ldots,k$ ,  $1 \le k \le \lfloor p/2 \rfloor$  be independent edges of the complete graph  $K_p$ ,  $p \ge 3$ . The graph  $K_p$ (k) is obtained by deleting  $f_i$ ,  $i=1,2,\ldots,k$  from  $K_p$ . In addition  $K_p$ (0)  $\cong K_p$ .

<u>DEFINITION 3</u> [4]: Let  $V_k$  be a k-element subset of the vertex set of the complete graph  $K_p$ ,  $2 \le k \le p$ ,  $p \ge 3$ . The graph  $Kc_p(k)$  is obtained by deleting from  $K_p$  all the edges connecting pairs of vertices from  $V_k$ . In addition  $Kc_p(0) \cong Kc_p(1) \cong K_p$ .

<u>DEFINITION 4</u> [4]: Let  $3 \le k \le p$ ,  $p \ge 3$ . The graph  $Kd_p(k)$  is obtained by deleting from  $K_p$ , the edges belonging to a k-membered cycle.

## *THEOREM 1* [4]:

For 
$$p \ge 3$$
 and  $0 \le k \le p - 1$ ,  

$$\phi(Ka_p(k) : \lambda) = (\lambda + 1)^{p-3} [\lambda^3 - (p-3)\lambda^2 - (2p-k-3)\lambda + (k-1)(p-1-k)].$$
(2.1)

### THEOREM 2 [4]:

For 
$$p \ge 3$$
 and  $0 \le k \le \lfloor p/2 \rfloor$ ,

$$\phi(Kb_{p}(k):\lambda) = \lambda^{k}(\lambda+1)^{p-2k-1}(\lambda+2)^{k-1}[\lambda^{2}-(p-3)\lambda-2(p-k-1)]. \tag{2.2}$$

### *THEOREM 3* [4]:

For 
$$p \ge 3$$
 and  $0 \le k \le p$ ,

$$\phi(Kc_p(k):\lambda) = \lambda^{k-1}(\lambda+1)^{p-k-1}[\lambda^2 - (p-k-1)\lambda - k(p-k)]. \tag{2.3}$$

### *THEOREM 4* [4]:

For  $p \ge 3$  and  $3 \le k \le p$ ,

$$\phi(Kd_p(k): \lambda) = (\lambda + 1)^{p-k-1} [\lambda^2 - (p-4)\lambda - (3p-2k-3)] \Pi(\lambda + 2\cos(2\pi i/k) + 1). \quad (2.4)$$

We introduce here another class of graph obtained from  $K_p$  and denote it by  $Ka_p(m,k)$ . Two subgraphs  $G_1$  and  $G_2$  of G are independent subgraphs if  $V(G_1) \cap V(G_2)$  is an empty set.

<u>DEFINITION 5</u>: Let  $(K_m)_i$ ,  $i=1,2,\ldots,k$ ,  $1 \le k \le \lfloor p/m \rfloor$ ,  $1 \le m \le p$ , be independent complete subgraphs with m vertices of the complete graph  $K_p$ ,  $p \ge 3$ . The graph  $Ka_p(m,k)$  is obtained from  $K_p$ , by deleting all edges of  $(K_m)_i$ ,  $i=1,2,\ldots,k$ . In addition  $Ka_p(m,0) \cong Ka_p(0,k) \cong Ka_p(0,0) \cong K_p$ .

Note that the graphs  $Kb_p(k)$  and  $Kc_p(k)$  are the special cases of the graph  $Ka_p(m,k)$ .

## THEOREM 5:

$$\begin{split} & \text{For } p \geq 3, \ 0 \leq k \leq \bigsqcup p/m \ \rfloor \ \text{and} \quad 1 \leq m \leq p, \\ & \varphi(Ka_p(m,k):\lambda) = \lambda^{mk-k} (\lambda + 1)^{p-mk-1} (\lambda + m)^{k-1} [\lambda^2 - (p-m-1)\lambda - m(p+k-mk-1)]. \ (2.5) \end{split}$$

PROOF: Without loss of generality we assume that the vertices of  $(K_m)_i$  are  $v_{m(i-1)+1}, v_{m(i-1)+2}, \ldots, v_{m(i-1)+m}, i=1,2,\ldots,k$ . Then the characteristic polynomial of  $Ka_p(m,k)$  is equal to the determinant (2.6).

$\mathbf{v}_1  \mathbf{v}_2 \qquad  \mathbf{v}_m  \mathbf{v}_{m+1}$	$v_{m+2}$ $v_{2m}$ $v_{m(k-1)}$	$v_{m(k-1)+m}$	$\mathbf{v}_{\mathrm{mk+1}}$ $\mathbf{v}_{\mathrm{p}}$	
λ 0 0 0 -1	-1 -111	-1 -11	-11	
$0 \lambda 0 \dots 0 -1$	-1 -111	-1 -11	-11	
$\begin{bmatrix} 0 & 0 & \lambda \dots 0 & -1 \end{bmatrix}$	-1 -111	<b>−1 −1 −1</b>	-11	
		•		
	-1 $-1$ $-1$ $-1$ 0 0 0 $-1$	-1 -11 -1 -11	-ll -ll	
	λ 0 01	-1 -11 -1 -11	-ll -ll	
-1 -1 -11 0 -1 -1 -11 0		-1 -11 -1 -11	-11 -11	
-1 -1 -11 0	υ	-1 -11	-11	
		•		
-1 -1 -11 0	0 0 λ1	-1 -11	-11 (i	2.6)
			•	
-1 -1 -11 -1		0 0 0	-11	
-1 -1 -11 -1		λ 0 0	-11	
-1 -1 -11 -1	-1 -11 0	$0  \lambda \dots  0$	-11	
		•		
		•	•	
-1 -1 -1 -1 -1	-1 -11 0	0 0 λ	-11	
	-1 -111		λ1	
		•		
-1 -1 -11 -1	-1 -111	-1 -11	$-1 \ldots \lambda$ .	

The last zeros are in the (mk)<sup>th</sup> row and (mk)<sup>th</sup> column of the determinant (2.6). Now we perform elementary transformations on the determinant (2.6) to prove the result (2.5).

Subtract the first column of (2.6) from all its other columns, to obtain (2.7) and let  $X = \lambda + 1$ .

					-XX				
0	λ	00	-1	-1	-11	-1	<b>−1 -1</b>	<b>−1 −1</b>	
0	0	$\lambda$ 0	-1	-1	-11	-1	-11	<b>−1 −1</b>	
		•							
.		•						•	
-		•					•		
- 1	0				-11				
-1		00			1 1 0		0 0		
-1	0				1 1 0		0 0		
-1	0	00	1	1	X 1 0	0	0 0	0 0	
-		•					•		
•		•					•	•	
	^		1			0			(2.7)
		0 0	1	1	1 X 0	0	0 0	0 0	(2.7)
•		•			•		•	•	
•		•					•	•	
.	Λ		Λ	Λ	v	1	1 1		
I .	0				0 0 X			0 0	
-1  -1		0 0 0 0		0	0 0 1		1 1 <b>v</b> 1	0 0	
	0	0 0	0	0	0 0 1	1	Λ 1	0 0	
•		•					•	•	
.		•					•	•	
-1	0	0 0	0	0	0 0 1	1	1 <b>Y</b>	0 0	
	0	0 0			000				
	U	0 0	U	U	0 0 0	U	0 0	Λ 0	
		•					•	•	
•		•					•	•	
-1	0	0 0	0	0	0 0 0	0	0 0	0 X	

Multiply the rows  $2, 3, \ldots, m$  of (2.7) by X to obtain (2.8).

	0 λ	X	00	–X -	-X	-XXX -XXX -XXX	-X	-X <b>-</b> X	-X <b>-</b> X	
	•									
	0 (	0	0 λΥ	_Y _	_ <b>Y</b>	 -XXX	$_{\mathbf{Y}}$	_Y _Y .	_Y _Y	
	-1	-						$0 \dots 0$		
	-1		00					0 0		
	-1	0	0 0	1	1	X 1 0	0	0 0	0 0	
	•							•		
1-m		_					•			(2.0)
$X^{1-m}$	-1	U	00	1	I	1 X 0	0	0 0	0 0	(2.8)
		Λ	0 0	0	Λ		1			
			0 0	0		0 0 X 0 0 1		1 1		
			0 0			0 0 1				
	٠									
	•		•							
			00			0 0 1				
	-1	0	0 0	0	0	0 0 0	0	0 0	X 0	
		_		_	_					
	-1	0	0 0	0	0	0 0 0	0	0 0	0 X	

Add the rows mk + 1, mk + 2, ..., p of (2.8) to the rows 1, 2, ..., m to obtain (2.9).

	λ+mk-	p -λ	-λλ	-X	-X	-X <b>-</b>	XX	-X	–X… <b>-</b> X	00	
	mk-p	λΧ	00	-X	-X	-X	·XX	-X	–XX	00	
	mk-p	0	λΧ0	-X	-X	-X	-XX	_X	−X… <b>-</b> Σ	00	
	٠		٠			•	•		•	•	
						•					
	mk-p	0	$0\lambda X$	X –X	-X	X –X	·XX	-X	–X… <b>-</b> X	00	
	-1	0	00	X	1	1	1 0	0	$0 \dots 0$	00	
	-1		00			1			00		
	-1	0	0 0	1	1	X	1 0	0	00	00	
			•						•		
	•		•			•	•		•	•	
$X^{1-m}$	-1	0	00	1	1	1 X	· 0	0	0 0	00	(2.9)
1		Ü		•	•			Ü			(2.)
	-1	0	00	0	0	0 0	) X	1	11	00	
	-1				0	0 (			11		
	-1	0	00	0	0	0 (	) 1	1	X1	00	
	•		٠			•	•		•	•	
	•		٠			•	•		•	•	
	-1	0	00	0	0	0 (		1	1X	0 0	
	-1	0		0		0 (			00		
							·				
	-						•		•		
	-1	0	0 0	0	0	0 0	· ) 0	0	00	0 X	

Evidently, expression (2.9) is equal to (2.10) in which the determinant is of order mk.

	mk-p	λΣ	X 00	-X	-X	-XX -XX -XX	-X	–X… <b>-</b> X	
	-1	0	0 0 0 0	X 1	1 X	-XXX 110 110 X10	0	$0 \dots 0 \\ 0 \dots 0$	
$X^{p-mk-m+1}$	-1	0	0 0	1	1		0	· · 0 0	(2.10)
	.1							1 1	
	-1 -1 ·	0	0 0 0 0	0	0	0 0 1 0 0 1			
	-1	0	0 0	0	0	0 0 1	1	1 X	

Extract  $\lambda$  from the columns 2, 3, ..., m of (2.10) to obtain (2.11).

Add columns 2, 3, . . . , m of (2.11) to the columns m+1, m+2, . . . , mk of (2.11) to obtain (2.12) and let Z=1-m-X.

	λ+mk-p	-1 -11 Z Z Z Z Z Z Z Z	
		$egin{array}{cccccccccccccccccccccccccccccccccccc$	
	ink p		
	mk-p	0 0 X 0 0 0 0 0 0 0 0	
	-1	0 00 X 1 110 0 00	
	-1	0 00 1 X 110 0 00	
	-1	0 0 0 1 1 X 1 0 0 0 0	
$\lambda^{m\text{-}1}X^{p\text{-}mk\text{-}m+1}$	-1	0 0 0 1 1 1 X 0 0 0 0	(2.12)
	-1	0 00 0 0 0 0 X 1 1 1	
	-1	0 00 0 0 0 0 1 X 1 1	
	-1	0 00 0 0 0 01 1 X1	
	-1	0 0 0 0 0 0 0 1 1 1 X	

Add the rows  $m+1,\ m+2,\ \ldots$ , mk of (2.12) to its first row to obtain (2.13).

The determinant (2.13) is in block – lower triangular form and it reduces to (2.14), in which each determinant is of order m.

Subtract second row from the rows 3, 4,  $\dots$ , m in both determinants of (2.14) to obtain (2.15).

Add the columns  $3, 4, \ldots, m$  to the second column in both determinants of (2.15) to obtain (2.16).

Expression (2.16) is same as

$$\begin{split} \lambda^{m-1} X^{p-mk-m+1} X^{m-2} & \left| \begin{array}{c} \lambda + m - p & 1 - m \\ mk - p & X \end{array} \right| (X-1)^{(m-2)(k-1)} \left| \begin{array}{c} X & m-1 \\ 1 & X + m-2 \end{array} \right|^{k-1} \\ &= \lambda^{m-1} X^{p-mk-1} (X-1)^{(m-2)(k-1)} \left| \begin{array}{c} \lambda + m - p & 1 - m \\ mk - p & X \end{array} \right| \left| \begin{array}{c} X & m-1 \\ 1 & X + m-2 \end{array} \right|^{k-1} \\ &= \lambda^{m-1} (\lambda+1)^{p-mk-1} \lambda^{(m-2)(k-1)} \left| \begin{array}{c} \lambda + m - p & 1 - m \\ mk - p & X \end{array} \right| \left| \begin{array}{c} \lambda + 1 & m-1 \\ 1 & \lambda + m-1 \end{array} \right|^{k-1} \\ &= \lambda^{mk-2k+1} (\lambda+1)^{p-mk-1} \lambda^{(m-2)(k-1)} \left| \begin{array}{c} \lambda + m - p & 1 - m \\ mk - p & \lambda + 1 \end{array} \right| \left| \begin{array}{c} \lambda + 1 & m-1 \\ 1 & \lambda + m-1 \end{array} \right|^{k-1} \\ &= \lambda^{mk-2k+1} (\lambda+1)^{p-mk-1} [(\lambda-p+m)(\lambda+1) - (1-m)(mk-p)] [(\lambda+1)(\lambda+m-1) - (m-1)]^{k-1} \end{split}$$

Simplification of this leads to the expression (2.5).

That expression (2.5) holds also for k = 0 is verified by direct calculation.

This completes the proof.

# SPECTRA AND ENERGY OF Kap(m,k)

From Theorem 5, it is elementary to obtain the spectra and energy of Ka<sub>p</sub>(m,k).

### **COROLLARY 6:**

For  $0 \le k \le \lfloor p/m \rfloor$  and  $1 \le m \le p$ , the spectrum of  $Ka_p(m,k)$  consists of 0 (mk – k times), -1(p-mk-1 times), -m (k – 1 times) and

$$\frac{p-m-1+\sqrt{(p-m-1)^2+4m(p+k-mk-1)}}{2}.$$

### **COROLLARY 7:**

For  $0 \le k \le \lfloor p/m \rfloor$  and  $1 \le m \le p$ ,

$$E(Ka_p(m,k)) = p - m - 1 + \sqrt{(p+m-1)^2 - 4mk(m-1)}$$
.

The energy of Ka<sub>p</sub>(m,k) is monotonically decreasing function of k. Hence we have following.

### **COROLLARY 8:**

For any integers m and p,  $1 \le m \le p$ ,

$$E(K_p) = E(Ka_p(m,0)) > E(Ka_p(m,1)) > E(Ka_p(m,2)) > \dots > E(Ka_p(m, \lfloor p/m \rfloor)).$$

From Corollary 8 it follows that the graph  $Ka_p(m,k)$  is not hyperenergetic.

### **REMARKS**

- 1. If k = 0, then the equation (2.5) reduces to  $(\lambda p + 1)(\lambda + 1)^{p-1}$ , the characteristic polynomial of the complete graph  $K_p$  [1, p.72].
- 2. If m = 1, then the equation (2.5) reduces to the characteristic polynomial of the complete graph  $K_p$ .
- 3. If m = p and k = 1, then the equation (2.5) reduces to the characteristic polynomial of  $\overline{K}_p$ , the complement of  $K_p$  [1, p.72].
- 4. If m=2 and k=p/2, then the equation (2.5) reduces to  $\lambda^{p/2}$  ( $\lambda+2$ )<sup>(p/2) 1</sup>( $\lambda-p+2$ ) which is the characteristic polynomial of the cocktail party graph [1, p.73].
- 5. If p = mk, then the equation (2.5) reduces to  $\lambda^{p-k}$  ( $\lambda + (p/k) p$ )( $\lambda + (p/k)$ )<sup>k-1</sup>, a characteristic polynomial of complete multipartite graph  $Kn_1, n_2, \ldots, n_k$  where,  $n_1 = n_2 = \ldots = n_k = (p/k)$  (see [1, p.73]).
- 6. If m = 2 and k = 1, then the equation (2.5) reduces to the characteristic polynomial of  $Ka_p(1)$ .
- 7. If m = 2, then the equation (2.5) reduces to the equation (2.2), the characteristic polynomial of  $Kb_p(k)$ .
- 8. If k = 1, then the equation (2.5) reduces to the characteristic polynomial of  $Kc_p(m)$ .
- 9. If k = 1 and m = 3, then the equation (2.5) reduces to the characteristic polynomial of  $Kd_p(3)$ .

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