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On the extremal energies of trees with a given maximum degree*

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Abstract

The energy of a graph is defined as the sum of the absolute values of all eigenvalues of the graph. Let $\mathcal{T}_n$ denote the set of trees with n vertices. When $n \geq 6$, for a given integer $\Delta \in [3, n-2]$, we characterize the tree in $\mathcal{T}_n$ with maximum degree Δ and maximal energy. Furthermore, for $\lceil \frac{n+1}{3} \rceil \leq \Delta(T) \leq n-2$ and $n \geq 7$, the tree in $\mathcal{T}_n$ with maximum degree Δ and minimal energy is also determined.

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1. Introduction

In the present paper we consider graphs without loops and multiple edges. Let G be such a graph with n vertices. A k-matching of G is a set of k independent edges in G, $k = 1,2,\cdots,\lfloor n/2 \rfloor$. And $m(G,k)$ will denote the number of k-matchings of G. It is both consistent and convenient to define $m(G,0)=1$, and $m(G,k)=0$ for $k > \lfloor n/2 \rfloor$.

Let G be a graph with vertex set $\{v_1, v_2, \cdots, v_n\}$. Its adjacency matrix $A(G)=(a_{ij})$ is defined to be the $n \times n$ matrix (a_{ij}), where $a_{ij}=1$ if v_i is adjacent to v_j, and $a_{ij}=0$ otherwise. The characteristic polynomial of G is just $\phi(G)=\det(xI - A(G))$, where I denote the identity matrix of order n. The n roots of the equation $\phi(G)=0$, denoted by $\lambda_1, \lambda_2, \cdots, \lambda_n$, are called the eigenvalues of graph G.

In chemistry the (experimentally determined) heats of formation of conjugated hydrocarbons are closely related to the total π-electron energy. And the calculation of the total energy of all π-electrons in conjugated hydrocarbons can be reduced to (within the framework of HMO approximation [15]) that of

$$E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n| .$$

If the characteristic polynomial of the graph G is $\phi(G) = \sum_{i=0}^{n} a_i x^{n-i}$, then $E(G)$ can be expressed in terms of the Coulson integral [15] as

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} x^{-2} \ln[(\sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^j a_{2j} x^{2j})^2 + (\sum_{j=0}^{\lfloor n/2 \rfloor} (-1)^j a_{2j+1} x^{2j+1})^2] dx .$$

Furthermore it is well known [2] that if T is a tree with n vertices then

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

$$E(T) = \frac{2}{\pi} \int_{0}^{+\infty} x^{-2} \ln[\sum_{k=0}^{\lfloor n/2 \rfloor} m(T,k) x^{2k}] dx . \qquad (*)$$

It is easily seen that $E(T)$ is a strictly monotonously increasing function of all matching numbers $m(T,k), k = 0,1,\cdots,\lfloor \frac{n}{2} \rfloor$. Based on this fact Gutman [4] introduced a quasi-ordering relation "$\succeq$" (i.e. reflexive and transitive relation) on the set of all forests (acyclic graphs) with n vertices: if T_1 and T_2 are two forests with n vertices, then $T_1 \succeq T_2 \Leftrightarrow m(T_1,k) \geq m(T_2,k)$ for all $k = 0,1,\cdots,\lfloor n/2 \rfloor$. If $T_1 \succeq T_2$ and there exists j such that $m(T_1, j) > m(T_2, j)$, then we write $T_1 \succ T_2$. If $T_1 \succeq T_2$ ($T_1 \succ T_2$), we also write $T_2 \preceq T_1$ (resp. $T_2 \prec T_1$). Hence by (*) we have $T_1 \succeq T_2 \Rightarrow E(T_1) \geq E(T_2)$ and $T_1 \succ T_2 \Rightarrow E(T_1) > E(T_2)$.

This quasi-ordering has been successfully applied in the study of the extremal values of energy over a significant class of graphs (see [3, 4, 5, 6-15]). In [4] Gutman determined the tree in $\mathcal{T}_n$ with the maximal energy, namely, the path P_n. Furthermore, he obtained the following result.

Lemma 1.1 [4]. Let T be a tree in $\mathcal{T}_n \setminus \{X_n, Y_n, Z_n, W_n\}$. If $n \geq 5$, then $E(X_n) < E(Y_n) < E(Z_n) < E(W_n) \leq E(T)$.

In Lemma 1.1, X_n is the star $K_{1,n-1}$, Y_n is the graph obtained by attaching a pendant vertex to a pendant vertex of $K_{1,n-2}$, Z_n by attaching two pendant vertex to a pendant vertex of $K_{1,n-3}$, W_n by attaching a P_2 to a pendant vertex of $K_{1,n-3}$. Fig.1 shows the trees X_9, Y_9, Z_9 and W_9.

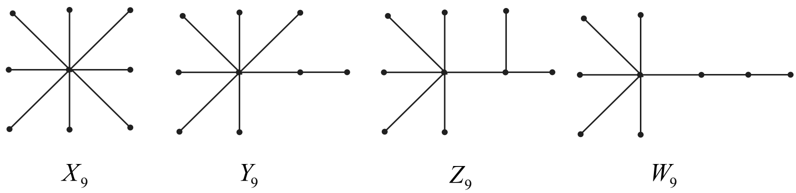

Fig 1. The trees X_9, Y_9, Z_9 and W_9.

In this paper we use the quasi-ordering to determine the trees with a given maximum degree and extremal energies. For a given integer $\Delta \in [3, n-2]$ and $n \geq 6$, the tree in $\mathcal{T}_n$ with maximum degree Δ and maximal energy is given. Furthermore, for $\lceil \frac{n+1}{3} \rceil \leq \Delta(T) \leq n-2$ and $n \geq 7$, the tree in $\mathcal{T}_n$ with maximum degree Δ and minimal energy is also determined.

2. Preliminaries

First we need the following notations.

The vertices of the path P_n will be labeled by $v_1, v_2, \cdots, v_n$ so that v_i and v_{i+1} are adjacent.

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.

Let u and v be two vertices of the graph G. Then $G(u,v)(a,b)$ denotes the graph obtained from G by attaching a pendant vertices to the vertex u and by attaching b additional pendant vertices to the vertex v.

Two vertices u and v of the graph G are called equivalent if the subgraphs $G-u$ and $G-v$ are isomorphic.

With the above notations, Gutman and Zhang [1] have shown the following results.

Lemma 2.1 [1]. If v is an arbitrary vertex of the graph G, then for $n = 4k+i$, $i \in \{-1, 0, 1, 2\}, k \geq 1$, $P_n(v_1, v)G \succ P_n(v_3, v)G \succ \cdots \succ P_n(v_{2k+1}, v)G$

$$\succ P_n(v_{2k}, v)G \succ P_n(v_{2k-2}, v)G \succ \cdots \succ P_n(v_2, v)G .$$

Lemma 2.2 [1]. If the vertices u and v of the graph G are equivalent, then

$G(u,v)(0,n) \prec G(u,v)(1,n-1) \prec \cdots \prec G(u,v)(\lfloor n/2 \rfloor, n-\lfloor n/2 \rfloor)$.

Definition 2.1. We call the transformation from $G_1 = P_n(v_r, v)G$ to $P_n(v_1, v)G$, where $r \geq 2$ and $n \geq 3$, the α_1-transformation of G_1.

Definition 2.2. 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.

Definition 2.3. 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 $G(u,v)(0,n)$ the β'-transformation of G_1, where $1 \leq a \leq b$, and u,v are equivalent in G.

By Lemmas 2.1 and 2.2, the following results are immediate.

Corollary 2.1. If G_0 can be obtained from G by one step of α_1- or α_3-transformation, then $G_0 \succ G$.

Corollary 2.2. If G_0 can be obtained from G by one step of β- or β'-transformation, then $G_0 \prec G$.

Definition 2.4. Let T be a tree in $\mathcal{T}_n$, 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 pendant vertex to the vertex u $(=v)$.

The procedures (1) and (2) are called [16] the edge-growing transformation of T (on edge $e = uv$), or e.g.t of T (on edge $e = uv$) for short.

Lemma 2.3. Let T be a tree in $\mathcal{T}_n$ 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 $T \succ T_0$ and $E(T) > E(T_0)$.

Proof. On one hand, each k-matching of T_0 corresponds a k-matching of T, $k=0,1,\cdots,\lfloor n/2\rfloor$, thus $m(T,k)\geq m(T_0,k)$ and $T\succeq T_0$. On the other hand, since $e=uv$ is a nonpendant edge of T, we can find a vertex adjacent to u (resp. v) in T_1 (resp. in T_2), say u_1 (resp. v_1). Then $\{u_1u, vv_1\}$ is a 2-matching of T, but not one of T_0, so $m(T,2)>m(T_0,2)$. Hence $T\succ T_0$, and $E(T)>E(T_0)$. □

Lemma 2.4 [1]. If $e=uv$ is an edge of G, then for all $k\geq 1$, $m(G,k)=m(G-u-v,k-1)+m(G-e,k)$.

The lemmas and corollaries above are often used to determine the quasi-order between two trees in the remainder of this paper.

In order to formulate our results, we need to define three trees: $S(n,m,r)$, where $n=2m+r+1\geq 5$, $m\geq 1$, $r\geq 0$, $m+r\geq 3$; $Y(n,m,r)$, where $n=2m+r+1$, $n\geq 8$, $m\geq 2$, $r\geq 3$; and $D(n,p,q)$ ($n\geq 4$, $p\geq q\geq 1$, $p+q=n-2$) as following: $S(n,m,r)$ is obtained from the star $K_{1,m+r}$ by attaching one pendant vertex to each of m pendant vertices of $K_{1,m+r}$. $Y(n,m,r)$ is obtained from the path P_{r+1} by attaching m P_2 to one end vertex of P_{r+1}. $D(n,p,q)$ is obtained from the star $K_{1,p+1}$ by attaching q pendant vertices to one pendant vertex of $K_{1,p+1}$. The three trees are shown in Fig.2.

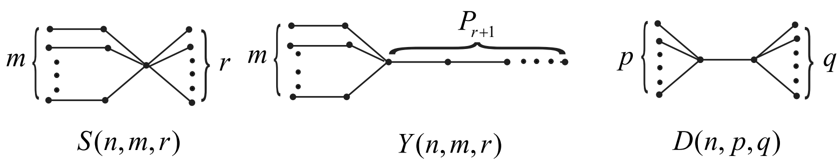

Fig.2. The trees $S(n,m,r)$, $Y(n,m,r)$ and $D(n,p,q)$.

For $S(n,m,r)$, Hou has shown the following result [17].

Lemma 2.5 [17]. Let T be a tree in $\mathcal{T}_n$ with m-matchings (i.e. $m(T,m)>0$).

Then $T \succeq S(n, m-1, n-2m+1)$ with the equality iff $T \cong S(n, m-1, n-2m+1)$.

Let $\overline{\mathcal{T}}_n^{\Delta} = \{T \in \mathcal{T}_n \,|\, T$ consists of Δ paths with a common end vertex$\}$, $\Delta = 3, 4, \cdots, n-1$. Then $S(n, n-\Delta-1, 2\Delta-n+1)$ and $Y(n, \Delta-1, n-2\Delta+1)$ are both in $\overline{\mathcal{T}}_n^{\Delta}$, and $P_n \notin \overline{\mathcal{T}}_n^{\Delta}$. Obviously, if $T \in \overline{\mathcal{T}}_n^{\Delta}$, then T has exact one vertex of degree more than 2. We call the vertex of degree $\Delta (> 2)$ the root of T, and call each of the Δ paths a pendant path of T (rooting at the root).

We also let $T^2_{r,s,t}$ and $T^3_{p,q,l,m}$ be the two trees shown in Fig. 3, where $r, s \geq 1$, $t \geq 0$ and $p, q \geq 0$, $l, m \geq 1$.

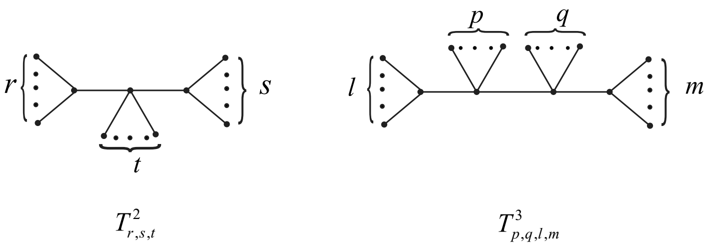

Fig 3. The trees $T^2_{r,s,t}$ and $T^3_{p,q,l,m}$.

3. Main results

We first determine the tree with a given maximum degree and maximal energy.

Theorem 3.1. Let T be a tree in $\mathcal{T}_n$ and $n \geq 4$. Then $T \preceq T_1^*(n, \Delta)$ and $E(T) \leq E(T_1^*(n, \Delta))$, with the equalities iff $T \cong T_1^*(n, \Delta)$, where $T_1^*(n, \Delta) = S(n, n-\Delta-1, 2\Delta-n+1)$ if $3 \leq \lfloor \frac{n}{2} \rfloor \leq \Delta(T) \leq n-2$, $T_1^*(n, \Delta) = Y(n, \Delta-1, n-2\Delta+1)$ if $3 \leq \Delta(T) < \lfloor \frac{n}{2} \rfloor$, and $T_1^*(n, \Delta) = P_n$ if $\Delta(T) = 2$.

Proof. If $\Delta(T) = 2$, then $T \cong P_n = T_1^*(n, \Delta)$, and the conclusion holds. So we suppose $\Delta(T) \geq 3$ hereafter. If $T \notin \overline{\mathcal{T}}_n^{\Delta}$, then T can be transformed into a tree

$T' \in \overline{\mathcal{T}}_n^{\Delta}$ by carrying out α_1 -transformation repeatedly. Thus $T \prec T'$ by Corollary 2.1. So it is sufficient to show that for any tree $\overline{T} \in \overline{\mathcal{T}}_n^{\Delta}$ and $\overline{T} \neq T_1^*(n,\Delta)$, $\overline{T} \prec T_1^*(n,\Delta)$.

We distinguish the following two cases.

Case 1. $\Delta(\overline{T}) = \Delta(T) \geq \lfloor n/2 \rfloor \geq 3$. Since $\overline{T} \neq T_1^*(n,\Delta) = S(n, n-\Delta-1, 2\Delta-n+1)$, then $\overline{T}$ has at least a pendant path with not less than 4 vertices. Moreover, there must exist at least a pendant path P_2 in $\overline{T}$. (Otherwise the number of vertices of $\overline{T}$ is $n \geq 2\Delta+2 \geq 2\lfloor n/2 \rfloor + 2 > n$, a contradiction.) So $\overline{T}$ can be transformed into $T_1^*(n,\Delta)$ by repeatedly carrying out α_3 -transformation, and $\overline{T} \prec T_1^*(n,\Delta)$ by Corollary 2.1.

Case 2. $\Delta(\overline{T}) = \Delta(T) < \lfloor n/2 \rfloor$. Since $\overline{T} \neq T_1^*(n,\Delta) = Y(n, \Delta-1, n-2\Delta+1)$, then either $\overline{T}$ has at least two different pendant paths with not less than 4 vertices, or $\overline{T}$ has at most one pendant paths with not less than 4 vertices and at least a pendant path P_2. If $\overline{T}$ is the former case, then $\overline{T}$ can be transformed into a tree $\overline{T}'$ with only one pendant path with not less than 4 vertices by carrying out α_3 -transformation repeatedly. Hence $\overline{T} \prec \overline{T}'$ by Corollary 2.1. If $\overline{T}' \cong T_1^*(n,\Delta) = Y(n, \Delta-1, n-2\Delta+1)$, then the result holds; otherwise, $\overline{T}'$ is the latter case. Thus it remains to show that $\overline{T}' \prec T_1^*(n,\Delta)$, where $\overline{T}'$ has at most one pendant path with not less than 4 vertices and at least a pendant path P_2. Then $\overline{T}'$ must have at least one pendant path with not less than 5 vertices. Otherwise, $\overline{T}'$ has at most one pendant path with 4 vertices and at least one pendant path P_2. Then, if n is odd, $n \leq 2\Delta+1 \leq 2\lfloor n/2 \rfloor < n$, a contradiction; if n is even, $n < 2\Delta+1 \leq 2\lfloor n/2 \rfloor = n$, again a contradiction. Thus $\overline{T}'$ can be transformed into a tree $\overline{T}''$ which has a pendant path with at least 4 vertices by a step of α_3 -transformation. If $\overline{T}''$ still contains a pendant path P_2, by the same reasoning, $\overline{T}''$ can be transformated into $T_1^*(n,\Delta) = Y(n,\Delta-1,n-2\Delta+1)$ by repeatedly carrying out α_3-transformations. Hence $\overline{T}' \prec T_1^*(n,\Delta)$ by Corollary 2.1.

The proof is thus completed. □

Noting that, for each Δ, $2 \le \Delta \le n-2$, $T_1^*(n,\Delta+1)$ can be transformed into $T_1^*(n,\Delta)$ by exact one step of α_1-transformation, we have $T_1^*(n,\Delta+1) \prec T_1^*(n,\Delta)$ by Corollary 2.1, and the next result follows from Theorem 3.1 immediately.

Corollary 3.1. Let T be a tree in $\mathcal{T}_n$ and $n \ge 5$. If $\Delta(T) \ge l \ge 3$, then $T \preceq T_1^*(n,l)$, with the equality iff $T \cong T_1^*(n,l)$.

Furthermore we can obtain the following interesting result.

Corollary 3.2. Let T_1 and T_2 be two trees in $\mathcal{T}_n$, and $n \ge 4$. If T_1 has m-matchings and $\Delta(T_2) \ge n-m$, then $T_1 \succeq T_2$, with the equality iff $T_1 \cong T_2 \cong S(n,m-1,n-2m+1)$.

Proof. Immediate from Lemma 2.5 and Corollary 3.1. □

Now we consider the tree with a given maximum degree and minimal energy.

Theorem 3.2. Let T be a tree in $\mathcal{T}_n$, and $n \ge 7$. If $\lceil \frac{n+1}{3} \rceil \le \Delta(T) \le n-2$, then $T \succeq T_2^*(n,\Delta)$ and $E(T) \ge E(T_2^*(n,\Delta))$, with the equalities iff $T \cong T_2^*(n,\Delta)$, where $T_2^*(n,\Delta) = D(n,\Delta-1,n-\Delta-1)$ if $\lceil \frac{n}{2} \rceil \le \Delta(T) \le n-2$, and $T_2^*(n,\Delta) = T^2_{\Delta-1,\Delta-1,n-2\Delta-1}$ if $\lceil \frac{n+1}{3} \rceil \le \Delta(T) \le \lceil \frac{n}{2} \rceil - 1$.

It is easy to see that, if $3 \le \lceil \frac{n}{2} \rceil \le \Delta \le n-2$, T can be transformed into $T_2^*(n,\Delta)$ by carrying out e.g.t and β-transformation repeatedly, so $T \succeq T_2^*(n,\Delta)$ with the equality iff $T \cong T_2^*(n,\Delta)$ by Lemma 2.3 and Corollary 2.2. However, in order to prove the conclusion of Theorem 3.2 for $\lceil \frac{n+1}{3} \rceil \le \Delta(T) \le \lceil \frac{n}{2} \rceil - 1$, we need more preparations.

Lemma 3.1. Let T be a tree in $\mathcal{T}_n$ with maximum degree Δ, where $\lceil \frac{n+1}{3} \rceil \le \Delta(T) \le \lceil \frac{n}{2} \rceil - 1$, and $n \ge 7$. If $T = T^2_{r,s,t}$ or $T = T^3_{p,q,l,m}$, then $T \succeq T^*_2(n,\Delta) = T^2_{\Delta-1,\Delta-1,n-2\Delta-1}$, with the equality iff $T \cong T^*_2(n,\Delta)$.

Proof. We prove the result by the following three cases.

Case 1. $T = T^2_{r,s,t}$. Then either $r = \Delta - 1$ and $s \le \Delta - 1$, $t \le \Delta - 2$, or $t = \Delta - 2$ and $s, r \le \Delta - 1$.

Subcase 1.1. $r = \Delta - 1$. Then $s + t = n - \Delta - 2$. By repeatedly applying Lemma 2.4 $\Delta - 1$ times, we have, for all $k \ge 1$,

$m(T,k) = (\Delta-1) \times m(D(n-\Delta, t, s), k-1) + m(D(n-\Delta+1, t+1, s), k)$, and

$m(T^*_2(n,\Delta), k) = (\Delta-1) \times m(D(n-\Delta, \Delta-1, n-2\Delta-1), k-1) + m(D(n-\Delta+1, \Delta-1, n-2\Delta), k)$.

Moreover by Lemma 2.2, $D(n-\Delta, t, s) \succeq D(n-\Delta, \Delta-1, n-2\Delta-1)$ and $D(n-\Delta+1, t+1, s) \succeq D(n-\Delta+1, \Delta-1, n-2\Delta)$, so $m(T,k) \ge m(T^*_2(n,\Delta), k)$, for all $k \ge 1$. Hence $T \succeq T^*_2(n,\Delta)$, with the equality iff $T \cong T^*_2(n,\Delta)$.

Subcase 1.2. $t = \Delta - 2$. Obviously, $r + s \ge \Delta$. Thus T can be transformed into $T^2_{\Delta-1,n-2\Delta,\Delta-2}$ by β-transformation, and by Corollary 2.2 and Subcase 1.1, $T \succeq T^2_{\Delta-1,n-2\Delta,\Delta-2} \succeq T^*_2(n,\Delta)$, with the equality iff $T \cong T^2_{\Delta-1,n-2\Delta,\Delta-2} \cong T^*_2(n,\Delta)$.

Case 2. $T = T^3_{p,q,l,m}$. Then either $l = \Delta - 1$, $p, q \le \Delta - 2$ and $m \le \Delta - 1$, or $p = \Delta - 2$, $q \le \Delta - 2$ and $l, m \le \Delta - 1$.

Subcase 2.1. $l = \Delta - 1$. By repeatedly applying Lemma 2.4 $\Delta - 1$ times, we have, for all $k \ge 1$, $m(T,k) = (\Delta-1) \times m(T^2_{p,m,q}, k-1) + m(T^2_{p+1,m,q}, k)$ and

$m(T^*_2(n,\Delta), k) = (\Delta-1) \times m(D(n-\Delta, \Delta-1, n-2\Delta-1), k-1) + m(D(n-\Delta+1, \Delta-1, n-2\Delta), k)$.

If $p + m \ge \Delta - 1$, and without loss of generality assuming $p \ge m$, then $T^2_{p,m,q}$ can be transformed into $D(n-\Delta, \Delta-1, n-2\Delta-1)$ by exact $(\Delta-1) - p = \Delta - p - 1$ steps of β-transformation, and followed one step of e.g.t if $p+m \geq \Delta$. So by Corollary 2.2 and 2.3**,** $T^2_{p,m,q} \succeq D(n-\Delta,\Delta-1,n-2\Delta-1)$. Otherwise $p+m<\Delta-1$, then $T^2_{p,m,q}$ can be transformed into $D(n-\Delta, p+m, q+1)$ by one step of β' -transformation, so $T^2_{p,m,q} \succeq D(n-\Delta, p+m, q+1) \succeq D(n-\Delta,\Delta-1,n-2\Delta-1)$ by Corollary 2.2 and Lemma 2.2. Similarly, $T^2_{p+1,m,q} \succ D(n-\Delta+1,\Delta-1,n-2\Delta)$. Therefore $m(T,k) \geq m(T_2^*(n,\Delta),k)$, and $T \succ T_2^*(n,\Delta)$.

Subcase 2.2. $p=\Delta-2$. We will show that $T=T^3_{\Delta-2,q,l,m} \succeq T'=T^3_{l-1,q,\Delta-1,m}$, then the case is deduced to Subcase 2.1. It is easy to see that for $k \geq 1$, $m(T,k)=m\times m(T^2_{l,q,\Delta-2},k-1)+m(T^2_{l,q+1,\Delta-2},k)$, and $m(T',k)=m\times m(T^2_{\Delta-1,q,l-1},k-1)+m(T^2_{\Delta-1,q+1,l-1},k)$. Similarly, we have, for all $k \geq 2$, $m(T^2_{l,q,\Delta-2},k-1)=q\times m(D(l+\Delta,l,\Delta-2),k-2)+m(D(l+\Delta+1,l,\Delta-1),k-1)$ and $m(T^2_{\Delta-1,q,l-1},k-1)=q\times m(D(l+\Delta,l-1,\Delta-1),k-2)+m(D(l+\Delta+1,l,\Delta-1),k-1)$. Noting that $l \leq \Delta-1$, for $k \geq 2$, we have $m(D(l+\Delta,l,\Delta-2),k-2) \geq m(D(l+\Delta,l-1,\Delta-1),k-2)$, so $m(T^2_{l,q,\Delta-2},k) \geq m(T^2_{l-1,\Delta-1,q},k)$. Similarly $m(T^2_{\Delta-2,l,q+1},k-1) \geq m(T^2_{l-1,\Delta-1,q+1},k-1)$ for all $k \geq 2$. Therefore $m(T,k) \geq m(T',k)$ for all $k \geq 2$, and $T \succeq T'$.

The proof is thus completed. □

Let $\varepsilon(G)$ denote the number of edges of the graph G. Let $K_{1,\Delta}$ be a star, and $v_1,v_2,\cdots,v_\Delta$ its vertices of degree 1. Let H_i be a tree with maximum degree at most Δ, and u_i a vertex of H_i, $i=1,2,\cdots,\Delta$, with degree at most $\Delta-1$. Then $T(n,\Delta;H_1,H_2,\cdots,H_\Delta)$ will denote the tree $K_{1,\Delta}(v_1,u_1)H_1(v_2,u_2)H_2\cdots(v_\Delta,u_\Delta)H_\Delta$. Let $\varepsilon_i=\varepsilon(H_i)$, $i=1,2,\cdots,\Delta$. Without loss of generality we assume that $\varepsilon_1 \geq \varepsilon_2 \geq \cdots \geq \varepsilon_\Delta$. When $\varepsilon_i=0$, H_i is an isolated vertex u_i, which will be denoted by K_1. If H_i is a star K_{1,ε_i} with the center u_i, then we write H_i as C_{ε_i}. (A center of a star is the vertex of the star with maximum degree.)

Obviously $T(n,\Delta;H_1,H_2,\cdots,H_\Delta)$ has maximum degree Δ, while every tree in

$\mathcal{T}_n$ with maximum degree Δ has the form $T(n,\Delta;H_1,H_2,\cdots,H_\Delta)$.

Lemma 3.2. Let $T=T(n,\Delta;H_1,H_2,\cdots,H_\Delta)$ with $\varepsilon_3>0$ and $\lceil\frac{n+1}{3}\rceil\le\Delta(T)\le\lceil\frac{n-2}{2}\rceil$. Then there exists a tree $T'=T(n,\Delta;H_1',C_t,K_1,\cdots,K_1)$, where $\varepsilon(H_1')\ge\Delta-1$, $t=n-\Delta-\varepsilon(H_1')-1\le\Delta-1$, such that $T\succ T'$.

Proof. If $\varepsilon_1\le\Delta-1$, then $\varepsilon_i\le\Delta-1$, $i=2,3,\cdots,\Delta$. Thus T can be transformed into $T'=T(n,\Delta;C_{\Delta-1},C_{n-2\Delta},K_1,\cdots,K_1)$ by a number of e.g.t and β-transformations, so the conclusion holds from Corollary 2.2 and Lemma 2.3. If $\varepsilon_1\ge\Delta$, then $t=\sum_{i=2}^{\Delta}\varepsilon_i\le\Delta-1$. (Otherwise $\varepsilon(T)=n-1\ge3\Delta\ge3\lceil\frac{n+1}{3}\rceil>n$, a contradiction.) Thus T can be transformed into $T'=T(n,\Delta;H_1,C_t,K_1,\cdots,K_1)$ by a number of e.g.t and β-transformations, and so $T\succ T'$. □

Now we give the proof of Theorem 3.2.

Proof of Theorem 3.2. We have mentioned that the conclusion holds if $\lceil\frac{n-2}{2}\rceil+1\le\Delta\le n-2$. Now we only deal with the case when $\lceil\frac{n+1}{3}\rceil\le\Delta(T)\le\lceil\frac{n}{2}\rceil-1$ here. By Lemma 3.2, it suffices to show the following statement: for each tree $T=T(n,\Delta;H_1,C_t,K_1,\cdots,K_1)$ with $\varepsilon_1=\varepsilon(H_1)\ge\Delta-1$ and $t=n-\Delta-\varepsilon_1-1\le\Delta-1$, $T\succeq T_2^*(n,\Delta)=T^2_{\Delta-1,\Delta-1,n-2\Delta-1}$, with the equality iff $T\cong T_2^*(n,\Delta)$.

If $\varepsilon_1=\Delta-1$, then T can be transformed into $T_1=T_{\Delta-1,t,\Delta-2}$ by e.g.t, and the conclusion holds from Lemma 2.3 and 3.1.

Hence assume $\varepsilon_1\ge\Delta$. Then we can find an edge $e=wu_1$ in H_1 such that the degree of w is more than 1 in H_1. Let L_1 and L_2 be the two components of H_1-e such that w is in L_1 (L_2 may be K_1). We complete the proof by induction on $\tau(T)$, the number of nonpendant edges of T. When $\tau=2$, $T=T^2_{r,s,t}$ for some r, s and t with $\Delta(T)=\Delta$, so the result holds from Lemma 3.1. Assume that the statement is true when $\tau=l-1$. Now let

$T = T(n,\Delta; H_1, C_t, K_1, \cdots, K_1)$ be a tree with $\tau(T) = l$. We distinguish the following two cases.

Case 1. $t > 0$, i.e. $C_t \neq K_1$.

Subcase 1.1. $\varepsilon(L_1) \leq \Delta - 1$ and $\varepsilon(L_2) \leq \Delta - 2$. Thus by e.g.t T can be transformed into $T^3_{\Delta-2,\varepsilon(L_2),t,\varepsilon(L_1)}$, so the statement is true by Lemma 3.1.

Subcase 1.2. $\varepsilon(L_1) \geq \Delta$. Thus $\varepsilon(L_2) + t \leq \Delta - 2$. By e.g.t, T can be transformed into $\hat{T}$ so that L_2 becomes $K_{1,\varepsilon(L_2)}$ with the center u_1. Then $T \succeq \hat{T}$ by Lemma 2.3. Let T_1 be the tree obtained from $\hat{T}$ by moving all the t pendant edges at vertex u_2 to u_1. By induction hypothesis $T_1 \succeq T_2^*(n,\Delta)$, with the equality iff $T_1 \cong T_2^*(n,\Delta)$, so it remains to show that $\hat{T} \succeq T_1$. Let $m'(L_1,i)$ denote the number of i-matchings of L_1 in which at least one edge is incident with the vertex w, and $m''(L_1, j)$ the number of j-matchings of L_1 which consist of edges not incident with the vertex w. Let $T' = T^2_{\varepsilon(L_2),t,\Delta-2}$ and $T'' = T^2_{\varepsilon(L_2)+1,t,\Delta-2}$. Then for all $k \geq 0$,

$$m(\hat{T},k) = \sum_{i=1}^{k} m'(L_1,i) \times m(T',k-i) + \sum_{j=0}^{k} m''(L_1, j) \times m(T'',k-j).$$

Similarly, $D' = D(\Delta + \varepsilon(L_2) + t + 3, \Delta + 1, \varepsilon(L_2) + t)$ and $D'' = D(\Delta + \varepsilon(L_2) + t + 4, \Delta + 1, \varepsilon(L_2) + t + 1))$.

$$m(T_1,k) = \sum_{i=0}^{k} m'(L_1,i) \times m(D',k-i) + \sum_{j=0}^{k} m''(L_1, j) \times m(D'',k-j).$$

Moreover by Lemma 2.2, $T' \succeq D'$ and $T'' \succ D''$, so $m(\hat{T},k) \geq m(T_1,k)$ for all $k \geq 0$. Hence $T \succeq \hat{T} \succ T_1 \succeq T_2^*(n,\Delta)$.

Subcase 1.3. $\varepsilon(L_2) \geq \Delta - 1$. Thus $\varepsilon(L_1) + t \leq \Delta - 1$. By e.g.t, T can be transformed into $\hat{T}$ so that L_1 becomes $K_{1,\varepsilon(L_1)}$ with the center w. Let T_1 be the tree obtained from $\hat{T}$ by moving all the $\varepsilon(L_1)$ at vertex w to u_2. Similar to Subcase 1.2, we have $T \succ T_1$, and the statement holds.

Case 2. $t = 0$, i.e. $C_t = K_1$.

Subcase 2.1. $\varepsilon(L_1)\le\Delta-1$ and $\varepsilon(L_2)\le\Delta-2$. Thus by e.g.t T can be transformed into $T^2_{\Delta-1,\varepsilon(L_1),\varepsilon(L_2)}$, and the statement holds by Lemma 3.1.

Subcase 2.2. $\varepsilon(L_1)\ge\Delta$. Thus $\varepsilon_2\le\Delta-2$. By e.g.t, T can be transformed into $\hat{T}$ so that L_2 becomes $K_{1,\varepsilon(L_2)}$ with the center u_1. Let $e'=yw$ be a nonpendant edge with an end vertex y in L_1. Let I_1 and I_2 be the two components of L_1-e' such that y is in I_1 (I_2 may be K_1).

Subsubcase 2.2.1. $\varepsilon(I_1)\le\Delta-1$ and $\varepsilon(I_2)\le\Delta-2$. Thus by e.g.t $\hat{T}$ can be transformed into $T^3_{\varepsilon(L_2),\varepsilon(I_2),\Delta-1,\varepsilon(I_1)}$, and the statement holds by Lemma 3.1.

Subsubcase 2.2.2. $\varepsilon(I_1)\ge\Delta$. Thus $\varepsilon(I_2)+\varepsilon(L_2)+1\le\Delta-2$. Let T_1 be the tree obtained from $\hat{T}$ by e.g.t on edge $e=wu_1$ and nonpendant edges in L_2. Then $T\succ T_1\succeq T_2^*(n,\Delta)$ by Lemma 2.3 and induction hypothesis.

Subsubcase 2.2.3. $\varepsilon(I_2)\ge\Delta-1$. Thus $\varepsilon(I_1)+\varepsilon(L_2)+1\le\Delta-2$. Let T_1 be the tree obtained from $\hat{T}$ by e.g.t on nonpendant edges in I_1 and then moving all the $\varepsilon(I_1)$ pendant edges at vertex y to u_1. Similar to Subcase 1.2, we have $\hat{T}\succ T_1$, and the conclusion holds.

Subcase 2.3. $\varepsilon(L_2)\ge\Delta-1$. Then $\varepsilon(L_1)\le\Delta-2$. By e.g.t, T can be transformed into $\hat{T}$ so that L_1 becomes $K_{1,\varepsilon(L_1)}$ with the center w. Let $e''=zu_1$ be a nonpendant edge with an end vertex u_1 in H_1. Let N_1 and N_2 be the two components of L_2-e'' such that z is in N_1 (N_2 may be K_1).

Subsubcase 2.3.1. $\varepsilon(N_1)\le\Delta-1$ and $\varepsilon(N_2)\le\Delta-3$. By e.g.t, $\hat{T}$ can be transformed into T_1 so that N_1 becomes $K_{1,\varepsilon(N_1)}$ with the center z and N_2 becomes $K_{1,\varepsilon(N_2)}$ with the center u_1. If $s=\varepsilon(L_1)+\varepsilon(N_1)\le\Delta-1$, then by Lemma 2.2 and Lemma 3.1 we have $T\succeq\hat{T}\succ T_1\succ T_{\Delta-1,s,\varepsilon(N_2)+1}\succeq T_2^*(n,\Delta)$. Otherwise $s\ge\Delta$. Then T_1 can be transformed into $T_2^*(n,\Delta)=T^2_{\Delta-1,\Delta-1,n-2\Delta-1}$ by exact $\Delta-1-\varepsilon(L_1)$

steps of β-transformation and followed a step of e.g.t. on edge $e''=zu_1$. Hence by Corollary 2.2, Lemma 2.3 and Lemma 3.1, $T \succ T_2^*(n,\Delta)$.

Subsubcase 2.3.2. $\varepsilon(N_1)\geq\Delta$. Thus $\varepsilon(L_1)+\varepsilon(N_2)\leq\Delta-3$. Let T_1 be the tree obtained from $\hat{T}$ by repeatedly carrying out e.g.t so that N_2 becomes $K_{1,\varepsilon(N_2)}$ with the center u_1, and followed a step of e.g.t on edge $e=wu_1$. Hence $T \succeq \hat{T} \succ T_1 \succeq T_2^*(n,\Delta)$ by Lemma 2.3 and induction hypothesis.

Subsubcase 2.3.3. $\varepsilon(N_2)\geq\Delta-2$. Thus $\varepsilon(L_1)+\varepsilon(N_1)\leq\Delta-1$. Let T_1 be the tree obtained from $\hat{T}$ by repeatedly carrying e.g.t such that N_1 becomes $K_{1,\varepsilon(N_1)}$ with the center z, and then moving all the $\varepsilon(N_1)$ pendant edges at vertex z to w (i.e. a step of β'-transformation). Then $T \succeq \hat{T} \succ T_1 \succeq T_2^*(n,\Delta)$ by Corollary 2.2, Lemma 2.3 and induction hypothesis.

The proof is completed. □

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