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On the Energy of Blossomed Stars

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Abstract

The energy of a graph is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix. Given p integers $n_1 \geq n_2 \geq \cdots \geq n_p \geq 0$, let $SC(n_1, n_2, \ldots, n_p)$ be a tree obtained from a star $K_{1,p}$ with p vertices $v_1, v_2, \ldots, v_p$ of degree one by attaching n_i pendent edges to vertex v_i for $1 \leq i \leq p$, which is called a blossomed star. Let $\mathcal{SC}(n; n_1, n_2, \ldots, n_p) = \{SC(n_1, n_2, \ldots, n_p) | \sum_{i=1}^{p} n_i = n-p-1\}$. In this paper, we show that, among all blossomed stars in $\mathcal{SC}(n; n_1, n_2, \ldots, n_p)$, $SC(n-p-1, 0, \ldots, 0)$ has minimal energy and $SC(\underbrace{r+1, \ldots, r+1}_{t}, \underbrace{r, \ldots, r}_{p-t})$ has maximal energy, where $n-p-1 = pr+t$, $0 \leq t \leq r-1$.

1 Introduction

Let G be a simple graph of order n and $A(G)$ the adjacency matrix of G. Denote the characteristic polynomial of $A(G)$ by $\phi(G; x) = det(xI - A(G))$. Assume that $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G, i.e. the zeros of $\phi(G; x)$.

In chemistry, the total energy of HMO π-electron plays an important role as a parameter of conjugated molecule, which is related to the thermodynamic stability of conjugated structures. And the total energy of HMO π-electron in conjugated hydrocarbons can be reduced to the sum of absolute values of all eigenvalues of the constructed molecular graph. In 1977, Gutman [8] first defined the energy of a graph G as

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

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Since then, the graph energy has been widely studied because it can be used to approximate the total π-electron energy of molecules [8, 9, 18]. One of the vital problems of the graph energy is the ordering of graphs with respect to their energies. Until now, numerous results relevant to the maximal or minimal energies of graphs have been obtained, see for example [1–3, 5, 6, 10, 11, 13–16, 19–21, 23–25].

It is well known that for an acyclic graph T of order n, the matching polynomial and the characteristic polynomial are the same. Hence

$$\phi(T;x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i m(T,i) x^{n-2i}, \tag{2}$$

where $m(T,i)$ is the number of matchings of size i in T.

The energy of a tree T with n vertices can be expressed as the Coulson integral formula [12] as follow:

$$E(T) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} m(T,i) x^{2i} \right] dx. \tag{3}$$

In fact, we can see that $E(T)$ is a strictly monotonically function in terms of $m(T,i)$. Gutman [7] also introduced a quasi-ordering relation which makes great effects on comparing the energy of acyclic graphs as follows:

If T_1 and T_2 are both acyclic graphs, then $T_1 \succeq T_2$ if and only if for any $i \geq 0$, $m(T_1,i) \geq m(T_2,i)$.

If $T_1 \succeq T_2$ and for some $j \geq 0$ such that $m(T_1,j) > m(T_2,j)$, then we say $T_1 \succ T_2$.

We thus have

$$T_1 \succeq T_2 \Rightarrow E(T_1) \geq E(T_2);$$

$$T_1 \succ T_2 \Rightarrow E(T_1) > E(T_2).$$

Let $T_n^d(n_1, n_2, \ldots, n_{d-1})$ $(n_i \geq 0)$ denote a caterpillar of order n and diameter d, which is obtained from a path P_{d+1} whose vertices ordered from 0 to d by attaching n_i pendent edges to i-th vertex for $i = 1, 2, \ldots, d-1$. By the quasi-ordering relation above, Zhang and Guo [22] proved that among all caterpillars of order n and diameter d, $T_n^d(n_1, n_2, \ldots, n_{d-1})$ satisfying $n_1 \geq n_{d-1} \geq n_2 \geq n_{d-2} \geq \cdots \geq n_{[\frac{d}{2}]}$ and $n_1 - n_{[\frac{d}{2}]} \leq 1$ has the maximum energy for $d \leq 5$. Recently, Che [4] extended this result to caterpillars of diameter 6.

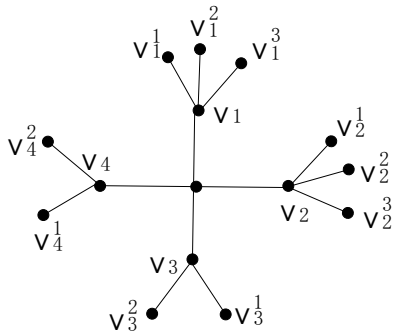

Figure 1. (a) A blossomed star $SC(3,3,2,2)$.

Given p integers $n_1 \geq n_2 \geq \cdots \geq n_p \geq 0$, let $SC(n_1, n_2, \ldots, n_p)$ be a blossomed star of order n, which is obtained from a star $K_{1,p}$ $(p > 1)$ with vertices $v_1, \ldots, v_p$ of degree one by attaching n_i pendent edges to vertex v_i for $i = 1, 2, \ldots, p$. Figure 1 illustrates $SC(3,3,2,2)$. Let $\mathcal{SC}(n; n_1, n_2, \ldots, n_p) = \{SC(n_1, n_2, \ldots, n_p) | \sum_{i=1}^{p} n_i = n - p - 1\}$.

In this paper, we mainly prove the following results.

Theorem 1.1. Among $\mathcal{SC}(n; n_1, n_2, \ldots, n_p)$, the energy of $SC(n-p-1, 0, \ldots, 0)$ is minimal.

Theorem 1.2. Among $\mathcal{SC}(n; n_1, n_2, \ldots, n_p)$, the energy of $SC(\underbrace{r+1, \ldots, r+1}_{t}, \underbrace{r, \ldots, r}_{p-t})$ is maximal, where $n - p - 1 = pr + t$, $0 \leq t \leq r - 1$.

2 Proofs of main results

We first need to introduce some lemmas.

Lemma 2.1. [17] Let T be a tree and u a vertex of T. Then

$$\phi(T; x) = x\phi(T - u; x) - \sum_{v \in N_T(u)} \phi(T - u - v; x),$$

where $T - u$ is the subgraph of T by deleting vertex u and $N_T(u) = \{v | (u, v) \in E(T)\}$, $E(T)$ is the edge set of T.

Lemma 2.2. Given p integers $n_1 \geq n_2 \geq \cdots \geq n_p \geq 0$, let $f(x) = \prod_{i=1}^{p}(x^2 - n_i)$ and $g(x) = \sum_{i=1}^{p} f(x)/(x^2 - n_i)$. Then

$$f(x) - g(x) = x^{2p} + \sum_{i=1}^{p}(-1)^i[a_i + (p-i+1)a_{i-1}]x^{2(p-i)},$$

where $a_0 = 1$, $a_i = \sum_{1 \leq s_1 < \cdots < s_i \leq p} n_{s_1} n_{s_2} \cdots n_{s_i}$, $i = 1, 2, \ldots, p$.

Proof. Note that

$$\begin{aligned} f(x) &= (x^2 - n_1)(x^2 - n_2)\cdots(x^2 - n_p) \\ &= x^{2p} - \left(\sum_{i=1}^{p} n_i\right) x^{2(p-1)} + \left(\sum_{1 \leq i < j \leq p} n_i n_j\right) x^{2(p-2)} + \cdots + (-1)^p \prod_{i=1}^{p} n_i \\ &= \sum_{i=0}^{p}(-1)^i a_i x^{2(p-i)}. \end{aligned}$$

Let $f_k(x) = f(x)/(x^2 - n_k) = \prod_{\substack{i=1 \\ i \neq k}}^{p}(x^2 - n_i) = \sum_{i=0}^{p-1}(-1)^i b_{ki} x^{2(p-1-i)}$, where $b_{k0} = 1$ and for $1 \leq i \leq p-1$,

$$b_{ki} = \sum_{\substack{1 \leq s_1 < \cdots < s_i \leq p \\ s_j \neq k, j=1,2,\ldots,i}} n_{s_1} n_{s_2} \cdots n_{s_i}.$$

Note that

$$\begin{aligned} \sum_{k=1}^{p} b_{ki} &= b_{1i} + b_{2i} + \cdots + b_{pi} \\ &= (p-i) \sum_{1 \leq s_1 < \cdots < s_i \leq p} n_{s_1} n_{s_2} \cdots n_{s_i} \\ &= (p-i)a_i. \end{aligned}$$

Thus,

$$\begin{aligned} f(x) - g(x) &= f(x) - \sum_{k=1}^{p} f_k(x) \\ &= \sum_{i=0}^{p}(-1)^i a_i x^{2(p-i)} - \sum_{i=0}^{p-1}(-1)^i \Big(\sum_{k=1}^{p} b_{ki}\Big) x^{2(p-1-i)} \\ &= \sum_{i=0}^{p}(-1)^i a_i x^{2(p-i)} - \sum_{i=0}^{p-1}(-1)^i (p-i) a_i x^{2(p-1-i)} \\ &= x^{2p} + \sum_{i=1}^{p}(-1)^i a_i x^{2(p-i)} - \sum_{i=1}^{p}(-1)^{i-1}(p-i+1)a_{i-1}x^{2(p-i)} \\ &= x^{2p} + \sum_{i=1}^{p}(-1)^i[a_i + (p-i+1)a_{i-1}]x^{2(p-i)}. \end{aligned}$$

■

Lemma 2.3. Let $SC(n_1, n_2, \ldots, n_p)$ be a blossomed star of order n. Then the characteristic polynomial of $SC(n_1, n_2, \ldots, n_p)$ is

$$\phi(SC(n_1, n_2, \ldots, n_p); x) = x^n + \sum_{i=1}^{p} (-1)^i [a_i + (p - i + 1)a_{i-1}] x^{n-2i}, \tag{4}$$

where $a_0 = 1, a_i = \sum_{1 \le s_1 < \cdots < s_i \le p} n_{s_1} n_{s_2} \cdots n_{s_i}, i = 1, 2, \ldots, p$.

Proof. It is obvious that

$$\phi(K_{1,n_i}; x) = x^{n_i+1} - n_i x^{n_i-1}.$$

By lemma 2.1,

$$\begin{aligned}
\phi(SC(n_1, n_2, \ldots, n_p); x) &= x \prod_{i=1}^{p} \phi(K_{1,n_i}; x) - \sum_{i=1}^{p} \frac{x^{n_i} \prod_{i=1}^{p} \phi(K_{1,n_i}; x)}{\phi(K_{1,n_i}; x)} \\
&= x \prod_{i=1}^{p} x^{n_i-1}(x^2 - n_i) - \sum_{i=1}^{p} \frac{x^{n_i} \prod_{i=1}^{p} x^{n_i-1}(x^2 - n_i)}{x^{n_i-1}(x^2 - n_i)} \\
&= x^{n-2p} \left[\prod_{i=1}^{p} (x^2 - n_i) - \sum_{i=1}^{p} \prod_{\substack{j=1 \\ j \ne i}}^{p} (x^2 - n_j) \right].
\end{aligned}$$

Therefore, by Lemma 2.2, the result is proved. ■

Lemma 2.4. Given p integers $n_1 \ge n_2 \ge \cdots \ge n_p \ge 0$ satisfying $n_i - n_j \ge 2$ for some i and j $(1 \le i < j \le p)$, define p integers $m_1, m_2, \ldots, m_p$ such that $m_s = n_s$ if $s \ne i, j$ and $m_i = n_i - 1$, $m_j = n_j + 1$. For any $1 \le k \le p$, let $a_k = \sum_{1 \le s_1 < \cdots < s_k \le p} n_{s_1} n_{s_2} \cdots n_{s_k}$ and $b_k = \sum_{1 \le s_1 < \cdots < s_k \le p} m_{s_1} m_{s_2} \cdots m_{s_k}$. Then

$$a_k < b_k, \text{ if } 2 \le k \le \alpha \ ; \ a_k = b_k = 0, \text{ if } \alpha < k \le p,$$

where $\alpha = |\{m_s | m_s \ne 0, 1 \le s \le p\}|$.

Proof. Obviously, if $k > \alpha$ then $a_k = b_k = 0$.

For fixed $1 \le i < j \le p$, let

$$\Delta_k = \sum_{\substack{1 \le s_1 < \cdots < s_k \le p \\ s_h \notin \{i,j\}, h=1,2,\ldots,k}} n_{s_1} n_{s_2} \cdots n_{s_k}.$$

Note that $n_i + n_j - m_i - m_j = 0$ and $n_i n_j - m_i m_j = -(n_i - n_j - 1) < 0$. Thus, if $k = 2$, then $a_2 - c_2 = (n_i + n_j - m_i - m_j)\Delta_1 + (n_i n_j - m_i m_j) < 0$.

For $2 < k \leq \alpha$,

$$\begin{aligned} a_k - c_k &= (n_i + n_j - m_i - m_j)\Delta_{k-1} + (n_i n_j - m_i m_j)\Delta_{k-2} \\ &= -(n_i - n_j - 1)\Delta_{k-2}. \end{aligned}$$

Since $\Delta_{k-2} > 0$, $a_k < c_k$.

Hence, the result follows. ■

Moreover, by Lemmas 2.3, 2.4 and the quasi-ordering relation, we have the following helpful lemma directly.

Lemma 2.5. Let $SC(m_1, m_2, \ldots, m_p)$ be a blossomed star of order n. If $m_i - m_j \geq 2$ for fixed $1 \leq i < j \leq p$, then the energies of $SC(m_1, m_2, \ldots, m_p)$ and $SC(m_1, \ldots, m_i - 1, \ldots, m_j + 1, \ldots, m_p)$ satisfying

$$E(SC(m_1, m_2, \ldots, m_p)) < E(SC(m_1, \ldots, m_i - 1, \ldots, m_j + 1, \ldots, m_p)).$$

Now, we can prove our results.

Proof of Theorem 1.1. Assume that $SC(m_1, m_2, \ldots, m_p)$ is the blossomed star whose energy is minimal. If there exists $1 \leq i < j \leq p$ such that $m_i \geq m_j \geq 1$, then $(m_i + 1) - (m_j - 1) \geq 2$. By Lemma 2.5,

$$E(SC(m_1, \ldots, m_i + 1, \ldots, m_j - 1, \ldots, m_p)) < E(SC(m_1, \ldots, m_i, \ldots, m_j, \ldots, m_p))$$

contradicting the choice of $SC(m_1, m_2, \ldots, m_p)$. Note that $m_1 \geq m_2 \geq \cdots \geq m_p \geq 0$, thus $m_2 = m_3 = \cdots = m_p = 0$, i.e. $SC(n-p-1, 0, \ldots, 0)$ has the minimal energy among $\mathcal{SC}(n; n_1, n_2, \ldots, n_p)$.

Proof of Theorem 1.2. Similarly, assume that $SC(m_1, m_2, \ldots, m_p)$ is the blossomed star whose energy is maximal. By Lemma 2.5, $|m_i - m_j| \leq 1$ for any $i \neq j$, implying that all the values of m_i equal to $\lfloor \frac{n-p-1}{p} \rfloor$ or $\lceil \frac{n-p-1}{p} \rceil$, i.e. $SC(m_1, m_2, \ldots, m_p) = SC(\underbrace{r+1, \ldots, r+1}_{t}, \underbrace{r, \ldots, r}_{p-t})$, where $n - p - 1 = pr + t$, $0 \leq t \leq r - 1$.

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