International Journal of Innovation in Science and Mathematics
Volume 2, Issue 6, ISSN (Online): 2347–9051

Maxmimal and Minimal Energies of Noncaterpillar

Bing Zhang
Department of Computer Science
Guangdong Polytechnic Normal University, Guanzghou 510665, P.R.China

Abstract **– If G is a graph and $\lambda_1,\lambda_2,\ldots,\lambda_n$ are its eigenvalue, then the energy of G is defined as $E(G)=|\lambda_1|+|\lambda_2|+\ldots+|\lambda_n|$. Recall that a caterpillar is a tree in which removal of all pendant vertices gives a path. Let R_n be the set of all noncaterpillar trees with n vertices. In this paper, we determine the graphs in R_n with maximal and minimal energies.**

Keywords **– Energy, Eigenvalue, Noncarterpillar.**

I. Introduction

Let G be a simple graph with n vertices and $A(G)$ the adjacency matrix of G. The characteristic polynomial of G is $\phi(G,x)=\det(xT-A(G))$, where I stands for the unit matrix of order n .The roots $\lambda_1(\mathrm{G}),\lambda_2(\mathrm{G}),\ldots,\lambda_n(G)$ of the equation $\phi(G,x)=0$ are called the eigenvalues of the graph G .The energy of the graph G is then defined as

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

In chemistry the energy of a graph is extensively studied since it can be used to approximate the total π-electron energy of a molecule [1]. For a survey of the mathematical properties of
$E(G)$ see the review [2].

If G is a bipartite graph with n vertices, then

$$\phi(\mathrm{G},x)=\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k\,\mathrm{m}(\mathrm{G},k)x^{n-2k}, \quad (1)$$

and

$$E(G)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln\left(\sum_{k=0}^{\lfloor n/2\rfloor}\mathrm{m}(G,k)x^{2k}\right)dx \quad (2)$$

Let G and H be bipartite graphs with n vertices. If

$$\mathrm{m}(G,k)\le m(H,k),\ \text{for all } k=0,1,\ldots,\lfloor n/2\rfloor \quad (3)$$

then from (2) it follows that $E(G)\le E(H)$. Further if there is a k_0 such that $\mathrm{m}(G,k_0)<m(H,k_0)$, then (3) implies that E(G)<E(H). (See [1 , 3].)

Let G_1,G_2 be two bipartite graphs of order n ,whose characteristic polynomials are

$$\varphi(G_1)=\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k b(G_1,k)x^{n-2k},\varphi(G_2)=\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k b(G_2,k)x^{n-2k} \quad (4)$$

If $b(G_1,k)\ge b(G_2,k)$ holds for all $k\ge 0$, we call $G_1\ge G_2$ or $G_2\le G_1$. If $G_1\ge G_2$ and there is a k such that $b(G_1,k)>b(G_2,k)$, we call $G_1>G_2$. By the strict monotonicity of $E(G)$, if $G_1\ge G_2$, then $E(G_1)\ge E(G_2)$; if $G_1>G_2$, then $E(G_1)>E(G_2)$. In order to state our results, we introduce some notation and terminology. Other undefined notation may refer to [4].We denote by P_n and S_n the path and star on vertices, respectively. For $x\in v(T), d_T(x)$ (or $d(T)$) denote the degree of x. Let T_n denote the set of trees with n vertices. Recall that a caterpillar is a tree in which removal of all pendant vertices gives a path. Let R_n be the set of all noncaterpillar trees with n vertices and $R_{n,d}$ be the set of all graphs in R_n with diameter d.

II. Preliminaries

Lemma 2.1. [5,6] Let G be a forest and v be a vertex of G. Then the characteristic polynomial of G satisfies

$$\phi(G)=x\phi(G-v)-\sum_u\phi(G-u,v), \quad (5)$$

where the summation extends over all vertices adjacent to v

Lemma 2.2. [5,6] Let G be a forest and e=uv be an edge of G .The characteristic polynomial of G satisfies

$$\phi(G)=\phi(G-e)-\phi(G-u,v) \quad (6)$$

Lemma 2.3. [5] If $G_1,G_2,\ldots,G_t$ are the components of a forest G, we have

$$\phi(G)=\prod_{i=1}^{t}\phi(G_i) \quad (7)$$

Lemma 2.4 [8]. Let G and G' betwo forests of order n with characteristic polynomials ,

$$\phi(G)=\sum_{k=0}^{\lfloor n/2\rfloor}a_k x^{n-2k},\phi(G')=\sum_{k=0}^{\lfloor n/2\rfloor}a'_k x^{n-2k} \quad (8)$$

respectively, then $G\ge G'$ if and only if $a_0-a'_0=0$ and $(-1)^k(a_k-a'_k)\ge 0$ for $k=1,2,\ldots,\lfloor n/2\rfloor$; $G>G'$ if and only if $G\ge G'$ and there is a k $\left(1\le k\le\lfloor n/2\rfloor\right)$ such that $(-1)^k(a_k-a'_k)>0$.

Lemma 2.5. [7]. Let G be a forest of order $n(n>1)$ and G' be a spanning subgraph (respectively a proper spanning subgraph) of G .Then $G \geq G'(G > G')$.

Let G and H be two graphs whose vertex sets are disjoint. If v is a vertex of G and w a vertex of H, then $G(v,w)H$ is the graph obtained by identifying the vertices v and w. In particular, the graph $P_n(v_r,v)G$ is obtained by identifying the vertex v_r of P_n with the vertex v of G .

Lemma 2.6. [11] If v is an arbitrary vertex of the graph G, then for $n=4k+i, i\in\{-1,0,1,2\}$,

$$P_n(v_1,v)G > P_n(v_3,v)G > \cdots > P_n(v_{2k+1},v)G$$
$$> P_n(v_{2k},v)G > P_n(v_{2k-2},v)G > \cdots > P_n(v_2,v)G$$

We call the transformation from $G_1 = P_n(v_r,v)G$ to $P_n(v_1,v)G$, where $r\geq 2, n\geq 3$, the α_1-transformation of G_1. We call the transformation from $G_1 = P_n(v_r,v)G$ to $P_n(v_3,v)G$, where $r\neq 1,3$ and $n\geq 6$, the α_3-transformation of G_1. Two vertices u and v of the graph G are called equivalent if the subgraph $G-u$ and $G-v$ are isomorphic. We call the transformation from $G_1 = G(u,v)(a,b)$ to $G(u,v)(a-1,b+1)$ the β-transformation of G_1, and the transformation from $G_1 = G(u,v)(a,b)$ to $G(u,v)(0,a+b)$ the β'-transformation of G_1, where $1\leq a\leq b$, and u,v are equivalent in G.

Lemma 2.7. [9] .If G_0 can be obtained from G by one step of α_1-or α_3-transformation, then $G_0 > G$.

Lemma 2.8. [9]. If G_0 can be obtained from G by one step of β-or β'-transformation, then $G_0 < G$.

Let $T\in T_n$ and $n\geq 3$. Let $e=uv$ be a nonpendant edge of T, and let T_1 and T_2 be the two components of $T-e, u\in T_1, v\in T_2$. T_0 is the tree obtained from T in the following way.

(1)Contract the edge $e=uv$ (i.e. identify u of T_1 with v of T_2.

(2) Attach a pendent vertex to the vertex $u(=v)$.

The procedures (1) and (2) are called the edge-growing transformation of T (on edge $e=uv$), or e.g.t of T (on edge $e=uv$) for short.

Lemma 2.9. [9]. Let T be a tree in T_n with at least a nonpendant edge, and $n\geq 3$. If T_0 can be obtained from T by one step of e.g.t (on edge $e=uv$), then $T > T_0$ and $E(T) > E(T_0)$.

Suppose $v_0v_1 \ldots v_d$ is a path, let T^* be the graph obtained by attaching P_2 to v_2. Suppose $v_0v_1v_2v_3v_4$ is a path, let T_1^* be the graph obtained by attaching P_2 to v_2 and n-7 pendent edges to v_1.

III. Main Results

Let $V_1(T)=\{x\in v(T) \mid d(x)\geq 3\}$. There are $d(x)$ components in $T-x$,each containing a vertex that is adjacent to vertex x in T. These components are called the branch of T at x.

Theorem 3.1. If $T\in R_n$, then $T\leq T^*$ and $E(T)\leq E(T^*)$ with the equalities if and only if $T\cong T^*$

Proof. Let $T\in R_n$, v is the maximal degree vertex in $V(T)$, $d(v)=\Delta$. We suppose all the branches at v are $B_1, B_2, \ldots, B_\Delta$. Then T can be transformed into a tree $T_1\in R_n$, $B_1,B_2,\ldots,B_\Delta$. can be transformed into three paths attaching v by carrying out α_1 - transformation repeatly, $V_1(T)=\{v\}$. Thus $T<T_1$ by Lemma 2.7. Then T_1 can be transformed into T^* by carrying our α_3-transformation twice. Thus $T_1 < T^*$ by
Lemma 2.7.

If $T, T'\in R_n$, where A_1, A_2 are two subtrees of T, A_2, A_3 are two subtrees of T'. If T' is obtained from T and satisfy that $A_1\geq A_3, A_3-u\geq A_1-u$ We say that T' is obtained from T by $\gamma-$ transformation.

Lemma 3.2. If T' is obtained from T by $\gamma-$ transformation, then $E(T)<E(T')$

Proof. Suppose A_1 contains y_1 vertices, A_2 contains y_2 vertices.

$$\phi(T)-\phi(T') = \sum_{l=0}^{\lfloor n/2 \rfloor}(a_l - a'_l)x^{n-2k}$$
$$= \phi(T-uv)-\phi(t-\{u,v\})-\phi(T'-uv) + \phi(T'-\{u,v\})$$
$$= \phi(A_1)\phi(A_2)-\phi(A_1-u)\phi(A_2-v) - \phi(A_2)\phi(A_3)+\phi(A_2-v)\phi(A_3-u)$$
$$= \phi(A_2)\left(\phi(A_1)-\phi(A_3)\right)+\phi(A_2-v) \left(\phi(A_3-u)-\phi(A_1-u)\right)$$

Let

$$\phi(A_1)-\phi(A_3)=\sum_{k=0}^{\lfloor y_1/2\rfloor}\varphi_k x^{y_1-2k}$$

$$\phi(A_3-u)-\phi(A_1-u)=\sum_{k=0}^{\lfloor y_1-1/2\rfloor}\varphi'_k x^{y_1-1-2k}$$

$$\phi(A_2)=\sum_{k=0}^{\lfloor y_2/2\rfloor}\xi_i x^{y_2-2k},\phi(A_2-v)=\sum_{k=0}^{\lfloor y_2-1/2\rfloor}\xi_i' x^{y_2-1-2k}.$$

Since $A_1\ge A_3$, by Lemma2.4, $(-1)^k\varphi_k\ge 0$ for $0\le k\le\lfloor y_1/2\rfloor$ and $\varphi_0=0$; $A_3-u\ge A_1-u$, by Lemma 2.4, $(-1)^k\varphi'_k\ge 0$ for $0\le k\le\lfloor y_1-1/2\rfloor$ and $\varphi'_0=0$. Recall $\phi(A_2),\phi(A_2-v)$,we have $(-1)^k\xi_i\ge 0,(-1)^k\xi_i'\ge 0.$ Thus $a_0-a_0'=0$, $(-1)^l(a_l-a'_l)\ge 0$ for $1\le l\le\lfloor n/2\rfloor$ and there is a l $(1\le l\le\lfloor n/2\rfloor)$ such that $(-1)^l(a_l-a'_l)>0$. By Lemma 2.4, we have $T>T'$, and then $E(T)>E(T')$.

Theorem 3.3. If $T\in R_n$, , then $T\ge T_1^*$ and $E(T)\ge E(T_1^*)$ with the equalities if and only if $T\cong T_1^*$

Proof. Let $T\in R_n$, v is the maximal degree vertex in $v(T)$, $d(v)=\Delta$. We suppose all the branch at v are $B_1,B_2,...,B_\Delta$. Then T can be transformed into a tree $T_1\in R_n$, B_1,B_2,B_3 can be transformed into three stars attaching v, $B_4,B_5,...,B_\Delta$ can be transformed into some pendent vertices attaching v by carrying out e.g.t-transformation repeatly. Then $T>T_1$ by Lemma 2.9. And T_1 can be transformed into T_2 by carrying out $\beta'-$transformation repeatly. Thus $T_1>T_2$ by Lemma 2.8. T_2 is a tree, we suppose a diameter path $v_1v_2v_3v_4v_5,v_3$ attaching tree stars and some pendent. Then T_2 can be transformed into T_1^* by carrying out $\gamma-$transformation.

References

[1] I. Gutman , O. E. Polansky. Mathematical Concepts in Organic Chemistry [M].Springer-Verlag, Berlin, 1986.
[2] I. Gutman. Algebraic Combinatorics and Applications, Springer-Verlag [M]. Berlin, 2001, pp.196-211.
[3] I. Gutman. Acyclic systems with extremal Huckle π -electron energy [M]. Berlin, 1977, 79-87.
[4] J.A.Bondy, U.S.A. Murty. Graph Theory with Applications [M]. New York, 1976.
[5] D.Cvetkovic, M.Doob, H.Sachs. Spectra of Graphs-Theory and Applications [M]. New York, 1980.
[6] A.J.Schwenk. Computing the characteristic polynomial of a graph, Graph and Combinatorics, in: R.A. Bari, F.Harary (Eds),Lecture Notes in Mathematics [M]. New York, 1974, pp. 153--173.
[7] Yan W G, Ye L Z . On the maximal energy and the Hosoya index of a type of trees with many pendant vertices [J]. MATCH Commun. Math. Comput. Chem, 2005, 53: 449--459.
[8] Zhang F J, Li H E. On acyclic conjugated moleculeswith minimal energies [J]. Discr. appl. Math, 1999 , 92: 71-- 84.
[9] Lin W S, Guo X F, Li H H. On the Extremal energies of trees with a given maximum degree [J], J. Math.Chem., 2005, 54: 363-- 378.
[10] Yu A M , Lv X Z. Minimum Energy on trees with k pendent vertices [J]. Linear Algebra and its Application , 2006.
[11] I. Gutman, Zhang F J . On the ordering of graphs with respect to their matching numbers [J]. Discrete Appl. Math.,1986, 15: 25--33.
[12] Jianbin Zhang, Bo Zhou . On Minimal Energies of non-starlike trees with given number of pendent vertices[M]. Match Commun.Math. Comput., 2009,62:481-490.

Author's Profile

Zhang Bing
1982-6-25, Department of Computer Science Guangdong Polytechnic Normal University, Guanzghou 510665, P.R.China Master's Degree, Research Field: Combinatorial Mathematics