Maximum Energy Trees with One Maximum and One Second Maximum Degree Vertex

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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. Later, in 2009 Li et al. characterized the maximum energy trees having two vertices of maximum degree Δ. In this paper we consider the general case and characterize the maximum energy trees with one maximum degree vertex and another second maximum degree vertex.

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]

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

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 [3–6]. 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 [6], 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 more information, refer to the survey [7] and the recent papers [8–14].

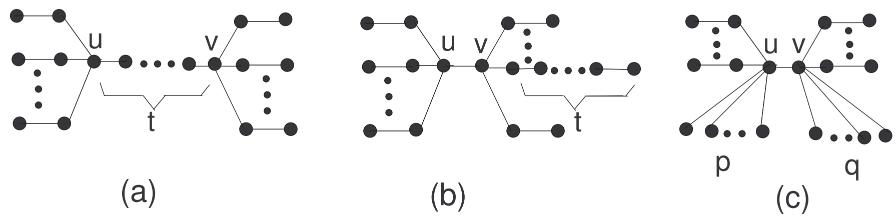
A vertex of a tree whose degree is three or greater will be called a *branching vertex*. A pendent vertex attached to a vertex of degree two will be called a *2-branch*.

For given maximum degree (Δ), Lin et al. [15] characterized the trees with the minimal energy among all trees of order n and $\lceil \frac{n+1}{3} \rceil \leq \Delta(T) \leq n-2$. Recently, Heuberger and Wagner ([16, 17]) completely characterized the trees with given maximum degree that minimize the energy for any $\Delta(T)$.

On the other hand, Lin et al. [15] showed that 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. In 2009 Li et al. [18] showed that a closely analogous result holds for trees with two maximum degree vertices (of degree Δ). In this paper we consider the general case and characterize the maximum energy trees with one maximum degree vertex and another second maximum degree vertex.

Theorem 1.1 *Among trees with a fixed number of vertices (n) and two vertices of maximum degree d_1 and second maximum degree d_2 ($d_1 > d_2$), the maximum energy tree has as many as possible 2-branches. (1) If $n \geq 2d_1 + 2d_2 - 1$, then the maximum energy tree is either the graph (a) or the graph (b), depicted in Figure 1. (2) If $n \leq$*

$2d_1+2d_2-2$, *then the maximum energy tree is among the graphs (c) depicted in Figure 1.*



$$d(u)=d_1, d(v)=d_2, t=n-2d_1-2d_2+4, p\le q.$$

Figure 1.1 The maximum energy trees with n vertices and two vertices u and v of degree d_1 and d_2

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 2.1 [6, 19]. *If for two trees T' and T'' ,*

$$m(T',k)\ge m(T'',k) \qquad \textit{holds for all} \quad k\ge 0 \tag{1}$$

then $E(T')\ge E(T'')$. Moreover, if at least one of the inequalities in (1) is strict (which happens in all non-trivial cases), then $E(T')>E(T'')$.

The fact that relations (1) are satisfied will be written in an abbreviated manner as: $T'\succcurlyeq T''$ or $T''\preccurlyeq T'$. Thus, $T'\succcurlyeq T''$ implies $E(T')\ge E(T'')$. If $T'\succcurlyeq T''$ and there is a k such that $m(T',k)>m(T'',k)$, we call $T'\succ T''$. Thus $T'\succ T''$ implies $E(T')>E(T'')$. For instance, in [6] 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 2.2 [20]. *Let G be an arbitrary graph, and let e be an edge of G connecting the vertices u and v. Then*

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

Lemma 2.3 [18]. *Let A_n and A_n^* be trees whose structures are depicted in Figure 2. 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. Then $A_n \succ A_n^*$.*

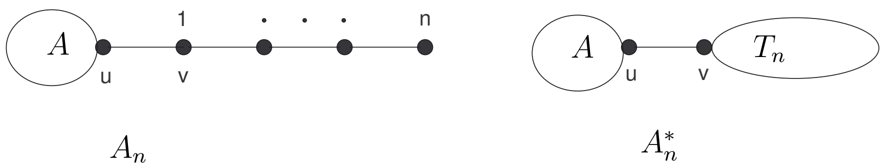


Figure 2.1 The trees considered in Lemma 2.3.

Lemma 2.4 [18]. *Let AB_n and AB_n^* be trees whose structures are depicted in Figure 2.2. By A and B are denoted arbitrary tree fragments and T_n denotes an n-vertex tree($n \neq 1$). Then $AB_n \succ AB_n^*$.*

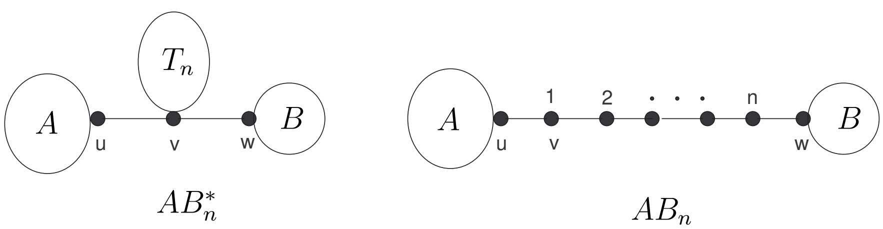


Figure 2.2 The trees considered in Lemma 2.4.

Lemma 2.5 [21]. *Let $X_{n,i}$ be the graph whose structure is depicted in Figure 2.3. For the fragment X being an arbitrary tree other than P_1,*

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

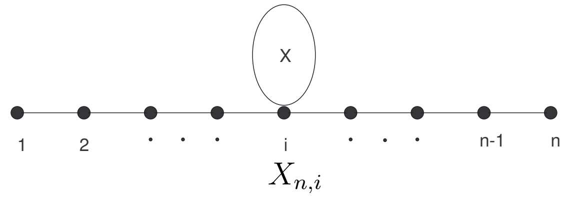


Figure 2.3 The tree considered in Lemma 2.5.

Lemma 2.6 [22]. *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 2.7 [18]. *Let $AX_{n,i}$ be the graph whose structure is depicted in Figure 2.4. For the fragments X and A being arbitrary trees other than P_1. Then $AX_{n,3} \succ AX_{n,i}$ for $2 \le i \le n-1,\ i \ne 3$.*

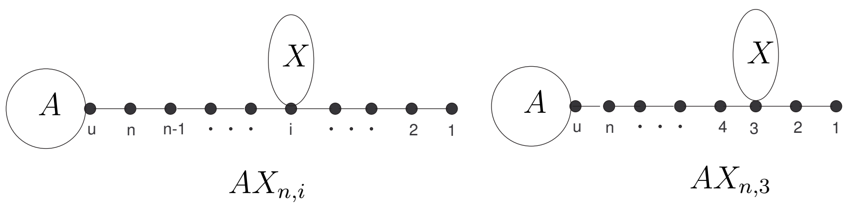


Figure 2.4 The trees considered in Lemma 2.7.

Let G be a graph and u, v be two vertices of G. 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. Then $G(u,v)(P_0,\ P_0) \cong G$.

Lemma 2.8 *Let T, T' be trees whose structure is shown in Figure 2.5. If $d_T(u) = d_{T'}(u) = d_1, d_T(v) = d_{T'}(v) = d_2,\ d_1 > d_2 \ge 3,\ t_1 \ge 3,\ t_2 \ge 1$, then $T' \succ T$.*

Proof. T and T' can be denoted by $G(u,v)(P_{t_1}, P_{t_2})$ and $G(u,v)(P_2, P_{t_1+t_2-2})$, respectively, where G is shown in Figure 2.5.

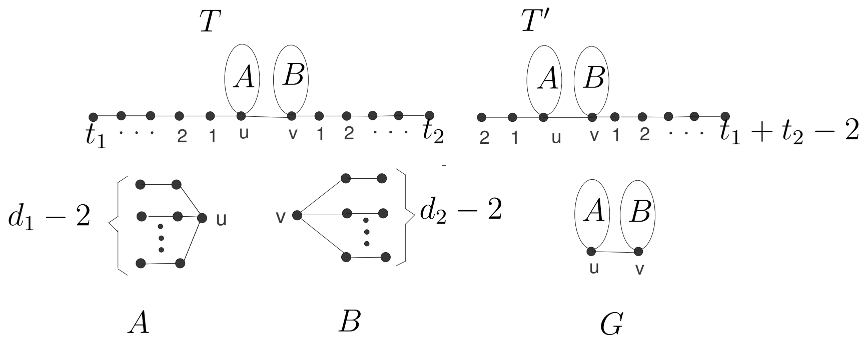


Figure 2.5 The trees considered in Lemma 2.8.

Applying Lemma 2.2 to T and T' , we get

$$\begin{aligned} & m(T',k) - m(T,k) \\ = \;& m(G(u,v)(P_2,P_{t_2}) \cup P_{t_1-2},k) + m(G(u,v)(P_2,P_{t_2-1}) \cup P_{t_1-3},k-1) \\ - \;& m(G(u,v)(P_2,P_{t_2}) \cup P_{t_1-2},k) + m(G(u,v)(P_1,P_{t_2}) \cup P_{t_1-3},k-1) \\ = \;& m(G(u,v)(P_2,P_{t_2-1}) \cup P_{t_1-3},k-1) - m(G(u,v)(P_1,P_{t_2}) \cup P_{t_1-3},k-1)\ . \end{aligned}$$

When $t_2 = 1$, a repeated application of Lemma 2.2 and using the same notations as in Lemma 2.3, we get

$$\begin{aligned} & m(T',k) - m(T,k) \\ = \;& m(G(u,v)(P_2,P_0) \cup P_{t_1-3},k-1) - m(G(u,v)(P_1,P_1) \cup P_{t_1-3},k-1) \\ = \;& m(G(u,v)(P_1,P_0) \cup P_{t_1-3},k-1) + m(G(u,v)(P_0,P_0) \cup P_{t_1-3},k-2) \\ - \;& m(G(u,v)(P_1,P_0) \cup P_{t_1-3},k-1) - m(A_1 \cup (B-v) \cup P_{t_1-3},k-2) \\ = \;& m(G(u,v)(P_0,P_0) \cup P_{t_1-3},k-2) - m(A_1 \cup (B-v) \cup P_{t_1-3},k-2)\ . \end{aligned}$$

Since $A_1 \cup (B-v)$ is a proper subgraph of $G(u,v)(P_0,P_0)$, we have $A_1 \cup (B-v) \prec G(u,v)(P_0,P_0)$ by Lemma 2.6. Then $m(G(u,v)(P_0,P_0) \cup P_{t_1-3},k-2) \geq m(A_1 \cup (B-v) \cup P_{t_1-3},k-2)$. Consequently, $m(T',k) \geq m(T,k)$ holds for all $k \geq 0$ and it is strict for $k = 3$. This implies $T' \succ T$.

When $t_2 = 2$, using Lemma 2.2 gives

$$\begin{aligned}
& m(T', k) - m(T, k) \\
= \; & m(G(u,v)(P_2, P_1) \cup P_{t_1-3}, k-1) - m(G(u,v)(P_1, P_2) \cup P_{t_1-3}, k-1) \\
= \; & m(G(u,v)(P_1, P_1) \cup P_{t_1-3}, k-1) + m(G(u,v)(P_0, P_1) \cup P_{t_1-3}, k-2) \\
- \; & m(G(u,v)(P_1, P_1) \cup P_{t_1-3}, k-1) - m(G(u,v)(P_1, P_0) \cup P_{t_1-3}, k-2) \\
= \; & m(G(u,v)(P_0, P_1) \cup P_{t_1-3}, k-2) - m(G(u,v)(P_1, P_0) \cup P_{t_1-3}, k-2) \\
= \; & m(G(u,v)(P_0, P_0) \cup P_{t_1-3}, k-2) + m(A \cup (B-v) \cup P_{t_1-3}, k-3) \\
- \; & m(G(u,v)(P_0, P_0) \cup P_{t_1-3}, k-2) - m((A-u) \cup B \cup P_{t_1-3}, k-3) \\
= \; & m(A \cup (B-v) \cup P_{t_1-3}, k-3) - m((A-u) \cup B \cup P_{t_1-3}, k-3) \ .
\end{aligned}$$

Since $(A-u) \cup B$ is a proper subgraph of $A \cup (B-v)$ when $d_1 > d_2$, then$A \cup (B-v) \cup P_{t_1-3} \succ (A-u) \cup B \cup P_{t_1-3}$ by Lemma 2.6. Consequently, $m(T', k) \geq m(T, k)$ holds for all $k \geq 0$ and it is strict for $k = 4$. Then we have $T' \succ T$.

When $t_2 \geq 3$, a repeated application of Lemma 2.2 and using the same notations as in Lemma 2.3, we get

$$\begin{aligned}
& m(T', k) - m(T, k) \\
= \; & m(G(u,v)(P_2, P_{t_2-1}) \cup P_{t_1-3}, k-1) - m(G(u,v)(P_1, P_{t_2}) \cup P_{t_1-3}, k-1) \\
= \; & m(G(u,v)(P_1, P_{t_2-1}) \cup P_{t_1-3}, k-1) + m(G(u,v)(P_0, P_{t_2-1}) \cup P_{t_1-3}, k-2) \\
- \; & m(G(u,v)(P_1, P_{t_2-1}) \cup P_{t_1-3}, k-1) - m(G(u,v)(P_1, P_{t_2-2}) \cup P_{t_1-3}, k-2) \\
= \; & m(G(u,v)(P_0, P_{t_2-1}) \cup P_{t_1-3}, k-2) - m(G(u,v)(P_1, P_{t_2-2}) \cup P_{t_1-3}, k-2) \\
= \; & m(G(u,v)(P_0, P_{t_2-2}) \cup P_{t_1-3}, k-2) + m(G(u,v)(P_0, P_{t_2-3}) \cup P_{t_1-3}, k-3) \\
- \; & m(G(u,v)(P_0, P_{t_2-2}) \cup P_{t_1-3}, k-2) - m((A-u) \cup B_{t_2-2} \cup P_{t_1-3}, k-3) \\
= \; & m(G(u,v)(P_0, P_{t_2-3}) \cup P_{t_1-3}, k-3) - m((A-u) \cup B_{t_2-2} \cup P_{t_1-3}, k-3) \\
= \; & m(A \cup B_{t_2-3} \cup P_{t_1-3}, k-3) + m((A-u) \cup (B-v) \cup P_{t_2-3} \cup P_{t_1-3}, k-4) \\
- \; & m((A-u) \cup B \cup P_{t_2-2} \cup P_{t_1-3}, k-3) \\
- \; & m((A-u) \cup (B-v) \cup P_{t_2-3} \cup P_{t_1-3}, k-4) \\
= \; & m(A \cup B_{t_2-3} \cup P_{t_1-3}, k-3) - m((A-u) \cup B \cup P_{t_2-2} \cup P_{t_1-3}, k-3) \ .
\end{aligned}$$

If $t_2 = 3$, $(A-u)\cup B\cup P_{t_2-2}\cup P_{t_1-3}$ is a proper subgraph of $A\cup B_{t_2-3}\cup P_{t_1-3}$, then $m(T',k)\geq m(T,k)$ holds for all $k\geq 0$ and it is strict for $k=4$. This implies $T'\succ T$.

When $t_2 > 3$,

$$\begin{aligned} & m(T',k)-m(T,k) \\ = \;& m(A\cup B\cup P_{t_2-3}\cup P_{t_1-3},k-3)+m(A\cup(B-v)\cup P_{t_2-4}\cup P_{t_1-3},k-4) \\ - \;& m((A-u)\cup B\cup P_{t_2-3}\cup P_{t_1-3},k-3)-m((A-u)\cup B\cup P_{t_2-4}\cup P_{t_1-3},k-4)\ . \end{aligned}$$

Since $(A-u)\cup B$ is a proper subgraph of $A\cup(B-v)$ when $d_1>d_2$ and $(A-u)\cup B$ is also a proper subgraph of $A\cup B$, then $m(T',k)\geq m(T,k)$ holds for all $k\geq 0$ and it is strict for $k=4$. Consequently, $T'\succ T$. Lemma 2.8 follows. ∎

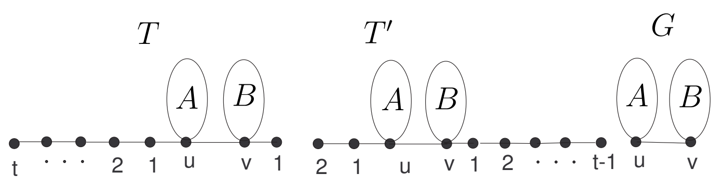


Figure 2.6 The trees considered in Lemma 2.9.

Lemma 2.9 *Let T, T' be trees whose structure is shown in Figure 2.6. For the fragments A and B being arbitrary trees other than P_1 and $t\geq 3$, we have $T'\succ T$.*

Proof. T and T' can be denoted by $G(u,v)(P_t,P_1)$ and $G(u,v)(P_2,P_{t-1})$, respectively, where G is shown in Figure 2.6. Applying Lemma 2.2 to T and T' and using the same notations as in Lemma 2.3, we get

$$\begin{aligned} & m(T',k)-m(T,k) \\ = \;& m(G(u,v)(P_2,P_1)\cup P_{t-2},k)+m(G(u,v)(P_2,P_0)\cup P_{t-3},k-1) \\ - \;& m(G(u,v)(P_2,P_1)\cup P_{t-2},k)-m(G(u,v)(P_1,P_1)\cup P_{t-3},k-1) \\ = \;& m(G(u,v)(P_1,P_0)\cup P_{t-3},k-1)+m(G(u,v)(P_0,P_0)\cup P_{t-3},k-2) \\ - \;& m(G(u,v)(P_1,P_0)\cup P_{t-3},k-1)-m(A_1\cup(B-v)\cup P_{t-3},k-2) \\ = \;& m(G(u,v)(P_0,P_0)\cup P_{t-3},k-2)-m(A_1\cup(B-v)\cup P_{t-3},k-2)\ . \end{aligned}$$

$A_1 \cup (B-v)$ is a proper subgraph of $G(u,v)(P_0,P_0) \cong G$, then $A_1 \cup (B-v) \prec G(u,v)(P_0,P_0)$ from Lemma 2.6. So we have $m(G(u,v)(P_0,P_0) \cup P_{t-3}, k-2) \geq m(A_1 \cup (B-v) \cup P_{t-3}, k-2)$, and then $m(T',k) \geq m(T,k)$ holds for all $k \geq 0$ and it is strict for $k=3$. The lemma follows. ▮

Lemma 2.10 *Let T, T' be trees whose structure is shown in Figure 2.7. If $d_T(u) = d_{T'}(u) = d_1, d_T(v) = d_{T'}(v) = d_2$, $d_1 > d_2 \geq 3$, $t \geq 3$, $d_1 - 2 \geq p \geq 0$, then $T' \succ T$.*

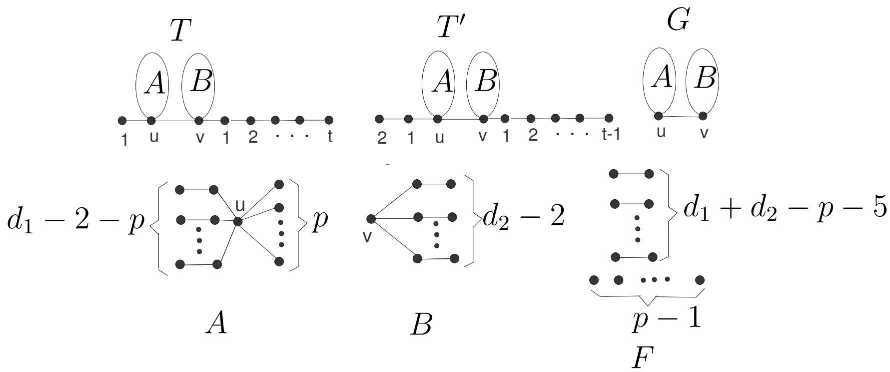


Figure 2.7 The trees considered in Lemma 2.10.

Proof. T and T' can be denoted by $G(u,v)(P_1,P_t)$ and $G(u,v)(P_2,P_{t-1})$, respectively, where G is shown in Figure 2.7. Applying Lemma 2.2 to T and T' and using the same notations as in Lemma 2.3, we get

$$\begin{aligned} m(T',k) - m(T,k) &= m(G(u,v)(P_1,P_{t-1}),k) + m(G(u,v)(P_0,P_{t-1}),k-1) \\ &\quad - m(G(u,v)(P_1,P_{t-1}),k) - m(G(u,v)(P_1,P_{t-2}),k-1) \\ &= m(G(u,v)(P_0,P_{t-2}),k-1) + m(G(u,v)(P_0,P_{t-3}),k-2) \\ &\quad - m(G(u,v)(P_0,P_{t-2}),k-1) - m((A-u) \cup B_{t-2},k-2) \\ &= m(G(u,v)(P_0,P_{t-3}),k-2) - m((A-u) \cup B_{t-2},k-2)\ . \end{aligned}$$

When $t=3$, the graph $(A-u) \cup B_{t-2}$ is a proper subgraph of $G(u,v)(P_0,P_{t-3})$, and then $m(T',,k) \geq m(T,k)$ holds for all $k \geq 0$ and it is strict for $k=3$. This implies $T' \succ T$.

When $t \geq 4$, a repeated application of Lemma 2.2 gives

$$\begin{aligned}
& m(T', k) - m(T, k) \\
= \; & m(A \cup B_{t-3}, k-2) + m((A-u) \cup (B-v) \cup P_{t-3}, k-3) \\
- \; & m((A-u) \cup B \cup P_{t-2}, k-2) - m((A-u) \cup (B-v) \cup P_{t-3}, k-3) \\
= \; & m(A \cup B \cup P_{t-3}, k-2) + m(A \cup (B-v) \cup P_{t-4}, k-3) \\
- \; & m((A-u) \cup B \cup P_{t-3}, k-2) - m((A-u) \cup B \cup P_{t-4}, k-3)\ .
\end{aligned}$$

Since $(A-u) \cup B$ is a proper subgraph of $A \cup B$, then $m(A \cup B \cup P_{t-3}, k-2) \geq m((A-u) \cup B \cup P_{t-3}, k-2)$. We claim that $A \cup (B-v) \succ (A-u) \cup B$ whose proof given below, then $m(A \cup (B-v) \cup P_{t-4}, k-3) \geq m((A-u) \cup B \cup P_{t-4}, k-3)$. Consequently, $m(T', k) \geq m(T, k)$ holds for all $k \geq 0$ and it is strict for $k = 3$. Lemma 2.10 follows.

Proof of Claim $A \cup (B-v) \succ (A-u) \cup B$.

When $p = 0$, $(A-u) \cup B$ is a proper subgraph of $A \cup (B-v)$, we have $A \cup (B-v) \succ (A-u) \cup B$ by Lemma 2.6.

When $p > 0$, Let $F_1 = (A-u) \cup B$ and $F_2 = A \cup (B-v)$, We show that $F_1 \prec F_2$. The orders of F_1 and F_2 are equal, i. e., $|V(T_1)| = |V(T_2)| = 2(d_1 + d_2) - p - 7$. The characteristic polynomials of F_1 and F_2 are denoted by $\phi(F_1)$ and $\phi(F_2)$, respectively. Then

$$\phi(F_1) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \, m(F_1, k) \, x^{n-2k} \quad , \quad \phi(F_2) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \, m(F_2, k) \, x^{n-2k}$$

where $n = 2(d_1 + d_2) - p - 7$ is the order of F_1 and F_2. The order of the graph F depicted in Figure 2.7 is $2(d_1 + d_2) - p - 11 = n - 4$. We have

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

On the other hand, direct calculation gives

$$\begin{aligned}
\phi(F_1) &= x^{p-1}(x^2-1)^{d_1+d_2-p-5}[x^4 - (d_2-1)x^2] \\
\phi(F_2) &= x^{p-1}(x^2-1)^{d_1+d_2-p-5}[x^4 - (d_1-1)x^2 + p] \\
\phi(F) &= x^{p-1}(x^2-1)^{d_1+d_2-p-5}\ .
\end{aligned}$$

Then

$$\phi(F_1) - \phi(F_2) = x^{p-1}(x^2-1)^{d_1+d_2-p-5}[(d_1-d_2)x^2-p] = \phi(F)[(d_1-d_2)x^2-p]\ .$$

So we have $m(F_1,k) - m(F_2,k) = -[(d_1-d_2)m(F,k-1) + p\cdot m(F,k-2)] \leq 0$ for $2 \leq k \leq \lfloor n/2 \rfloor$ and $m(F_1,0) = m(F_2,0) = 1,\ m(F_1,1) - m(F_2,1) = d_2 - d_1 < 0$. Therefore, $m(F_1,k) \leq m(F_2,k)$ holds for all $k \geq 0$ and it is strict for $k=1$. This implies $F_1 \prec F_2$. The claim follows. ∎

3 Proof of theorem

Suppose T is a tree of order n having exactly one vertex of maximum degree d_1 and another vertex of the second maximum degree $d_2\,(d_1 > d_2)$, with maximum energy. Let u and v be the two vertices in T with degree d_1 and d_2, respectively. Let P_t be the unique path connecting u and v. We can claim that there are no other branching vertices in P_t except u and v by Lemma 2.4 and there are d_1-1 and d_2-1 pendent paths at u and v, respectively, which follows from Lemma 2.3.

When $d_2 = 1$ or $d_2 = 2$, T has exactly one branching vertex u (of degree d_1) and as many as possible 2-branches by Lemma 2.5. So in what follows we assume $d_1 > d_2 \geq 3$.

We next claim that there is at most one pendent path with length ≥ 3 in T. Otherwise, assume there are two or more such paths. By Lemma 2.5, 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 2.5 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_3 and $P_{t_1+t_2-3}$, respectively. $T' \succ T$ follows from Lemma 2.8, a contradiction. If $t \geq 3$, then we can also construct 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 2.7, a contradiction. So the claim follows. By this claim we consider two cases according to the number of pendent paths of length ≥ 3 in T as follows.

Case 1. T has exactly one such path. We claim this path must be attached to the vertex v and all the other pendent paths are of length 2 and in addition u and v are adjacent, i. e., T has the structure (b) depicted in Figure 1.

By Lemma 2.7 , the length of the path P_t connecting u and v must be 1, i. e., u and v are adjacent in T . Otherwise, we can construct a new tree T' with greater energy than T as shown in Figure 2.4 , a contradiction.

The pendent path of length ≥ 3 must be attached to v . Otherwise, assume it is attached to u, then the other pendent paths at u are of length 2 from Lemma 2.5 and by Lemma 2.8 there must be at least one pendent path of length 1 at v. By Lemma 2.9 we can construct a new tree T' which has greater energy than T, a contradiction.

Thus the pendent path of length ≥ 3 must be attached to v and all the other pendent paths in T are of length 2 follows from Lemma 2.5 and Lemma 2.10. Consequently, the claim follows and T has the structure (b) depicted in Figure 1.

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 connecting u and v is greater than 1, then from Lemma 2.7 all the pendent paths in T are of length 2. Then T has the structure (a) depicted in Figure 1 .

If the length of the path P_t is equal to 1 , i. e., u and v are adjacent, then $n \leq 2d_1 + 2d_2 - 2$ since each pendent path is either P_3 or a pendent edge. Assume there are p pendent edges and $d_1 - p - 1$ pendent paths P_3 at u , q pendent edges and $d_2 - q - 1$ pendent paths P_3 at v . Then $p + q = 2d_1 + 2d_2 - n - 2 = m$. Direct calculation of the characteristic polynomial of T gives

$$\begin{aligned}\phi(T,x) &= x^{m-2}(x^2-1)^{d_1+d_2-m-4}\{x^8 - (d_1+d_2+1)\,x^6 \\ &+ (d_1d_2+m+2)\,x^4 - (d_1q+d_2p+1)\,x^2 + pq\}\ .\end{aligned}$$

Then in order that the E-value of T reaches the maximum, p must be less or equal to q. T is depicted in (c) of Figure 1. ∎

Remark. By using the method of comparing the matching number we cannot determine which graph of (a) and (b) in theorem have greater energy. Maybe one should find other methods to solve this problem.

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