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On the Energy of Some Graphs

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Abstract. Energy of a graph is an interesting parameter related to total π electron energy of the corresponding molecule. Recently Vaidya and Popat defined a pair of new graphs and obtained their energy in terms of the energy of original graph. In this paper we generalize the construction and obtain their energy. Also we discuss the spectrum of the first level thorn graph of a graph.

Keywords: Splitting graph, Shadow graph, Thorn graph, Energy of a graph

AMS Mathematics Subject Classification (2010): 05C50

1. Introduction

In quantum chemistry, the skeletons of certain non-saturated hydrocarbons are represented by graphs [1, 3]. Energy levels of electrons in such a molecule are, in fact, the eigenvalues of the corresponding graph. All the graphs considered here are finite, simple and undirected. The adjacency matrix $A(G)$ of a graph of order n with vertex set $\{v_1, v_2, \ldots\ldots v_n\}$ is an n x n matrix $[a_{ij}]$ with $a_{ij}=1$ if v_i is adjacent to v_j and 0 otherwise.

The eigenvalues of $A(G)$ are called eigenvalues of G. Eigenvalues along with their multiplicities form the spectrum of G. We denote spectrum of graph G by spec (G).The addition of absolute eigenvalues of G is defined as energy of G denoted by $E(G)$ [5]. It is a generalization of a formula valid for the total π-electron energy of a conjugated hydrocarbon as calculated with the Huckel molecular orbital (HMO) method [1-4]. For some bounds on the energy of a graph; one can refer [6-8].Two non isomorphic graphs on same number of vertices are said to be cospectral if they have the same spectrum. Two non isomorphic graphs are called equienergetic if they have same energy. Obviously cospectral graphs are equienergetic, so we look for non isomorphic non cospectral connected graphs which are equienergetic. For work on equienergetic graphs; one can refer [9-12].

For some work on energy of singular graphs, eccentric energy and degree sum energy; one can refer [13-15].

Let $A \in R^{m\,x\,n}$ and $B \in R^{n\,x\,p}$ then, the Kronecker product (tensor product) of A and B is defined as the matrix $A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix}$

Proposition 1.1[16]: Let $A \in M^{m}$ and $B \in M^{n}$.Furthermore; if λ is an eigenvalue of A with eigenvector x and μ is an eigenvalue of B with eigenvector y then $\lambda\mu$ is an eigenvalue of $A \otimes B$ with eigenvector $x \otimes y$.

The present work generalizes the two graphs defined by Vaidya, Popat [17], so that their results become particular cases.

2. Energy of *k* splitting graph

The splitting graph of a graph was defined in 1980 by Sampathkumar and Walikar [18]. Here we define the generalized version of the same.

Definition 2.1. The k splitting graph $S^k(G)$ $(k \geq 1)$ of a graph G of order n, is obtained from k copies of G by adding one set of n new vertices corresponding each vertex of G say $\{u_1, u_2, \ldots u_n\}$ and joining each u_i to neighbor of v_i^j for j=1,2,3,…, k. Here we assume that v_i^j denotes the i^{th} vertex in j^{th} copy of G. Also we join every v_i^j to neighbors of v_i^l $(j \neq l)$ for all $j = 1,2,\ldots,k$.

We prove the following.

Theorem 2.2. $E\left(S^k(G)\right) = \left(\sqrt{k^2+4k}\right)E(G)$.

Proof: With pertinent labeling of vertices the adjacency matrix of $S^k(G)$ takes the form

$$A(\mathrm{S}^{\mathrm{k}}(G)) = \begin{bmatrix} A(G) & A(G) & \cdots & \cdots & A(G) \\ A(G) & A(G) & \cdots & \cdots & A(G) \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A(G) & A(G) & \cdots & \cdots & O \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & \cdots & 1 \\ 1 & 1 & \cdots & \cdots & 1 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & \cdots & 0 \end{bmatrix} \otimes A(G)$$

where $A(G)$ is adjacency matrix of G and O is a zero matrix of order n.

the matrix $\begin{bmatrix} 1 & 1 & \cdots & \cdots & 1 \\ 1 & 1 & \cdots & \cdots & 1 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & \cdots & 0 \end{bmatrix}$ of order k+1 by k+1 coincides with minimum covering matrix of K_{k+1} (complete graph of order k +1) with characteristic polynomial $\lambda^{k-1}[\lambda^2 - k\lambda - k]$ and eigenvalues 0 k-1 times and $(k \pm \sqrt{k^2+4k})/2$ once (see [19]). Using proposition 1.1,we have the spectrum of $S^k(G)$

$$=\begin{pmatrix} \left(\frac{k+\sqrt{k^2+4k}}{2}\right)\lambda_i & (\frac{k-\sqrt{k^2+4k}}{2})\lambda_i \\ n & n \end{pmatrix}$$ where λ_i $i=1,2,\ldots n$ are the eigenvalues of G.

So that

$$E(S^k(G))\sum_{i=1}^{n}|\lambda_i|\,(\frac{k\pm\sqrt{k^2+4k}}{2})=\sqrt{k^2+4k}\times\sum_{i=1}^{n}|\lambda_i|=\sqrt{k^2+4k}\ E(G). \qquad (1)$$

Corollary 2.3. From equation (1) it's easy to see that if G_1 and G_2 are two equienergetic graphs, then $S^k(G_1)$ and $S^k(G_2)$ are equienergetic for all k.

Corollary 2.4. If $k=1$ in equation (1) we get the splitting graph of G and the corresponding result for energy as in [17] .
Illustration: If G is K_2 and $k=2$ the graph $S^2(K_2)$ is as shown below

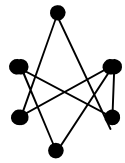


Figure 1:

The spectrum of $K_2=\begin{pmatrix}1 & -1\\ 1 & -1\end{pmatrix}$ so that spectrum of $S^2(K_2)$ is $\begin{pmatrix}1\pm\sqrt{3} & -(1\pm\sqrt{3}\\ 1 & -1\end{pmatrix}$
$E(S^2(K_2)) = \sqrt{2^2+8}\ E(K_2)=4\sqrt{3}.$

3. Energy of a *k* shadow graph

We now define the k shadow graph of a graph as follows.

Definition 3.1. The k shadow graph $D_k(G)$ of a connected graph G is constructed by taking k (≥ 2) copies of G. Join each vertex of every copy with the neighbors of corresponding vertex in all remaining k-1 copies.

Theorem 3.1. $E(D_k(G)) = kE(G)$.
Proof: With pertinent labeling the adjacency matrix of $D_k(G)$ takes the form

$$A(D_k(G))=\begin{bmatrix} A(G) & A(G) & \cdots & \cdots & A(G)\\ A(G) & A(G) & \cdots & \cdots & A(G)\\ \vdots & \vdots & \ddots & \cdots & \vdots\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ A(G) & A(G) & \cdots & \cdots & A(G)\end{bmatrix}=\begin{bmatrix} 1 & 1 & \cdots & \cdots & 1\\ 1 & 1 & \cdots & \cdots & 1\\ \vdots & \vdots & \ddots & \cdots & \vdots\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ 1 & 1 & \cdots & \cdots & 1\end{bmatrix}\otimes A(G)$$

where $A(G)$ is the adjacency matrix of G .

The matrix $\begin{bmatrix} 1 & 1 & \cdots & \cdots & 1 \\ 1 & 1 & \cdots & \cdots & 1 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & \cdots & 1 \end{bmatrix}$ of order k by k, having the characteristic polynomial $\lambda^{k-1}(\lambda - k)$ and hence has eigenvalues 0 k-1 times and k once.

Using proposition 1.1 we have the spectrum of $D_k(G) = \begin{pmatrix} k\lambda_i & 0 \\ n & n \end{pmatrix}$ where λ_i i =1,2,…n are the eigenvalues of G. Hence, $E\,[D_k(G)] = \sum_{i=1}^{n} k|\lambda_i| = k\,E(G)$. (2)

Corollary 3.2. From equation (2) it's easy to see that if G_1 and G_2 are two equienergetic graphs, then $D_k(G_1)$ and $D_k(G_2)$ are equienegetic for all k.

Corollary 3.3. If k = 2 in equation (2) we get the shadow graph of G as defined in [17] and the corresponding result for energy.

Illustration: If G is K_2 and k = 3 then $D_3(K_2)$ is as shown below

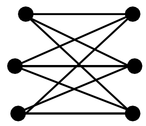


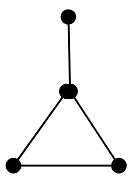
Figure 2:

The spectrum of $K_2 = \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}$ so that spectrum of $D_3(K_2)$ is $\begin{pmatrix} 3 & -3 \\ 1 & -1 \end{pmatrix}$. Also $E(D_3(K_2)) = 3E(K_2) = 6$.

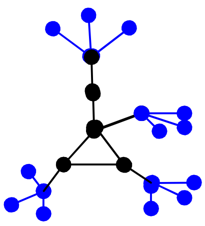
4. First level thorn graphs

We consider some class of graphs which are constructed by joining an edge to every vertex and then joining k pendent vertices to the end vertices of the edge joined. The graph obtained by this procedure from G we call, first level thorn graph denoted by $G^{1(+k)}$.

A graph G and first level thorn graph $G^{1(+3)}$ are shown below.



(a)



(b)

Figure 3:

The spectrum of 0 level thorn graphs is discussed in [20]. In this chapter we compute characteristic polynomial of first level thorn graphs.

Lemma 4.1. [21] If M is any nonsingular matrix then

$$\begin{vmatrix} M & N \\ P & Q \end{vmatrix} = |M|\,|Q - PM^{-1}N|$$

Theorem 4.2. The adjacency polynomial of a first level thorn graph of a graph G is related with adjacency polynomial of G by $P(G^{1(+k)},\lambda) = \lambda^{nk-n}(\lambda^2 - k)^n P(G, \frac{\lambda(\lambda^2-k-1)}{\lambda^2-k})$.

Proof: Let $G^{1(+k)}$ denote the graph obtained from G by attaching an edge to each vertex of G and then attaching k pendent vertices to ends of edges joined. With pertinent labeling the adjacency matrix of $G^{1(+k)}$ has the form,

$$G^{1(+k)}) = \begin{bmatrix} O_{nk} & P & O_{nk\times n} \\ P^T & O_n & I_n \\ O_{n\times nk} & I_n & A(G) \end{bmatrix}$$

where P is a matrix of order nk by n with i^{th} column having1's in $(i-1)k^{th}$ row to ik^{th} row for $i = 1,2,3\ldots\ldots.n$, O_n denotes a zero matrix and I_n denotes the identity matrix of order n.

The characteristic equation of $G^{1(+k)}$ is then

$$|\lambda I - A(G^{1(+k)})| = \begin{vmatrix} \lambda I_{nk} & -P & -O_{nk\times n} \\ -P^T & \lambda I_n & -I_n \\ -O_{n\times nk} & -I_n & \lambda I - A(G) \end{vmatrix}.$$

From Lemma 4.1 we have

$$|\lambda I - A(G^{1(+k)})| = |\lambda I_{nk}| \begin{vmatrix} \lambda I_n & -I_n - \frac{\begin{vmatrix} kI_n & O_n \\ O_n & O_n \end{vmatrix}}{\lambda} \\ -I_n & \lambda I - A(G) \end{vmatrix}$$

$$= \lambda^{nk-n} \begin{vmatrix} (\lambda^2 - k)I_n & -\lambda I_n \\ -\lambda I_n & \lambda^2 I - \lambda A(G) \end{vmatrix}.$$

Again from Lemma 4.1 we have

$$|\lambda I - A(G^{1(+k)})| = \lambda^{nk-n}(\lambda^2 - k)^n \left| \frac{\lambda(\lambda^2-k-1)}{\lambda^2-k} - A(G) \right| \tag{3}$$

Hence the theorem.

Corollary 4.3. From equation (3) the spectrum of $G^{1(+k)}$ is given by

$$spec(G^{1(+k)} = \begin{pmatrix} 0 & roots\ of\ \ cubic\ equation\ \lambda^3 - \lambda_i\lambda^2 - (k+1)\lambda + k\lambda_i = 0 \\ nk-n & 1 \end{pmatrix}$$

for each eigenvalue of G , $\lambda_i \;\; i = 1,2,..n$.

So that the energy of $G^{1(+k)}$, $E(G^{1(+k)}) = \sum_{j=1}^{3} |\alpha_{ij}|$ where α_{ij} denotes root of the cubic equation $\lambda^3 - \lambda_i\lambda^2 - (k+1)\lambda + k\lambda_i = 0$ for each eigenvalue $\lambda_i \;\; i = 1,2,..n$ of G.

Also from the cubic equation, it can be observed that if nullity of G (number of zero eigenvalues) is p then $G^{1(+k)}$ has nullity $nk - n + 2p$ and contains $'k+1'$ p times in its spectrum.

Corollary 4.4. If $k = 1$ from equation (3) we get $G^{1(+1)}$ which is same as the graph G with path of length 2 attached to each vertex, having the polynomial

$P(G^{1(+1)}, \lambda) = (\lambda^2 - 1)^n P(G, \frac{\lambda(\lambda^2-2)}{\lambda^2-1})$.

Note: from the relations above its clear that, if G has singularity 'p' then $G^{1(+1)}$ will have singularity '$2p$' and $\pm\sqrt{2}$ 'p' times in it's specctrum .

Further if $G \cong C_n$ then, $G^{1(+1)}$ is a unicyclic graph of diameter $\left\lfloor \frac{n}{2} \right\rfloor + 4$ having adjacency polynomial $P_G(C_n^{(+1)}, \lambda) = (\lambda^2 - 1)^n P(C_n, \frac{\lambda(\lambda^2-2)}{\lambda^2-1}) = (\lambda^2-1)^n \prod_{i=0}^{n-1}[\frac{\lambda(\lambda^2-2)}{\lambda^2-1} - 2\cos(\frac{2\pi i}{n})]$.

Corollary 4.5. When $k = 0$ from equation (3) we have, $P(G^{1(+0)}, \lambda) = \lambda^n P(G, \lambda - \frac{1}{\lambda})$ coincides with the characteristic polynomial of G^{+1} in [19] as required.

5. Conclusion

The paper deals with general version of splitting graph and shadow graph of a graph; consequently we have graphs, whose energy is positive integral multiple of energy of any given graph *G*. Also we obtained infinite family of equienergetic graphs starting with a pair of equienergetic graphs. Also we give a relation between the characteristic polynomial of first level thorn graph of *G* with that of *G*.

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