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Maximum energy trees with two maximum degree vertices

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Abstract The energy E of a graph G is equal to the sum of the absolute values of the eigenvalues of G . In 2005 Lin et al. determined the trees with a given maximum vertex degree Δ and maximum E, that happen to be trees with a single vertex of degree Δ. We now offer a simple proof of this result and, in addition, characterize the maximum energy trees having two vertices of maximum degree Δ.

Keywords Energy of graph · Tree · Maximum degree

1 Introduction

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a graph G [1], then the *energy* of G is defined in 1978 as [2,3]

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

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This definition was motivated by a large number of earlier results for the Hückel molecular orbital total π-electron energy, bond orders, and related quantities [4–13]. In all these works it was, explicitly or tacitly, assumed that the total π-electron energy satisfies the relation (1) (which is tantamount to the requirement that all bonding MOs are doubly filled and all antibonding MOs are empty). The expression on the right–hand side of (1) has a certain mathematical beauty, and in our time graph energy became a popular topic of research in mathematical chemistry and mathematics.

One of the fundamental questions that is encountered in the study of graph energy is which graphs (from a given class) have greatest and smallest E-values. The first such result was obtained for trees [13], when it was demonstrated that the star has minimum and the path maximum energy. In the meantime, a remarkably large number of papers were published on such extremal problems: for general graphs [4–17], trees and chemical trees [18–27], unicyclic [28–40], bicyclic [41–45], and tricyclic graphs [46], as well as for benzenoid and related polycyclic systems [47–50].

In 2005 Lin et al. [20] showed that among trees with a fixed number n of vertices and fixed maximum vertex degree Δ, the species with maximum energy are those depicted in Fig. 1.

A vertex of a tree whose degree is three or greater will be calle a *branching vertex*. A pendent vertex attached to a vertex of degree two will be called a *2-branch*.

In what follows we offer a simplified proof of the result of Lin et al. [20], from which it will become evident that it can be stated as:

Theorem 1 *Among trees with a fixed number of vertices* (n) *and of maximum vertex degree* (Δ)*, the maximum energy tree has exactly one branching vertex (of degree* Δ) *and as many as possible 2-branches.*

Using the same way of reasoning we show that a closely analogous result holds for trees with two maximum degree vertices:

Theorem 2 *Among trees with a fixed number of vertices* (n) *and two vertices of maximum degree* (Δ)*, the maximum energy tree has as many as possible 2-branches. (1) If* $n \geq 4\Delta - 1$*, then the maximum energy tree is either the graph* (a) *or the graph* (b)*, depicted in Fig. 2. (2) If* $n \leq 4\Delta - 2$*, then the maximum energy tree is the graph (c) depicted in Fig. 2, in which the numbers of pendent vertices attached to the two branching vertices u and v differ by at most* 1.

In order to prove Theorems 1 and 2 we need some preparations.

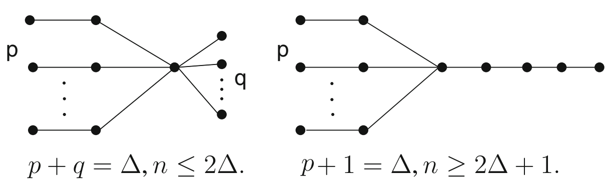
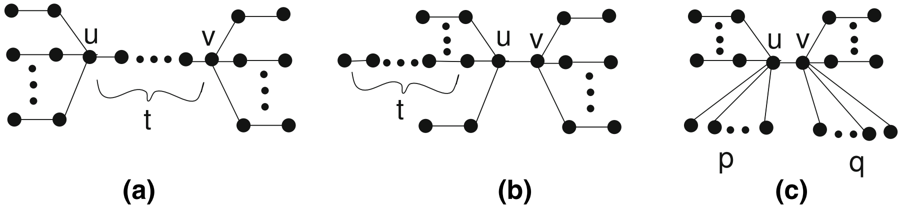


Fig. 1 The maximum energy trees with n vertices and maximum vertex degree Δ, according to Lin et al. [20]



$$d(u) = d(v) = \Delta, t = n - 4\Delta + 4, |p - q| \leq 1.$$

Fig. 2 The maximum energy trees with n vertices and two vertices u and v of maximum degree Δ

2 Preliminaries

Denote by $m(G, k)$ the number of selections of k mutually independent edges in the graph G. This quantity is also known as the k-th matching number of G. The proofs in this paper are based on the applications of the following long–time known results:

Lemma 1 [13,51]. *If for two trees T' and T'',*

$$m(T', k) \geq m(T'', k) \qquad \text{holds for all } k \geq 0 \tag{2}$$

then $E(T') \geq E(T'')$. Moreover, if at least one of the inequalities in (2) is strict (which happens in all non-trivial cases), then $E(T') > E(T'')$.

The fact that relations (2) are satisfied will be written in an abbreviated manner as: $T' \succ T''$ or $T'' \prec T'$. Thus, $T' \succ T''$ implies $E(T') > E(T'')$. For instance, in [13] it was demonstrated that for T_n being any n-vertex tree, different from the path (P_n) and the star (S_n), then $P_n \succ T_n \succ S_n$, implying that P_n and S_n are the n-vertex trees with, respectively, maximum and minimum energy.

Lemma 2 [52]. *Let $X_{n,i}$ be the graph whose structure is depicted in Fig. 3. For the fragment X being an arbitrary tree (or more generally: an arbitrary bipartite graph),*

$$X_{n,1} \succ X_{n,3} \succ X_{n,5} \succ \cdots \succ X_{n,4} \succ X_{n,2} .$$

The next lemma states a well known recursion relation (see, e.g. in [53]):

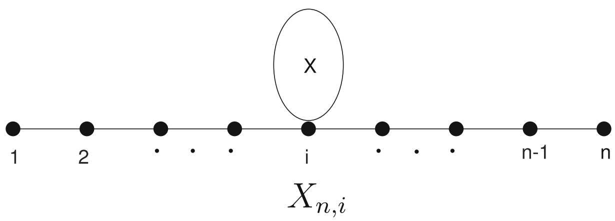


Fig. 3 The tree considered in Lemma 2

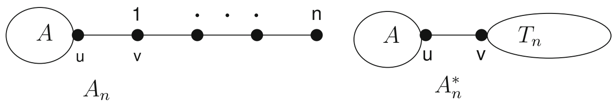


Fig. 4 The trees considered in Lemma 4

Lemma 3 *Let G be an arbitrary graph, and let e be an edge of G connecting the vertices u and v. Then*

$$m(G, k) = m(G - e, k) + m(G - u - v, k - 1) .$$

Let A_n and A_n^* be trees whose structures are depicted in Fig. 4. By A is denoted an arbitrary tree. In A_n the fragment A is attached via the vertex u to a terminal vertex v of the path P_n. In A_n^* the fragment A is attached to some n-vertex tree other than P_n.

Lemma 4 $A_n \succ A_n^*$.

Proof Apply Lemma 3 to the edges of A_n and A_n^*, connecting the vertices u and v (as shown in Fig. 4). Then

$$m(A_n, k) = m(A \cup P_n, k) + m(A - u \cup P_{n-1}, k - 1)$$

$$m(A_n^*, k) = m(A \cup T_n, k) + m(A - u \cup T_n - v, k - 1) .$$

Since $P_n \succ T_n$ and $P_{n-1} \succ T_n - v$, we have that

$$m(A \cup P_n, k) \geq m(A \cup T_n, k)$$

$$m(A - u \cup P_{n-1}, k - 1) \geq m(A - u \cup T_n - v, k - 1)$$

and therefore

$$m(A_n, k) \geq m(A_n^*, k) .$$

Lemma 4 follows. □

Let AB_n and AB_n^* be trees whose structures are depicted in Fig. 5. By A and B are denoted arbitrary tree fragments and T_n denotes an n-vertex tree.

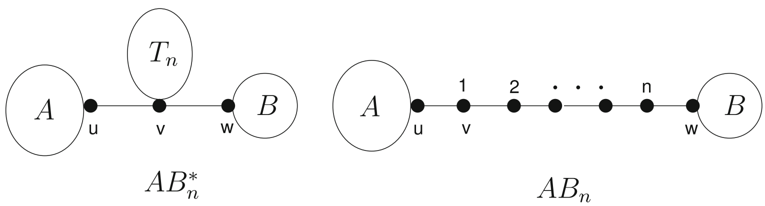


Fig. 5 The trees considered in Lemma 5

Lemma 5 $AB_n \succ AB_n^*$.

Proof Apply Lemma 3 to the edge connecting the vertices v and w of AB_n^*. Using the same notation as in Lemma 4, we get

$$m(AB_n^*, k) = m(A_n^* \cup B, k) + m(A \cup B - w \cup T_n - v, k - 1)$$

and in an analogous manner

$$m(AB_n, k) = m(A_n \cup B, k) + m(A_{n-1} \cup B - w, k - 1) \ .$$

By a repeated application of Lemma 3 and by $P_{n-1} \succ T_n - v$, we get

$$\begin{aligned} &m(A_{n-1} \cup B - w, k - 1) \\ &\quad = m(A \cup B - w \cup P_{n-1}, k - 1) + m(A - u \cup B - w \cup P_{n-2}, k - 2) \\ &\quad \geq m(A \cup B - w \cup T_n - v, k - 1) + m(A - u \cup B - w \cup P_{n-2}, k - 2) \ . \end{aligned}$$

On the other hand, by Lemma 4 it is $A_n \succ A_n^*$. Then $m(A_n \cup B, k) \geq m(A_n^* \cup B, k)$, which combined with the above relations yields

$$m(AB_n, k) \geq m(AB_n^*, k) + m(A - u \cup B - w \cup P_{n-2}, k - 2)$$

evidently implying

$$m(AB_n, k) \geq m(AB_n^*, k) \ .$$

Lemma 5 follows. □

Lemma 6 [19]. *Let G be a forest of order n $(n > 1)$ and G' be a spanning subgraph (respectively, a proper spanning subgraph) of G. Then $G \succeq G'$ (respectively, $G \succ G'$).*

Lemma 7 [22]. *Let $AX_{n,n}$, $AX_{n,2}$ be the trees shown in Fig. 6, in which X and A are denoted arbitrary tree fragments and $n \geq 3$. Then $AX_{n,n} \succ AX_{n,2}$.*

Lemma 8 *Let $AX_{n,i}$ be the graph whose structure is depicted in Fig. 7. For the fragments X and A being arbitrary trees, we have $AX_{n,3} \succ AX_{n,i}$ for $2 \leq i \leq n - 1$, $i \neq 3$.*

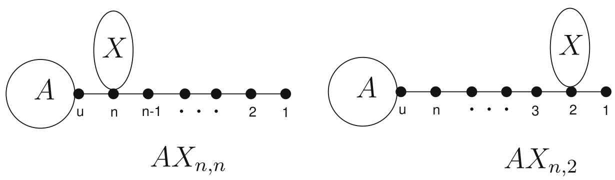


Fig. 6 The tree considered in Lemma 7

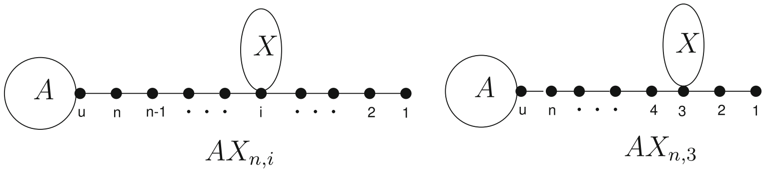


Fig. 7 The tree considered in Lemma 8

Proof Apply Lemma 3 to the edges of $AX_{n,i}$ and $AX_{n,3}$, connecting the vertex u of A and the n-th vertex of the path. Using the same notation as in Lemma 2, we get

$$m(AX_{n,i}, k) = m(A \cup X_{n,i}, k) + m(A - u \cup X_{n-1,i}, k-1)$$

$$m(AX_{n,3}, k) = m(A \cup X_{n,3}, k) + m(A - u \cup X_{n-1,3}, k-1).$$

When $2 \le i \le n-2,\ i \ne 3$, we have $X_{n,3} \succ X_{n,i},\ X_{n-1,3} \succ X_{n-1,i}$ from Lemma 2. So we have $m(A \cup X_{n,3}, k) \ge m(A \cup X_{n,i}, k),\ m(A - u \cup X_{n-1,3}, k-1) \ge m(A - u \cup X_{n-1,i}, k-1)$, and therefore $m(AX_{n,i}, k) \ge m(AX_{n,3}, k)$, that is, $AX_{n,3} \succ AX_{n,i}$.

When $i = n-1 \ge 2, i \ne 3$, we have $n \ge 3,\ n \ne 4$. If $n = 3$, then $i = 2$. From Lemma 7 we have $AX_{3,3} \succ AX_{3,2}$, and thus the result is true. If $n \ge 5$, a repeated application of Lemma 3 gives

$$\begin{aligned} m(AX_{n,n-1}, k) &= m(A \cup X_{n,n-1}, k) + m(A - u \cup X_{n-1,n-1}, k-1) \\ &= m(A \cup X_{n,2}, k) + m(A - u \cup X_{n-1,1}, k-1) \\ &= m(A \cup X_{n-1,2}, k) + m(A \cup X_{n-2,2}, k-1) \\ &\quad + m(A - u \cup X_{n-2,1}, k-1) + m(A - u \cup X_{n-3,1}, k-2) \end{aligned}$$

$$\begin{aligned} m(AX_{n,3}, k) &= m(A \cup X_{n,3}, k) + m(A - u \cup X_{n-1,3}, k-1) \\ &= m(A \cup X_{n-1,2}, k) + m(A \cup X_{n-2,1}, k-1) \\ &\quad + m(A - u \cup X_{n-2,2}, k-1) + m(A - u \cup X_{n-3,1}, k-2) \end{aligned}$$

and therefore

$$\begin{aligned} & m(AX_{n,3}, k) - m(AX_{n,n-1}, k) \\ &= m(A \cup X_{n-2,1}, k-1) + m(A - u \cup X_{n-2,2}, k-1) \\ &\quad - m(A \cup X_{n-2,2}, k-1) - m(A - u \cup X_{n-2,1}, k-1) \\ &= \sum_{j=0}^{k-1} [m(A, j) m(X_{n-2,1}, k-1-j) + m(A-u, j) m(X_{n-2,2}, k-1-j) \\ &\quad - m(A, j) m(X_{n-2,2}, k-1-j) - m(A-u, j) m(X_{n-2,1}, k-1-j)] \\ &= \sum_{j=0}^{k-1} [m(A, j) - m(A-u, j)][m(X_{n-2,1}, k-1-j) - m(X_{n-2,2}, k-1-j)]\,. \end{aligned}$$

By Lemma 6 and Lemma 2, we have $A \succ A-u$, $X_{n-2,1} \succ X_{n-2,2}$, and so $m(A, j) \geq m(A-u, j)$ and $m(X_{n-2,1}, k-1-j) \geq m(X_{n-2,2}, k-1-j)$. Hence $m(AX_{n,3}, k) \geq m(AX_{n,n-1}, k)$ and thus the lemma follows. □

Lemma 9 *Let A and B be the graphs whose structures are depicted in Fig. 8 such that* $d(u) = d(v) = \Delta-2,\ \Delta \geq 3,\ 0 < p \leq \Delta-2$. *Then* $(A-u)\cup B \succ A\cup(B-v)$.

Proof Let $T_1 = (A-u)\cup B$ and $T_2 = A\cup(B-v)$. We show that $T_1 \succ T_2$. The orders of T_1 and T_2 are equal, i.e., $|V(T_1)| = |V(T_2)| = 4\Delta - p - 7$. The characteristic polynomials of T_1 and T_2 are denoted by $\phi(T_1)$ and $\phi(T_2)$, respectively. It is known that if T is a forest of order n, then its characteristic polynomial can be written as [53]

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

When $0 < p \leq \Delta - 2$, direct calculation gives

$$\phi(T_1) = x^{p-1}(x^2-1)^{2\Delta-5-p}[x^4 - (\Delta-1)x^2 + p]$$
$$\phi(T_2) = x^{p-1}(x^2-1)^{2\Delta-5-p}[x^4 - (\Delta-1)x^2]\ .$$

Then

$$\phi(T_1) - \phi(T_2) = p\, x^{p-1}(x^2-1)^{2\Delta-5-p}\ .$$

Also by direct calculation, the characteristic polynomial of the graph C depicted in Fig. 8 is $\phi(C) = x^{p-1}(x^2-1)^{2\Delta-5-p}$. Therefore, $\phi(T_1) - \phi(T_2) = p\,\phi(C)$.

On the other hand,

$$\phi(T_1) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, m(T_1, k)\, x^{n-2k}, \qquad \phi(T_2) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k\, m(T_2, k)\, x^{n-2k}$$

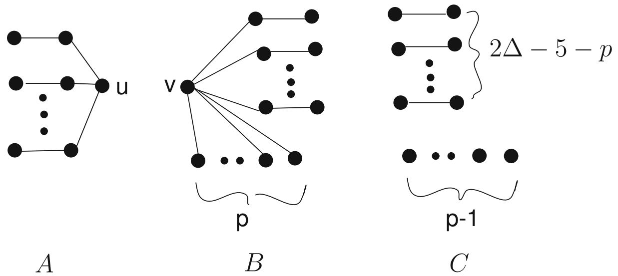


Fig. 8 The trees considered in Lemma 9

where $n = 4\Delta - p - 7$ is the order of T_1 and T_2. The order of the graph C is $p - 1 + 2(2\Delta - 5 - p) = n - 4$. Then we have

$$\phi(C) = \sum_{k=0}^{\lfloor \frac{n-4}{2} \rfloor} (-1)^k \, m(C, k) \, x^{n-4-2k} .$$

Since $\phi(T_1) - \phi(T_2) = p\,\phi(C)$, we have $m(T_1, k) - m(T_2, k) = p \cdot m(C, k-2) \geq 0$ for $2 \leq k \leq \lfloor n/2 \rfloor$ and $m(T_1, 0) = m(T_2, 0) = 1$, $m(T_1, 1) = m(T_2, 1) = n - 1$. Therefore, $m(T_1, k) \geq m(T_2, k)$ when $0 < p \leq \Delta - 2$, and thus $T_1 \succ T_2$. Lemma 9 follows. □

Let P_n be the path with n vertices and u, v be two vertices of a graph G. Two vertices u and v of G are said to be equivalent if the subgraphs $G - u$ and $G - v$ are isomorphic. The graph $G(u, v)(P_a, P_b)$ is obtained by joining the terminal vertices of P_a and P_b to u and v, respectively.

Lemma 10 [52]. *If the vertices u and v of a graph G are adjacent and equivalent, then for $n = 4k + i$, $i \in \{0, 1, 2, 3\}$, $k \geq 1$,*

$$\begin{aligned} G(u, v)(P_0, P_n) &\succ G(u, v)(P_2, P_{n-2}) \succ \cdots \succ G(u, v)(P_{2k}, P_{n-2k}) \\ &\succ G(u, v)(P_{2k+1}, P_{n-2k-1}) \succ G(u, v)(P_{2k-1}, P_{n-2k+1}) \\ &\succ G(u, v)(P_1, P_{n-1}) . \end{aligned}$$

Lemma 11 *Let T, T' be trees whose structure is shown in Fig. 9. If $d_T(u) = d_T(v) = d_{T'}(u) = d_{T'}(v) = \Delta$, $\Delta \geq 3$, $0 \leq p \leq \Delta - 2$, $t \geq 2$, then $T \succ T'$.*

Proof T and T' can be denoted by $G(u, v)(P_t, P_2)$ and $G(u, v)(P_{t+1}, P_1)$, respectively, where G is shown in Fig. 9. If $p = 0$, then $A \cong B$. The vertices u and v are equivalent in G, and then $T \succ T'$ by Lemma 10. So in what follows we assume that $0 < p \leq \Delta - 2$.

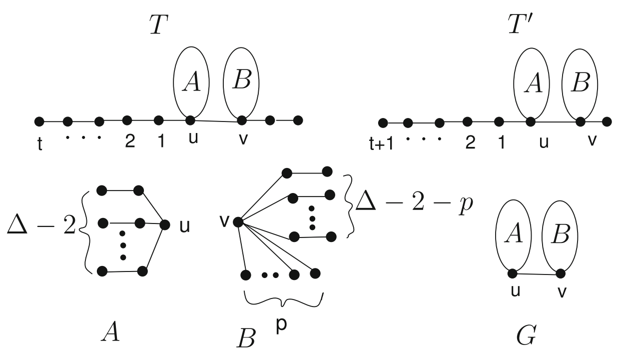


Fig. 9 The trees considered in Lemma 11

Applying Lemma 3 to T and T', and using the same notations as in Lemmas 4 and 8, we get

$$\begin{aligned} m(T,k) &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_t,P_0),k-1)\\ &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_{t-1},P_0),k-1)\\ &\quad + m(G(u,v)(P_{t-2},P_0),k-2) \end{aligned}$$

$$\begin{aligned} m(T',k) &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_{t-1},P_1),k-1)\\ &= m(G(u,v)(P_t,P_1),k) + m(G(u,v)(P_{t-1},P_0),k-1)\\ &\quad + m(A_{t-1}\cup(B-v),k-2)\ . \end{aligned}$$

Then $m(T,k) - m(T',k) = m(G(u,v)(P_{t-2},P_0),k-2) - m(A_{t-1}\cup B-v,k-2)$.

When $t=2$, the graph $A_{t-1}\cup(B-v)$ is a proper subgraph of $G(u,v)(P_{t-2},P_0)$, and then $m(T,k)\geq m(T',k)$ by Lemma 6.

When $t\geq 3$, a repeated application of Lemma 3 gives

$$\begin{aligned} m(T,k)-m(T',k) &= m(G(u,v)(P_{t-2},P_0),k-2) - m(A_{t-1}\cup(B-v),k-2)\\ &= m(A_{t-2}\cup B,k-2) + m((A-u)\cup(B-v)\cup P_{t-2},k-3)\\ &\quad -m(A\cup(B-v)\cup P_{t-1},k-2)\\ &\quad -m((A-u)\cup(B-v)\cup P_{t-2},k-3)\\ &= m(A_{t-2}\cup B,k-2) - m(A\cup(B-v)\cup P_{t-1},k-2)\\ &= m(A\cup B\cup P_{t-2},k-2) + m((A-u)\cup B\cup P_{t-3},k-3)\\ &\quad -m(A\cup(B-v)\cup P_{t-2},k-2)\\ &\quad -m(A\cup(B-v)\cup P_{t-3},k-3)\ . \end{aligned}$$

Since $A\cup(B-v)$ is a proper subgraph of $A\cup B$, we have $A\cup B\succ A\cup(B-v)$ and $m(A\cup B\cup P_{t-2},k-2)\geq m(A\cup(B-v)\cup P_{t-2},k-2)$. On the other hand, $(A-u)\cup B\succ A\cup(B-v)$ follows by Lemma 9. Then $m((A-u)\cup B\cup P_{t-3},k-3)\geq m(A\cup(B-v)\cup P_{t-3},k-3)$. Consequently, $m(T,k)\geq m(T',k)$. Lemma 11 follows. □

3 Proof of Theorem 1

Let T be a tree of order n and maximum degree Δ with maximum energy. Let u be a vertex of maximum degree Δ in T. By Lemma 4, T must contain Δ pendent paths at u, i.e., T is a starlike tree with a unique branching vertex of degree Δ. By Lemma 2, T has as many as possible 2-branches. This completes the proof of Theorem 1.

4 Proof of Theorem 2

Suppose T is a tree of order n having exactly two vertices of maximum degree, with maximum energy. Let u and v be the vertices of maximum degree. Let P_t be the unique path connecting u and v. We first claim that there are no branching vertices in P_t. Otherwise, suppose there is a branching vertex w in P_t and T_{n_1} is the tree attached to the path P_t at w. Assume ww_1, ww_2 are the two edges in the path P_t. Then we can obtain a new tree T' from T by deleting T_{n_1} and adding a path P_{n_1} whose two terminal vertices are adjacent to w_1, w_2, respectively. From Lemma 5, $T' \succ T$, a contradiction. By Lemma 4, we know that there are $\Delta - 1$ pendent paths at u and v, respectively.

Next we claim that there is not more than one pendent path with length ≥ 3 in T. Otherwise, assume there are two or more such paths. By Lemma 2, there is at most one pendent path of length ≥ 3 at each vertex of u and v. So we can assume that P_{t_1} and P_{t_2} ($t_1 \geq 4$, $t_2 \geq 4$) are the unique pendent paths of length ≥ 3 with terminal vertex u and v in T, respectively. From Lemma 2 the other pendent paths in T are all of length 2. If the length of the unique path P_t connecting u and v is equal to 1, i. e., $t = 2$, then u and v are adjacent. Then we can construct a new tree T' from T by changing the paths P_{t_1} and P_{t_2} to $P_{t_1+t_2-3}$ and P_3, respectively. $T' \succ T$ follows from Lemma 10, a contradiction. If $t \geq 3$, then we can also obtain a new tree T' from T by changing P_{t_2} and P_t to P_3 and P_{t+t_2-3}, respectively. $T' \succ T$ follows from Lemma 8, a contradiction. So the claim follows. From this claim we have that there is at most one pendent path of length ≥ 3 in T.

In what follows, we consider two cases.

Case 1 T has one such path. Without loss of generality we may assume that it is attached to vertex u. By Lemma 2, we know that the other pendent paths at u are all of length 2. By Lemma 8, the length of the path P_t connecting u and v must be 1, i.e., u and v are adjacent in T. Then from Lemma 11 we get that all the pendent paths at v are of length 2. Therefore T has the structure (b) depicted in Fig. 2.

Case 2 T has no pendent path of length ≥ 3. Then all the pendent paths at u and v are of length 1 or 2.

If the length of the path P_t is greater than 1, then from Lemma 8 all the pendent paths in T are of length 2. Then T has the structure (a) depicted in Fig. 2.

If the length of the path P_t is equal to 1, i.e., u and v are adjacent, then since each pendent path is either P_3 or a pendent edge, then $n \leq 4\Delta - 2$. Assume there are p pendent edges and $\Delta - p - 1$ pendent paths P_3 at u, q pendent edges and $\Delta - q - 1$ pendent paths P_3 at v. Then $p + q = 4\Delta - n - 2 = m$.

By direct calculation the characteristic polynomial of T is

$$\phi(T, x) = x^{m-2}(x^2 - 1)^{2\Delta-m-4}\{x^8 - (2\Delta + 1)\, x^6 + (\Delta^2 + m + 2)\, x^4 - (\Delta m + 1)\, x^2 + pq\}\,.$$

Thus, when p and q are almost equal, i.e., $|p - q| \leq 1$, then the E-value of T reaches the maximum which is depicted in (c) of Fig. 2. This completes the proof. □

Remark For $n > 4\Delta - 2$, one could ask a natural question: Which of the graphs (a) and (b) in Theorem 2 has the maximum energy? The examples in Fig. 10 shows that sometimes the energy of graph (a) is greater than that of graph (b), and sometimes the other round is true, i.e., the energy of graph (b) is greater than that of (a).

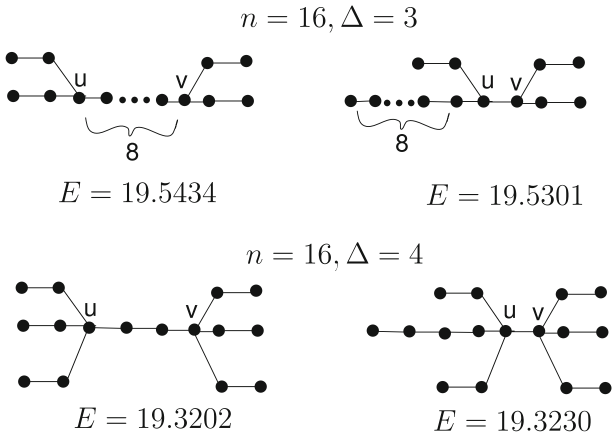


Fig. 10 The energy E of graph (**a**) and (**b**) in Theorem 2

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