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DISTANCE SPECTRAL RADIUS OF TREES WITH FIXED MAXIMUM DEGREE*

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Abstract. Distance energy is a newly introduced molecular graph-based analog of the total π-electron energy, and it is defined as the sum of the absolute eigenvalues of the molecular distance matrix. For trees and unicyclic graphs, distance energy is equal to the doubled value of the distance spectral radius. In this paper, we introduce a general transformation that increases the distance spectral radius and provide an alternative proof that the path P_n has the maximal distance spectral radius among trees on n vertices. Among the trees with a fixed maximum degree Δ, we prove that the broom $B_{n,\Delta}$ (consisting of a star $S_{\Delta+1}$ and a path of length $n-\Delta-1$ attached to an arbitrary pendent vertex of the star) is the unique tree that maximizes the distance spectral radius, and conjecture the structure of a tree which minimizes the distance spectral radius. As a first step towards this conjecture, we characterize the starlike trees with the minimum distance spectral radius.

Key words. Distance matrix, Distance spectral radius, Broom graph, Maximum degree.

AMS subject classifications. 05C05, 05C12.

1. Introduction. Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices. For vertices $u, v \in V$, the distance d_{uv} is defined as the length of the shortest path between u and v in G. The distance matrix $D = (d_{uv})_{u,v \in V}$ is a symmetric real matrix, with real eigenvalues [7]. The *distance spectral radius* $\varrho(G) = \varrho_G$ of G is the largest eigenvalue of the distance matrix D of a graph G.

Distance energy $DE(G)$ is a newly introduced molecular graph-based analog of the total π-electron energy, and it is defined as the sum of the absolute eigenvalues of the molecular distance matrix. For trees and unicyclic graphs, distance energy is equal to the doubled value of the distance spectral radius. For more details on distance matrices and distance energy, see [6, 11, 15, 16, 19, 23].

Let T be a tree with $n > 2$ vertices, and let $\Lambda_1 \geq \Lambda_2 \geq \cdots \geq \Lambda_n$ be the eigenvalues of $D = D(T)$ arranged in a non-increasing order. Merris in [18] obtained

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an interlacing inequality involving the distance and Laplacian eigenvalues of T,

$$0 > -\frac{2}{\mu_1} \geq \Lambda_2 \geq -\frac{2}{\mu_2} \geq \Lambda_3 \geq \cdots \geq -\frac{2}{\mu_{n-1}} \geq \Lambda_n,$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the Laplacian eigenvalues of T.

Let $e = (u, v)$ be an edge of G such that $G' = G - e$ is also connected, and let D' be the distance matrix of $G - e$. The removal of e may not create shorter paths than the ones in G, and therefore, $D_{ij} \leq D'_{ij}$ for all $i, j \in V$. Moreover, $1 = D_{uv} < D'_{uv}$ and by the Perron-Frobenius theorem, we conclude that

$$\varrho_G < \varrho_{G-e}. \tag{1.1}$$

In particular, for any spanning tree T of G, we have that

$$\varrho_G \leq \varrho_T. \tag{1.2}$$

Similarly, adding a new edge $f = (s, t)$ to G does not increase distances, while it does decrease at least one distance; the distance between s and t is one in $G + f$ and at least two in G. Again by the Perron-Frobenius theorem,

$$\varrho_{G+f} < \varrho_G. \tag{1.3}$$

The inequality (1.3) tells us immediately that the complete graph K_n has the minimum distance spectral radius among the connected graphs on n vertices, while the inequality (1.2) shows that the maximum distance spectral radius will be attained for a particular tree. Therefore, we focus our attention to trees in the rest of this paper.

Balaban et al. [1] proposed the use of ϱ_G as a molecular descriptor, while in [13], it was successfully used to infer the extent of branching and model boiling points of alkanes. Recently, in [25, 26], the authors provided the upper and lower bounds for $\varrho(G)$ in terms of the number of vertices, Wiener index and Zagreb index. Balasubramanian in [2, 3] pointed out that the spectra of the distance matrices of many graphs such as the polyacenes, honeycomb and square lattice have exactly one positive eigenvalue, and he computed the spectrum of fullerenes C_{60} and C_{70}. Bapat in [4, 5] showed various connections between the distance matrix $D(G)$ and Laplacian matrix $L(G)$ of a graph, and calculated the determinant and inverses of weighted trees and unicyclic graphs.

If the maximal degree of a graph is less than or equal to 4, graph G is called a chemical graph. The broom $B_{n,\Delta}$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n - \Delta - 1$ attached to an arbitrary pendent vertex of the star. It is proven in [17] that among trees with the maximum vertex degree equal to Δ, the broom $B_{n,\Delta}$

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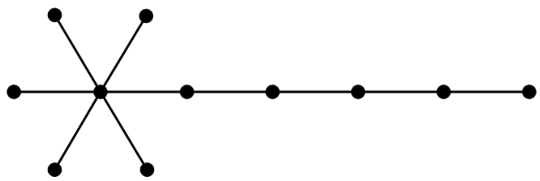

FIG. 1.1. *The broom tree $B_{n,\Delta}$ for $n = 11$ and $\Delta = 6$.*

uniquely minimizes the largest eigenvalue of the adjacency matrix. Further, within the same class of trees, the broom has the minimum Wiener index and Laplacian-energy like invariant [21]. In [24], it was demonstrated that the broom has minimum energy among trees with the fixed diameter.

Subhi and Powers in [22] proved that for $n \geq 3$, the path P_n has the maximum distance spectral radius among trees on n vertices. Here, we extend the result by introducing a transformation that strictly increases the distance spectral radius of a tree and present an alternative proof of this fact. In addition, we prove that among trees with a fixed maximum degree Δ, the broom graph $B_{n,\Delta}$ has the maximal distance spectral radius. As a corollary, we determine the unique tree with the second maximal distance spectral radius. We conclude the paper by posing a conjecture on the structure of the extremal tree that minimizes the distance spectral radius.

2. The star S_n has minimum distance spectral radius. The distance matrix of S_n has the form

$$D_{S_n} = \begin{bmatrix} 0 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & 2 & \cdots & 2 & 2 \\ 1 & 2 & 0 & \cdots & 2 & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 2 & 2 & \cdots & 0 & 2 \\ 1 & 2 & 2 & \cdots & 2 & 0 \end{bmatrix}.$$

Let x be an eigenvector of D_{S_n} corresponding to the spectral radius ϱ_{S_n}. Let a be the component of x at the center of S_n. Since ϱ_{S_n} is a simple eigenvalue of D_{S_n} by the Perron-Frobenius theorem, and all leaves are similar to each other, we may denote by b the component of x at each leaf of S_n. The eigenvalue equation $D_{S_n}x = \varrho_{S_n}x$ gives the system

$$\begin{aligned} (n-1)b &= \varrho_{S_n} a, \\ a + 2(n-2)b &= \varrho_{S_n} b, \end{aligned}$$

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which, after eliminating a and b, yields a quadratic equation in ϱ_{S_n}, whose positive solution is

$$\varrho_{S_n} = n - 2 + \sqrt{(n-2)^2 + (n-1)}.$$

The Wiener index of G is the sum of distances between all pairs of vertices,

$$W(G) = \sum_{u,v \in V} d(u,v).$$

The Wiener index is considered as one of the most useful topological indices having a high correlation with many physical and chemical properties of molecular compounds. The huge majority of chemical applications of the Wiener index deal with acyclic organic molecules. For recent results and applications of the Wiener index, see [8].

Theorem 2.1 ([14]). *Let G be a connected graph with $n > 2$ vertices. Then*

$$\varrho_G \geq \frac{2W(G)}{n}, \tag{2.1}$$

with equality if and only if the row sums of D are all equal.

For trees on $n \geq 3$ vertices, the strict inequality in (2.1) holds. Now, let $T \ncong S_n$ be an arbitrary tree on n vertices, with the distance matrix D.

According to [9], among the trees on $n \geq 4$ vertices, the star S_n has the smallest Wiener index, equal to $(n-1)^2$, and the next smallest Wiener index, equal to $n^2 - n - 2$, is attained by the star S_{n-1} with a pendent edge attached to one of its leaves. Thus,

$$\varrho_T \geq \frac{2}{n}(n^2 - n - 2) > n - 2 + \sqrt{(n-2)^2 + (n-1)} = \varrho_{S_n},$$

for $n \geq 4$.

3. The path P_n has the maximum distance spectral radius. Let G be a simple graph and v one of its vertices. For $k, l \geq 0$, we denote by $G(v,k)$ the graph obtained from $G \cup P_k$ by adding an edge between v and the end vertex of P_k (see Figure 3.1), and by $G(v,k,l)$ the graph obtained from $G \cup P_k \cup P_l$ by adding edges between v and one of the end vertices in both P_k and P_l (see Figure 3.2). The main ingredient of our proof will be the lemma that for $k \geq l \geq 1$,

$$\varrho_{G(v,k+1,l-1)} > \varrho_{G(v,k,l)}.$$

In order to prove this lemma, we first need an auxiliary result on the components of the principal eigenvector along P_k in $G(v,k)$.

Lemma 3.1. *Let x be a positive eigenvector of $G(v,k)$, $k \geq 1$, corresponding to $\varrho = \varrho_{G(v,k)}$. Denote by x_0 the component of x at v, and by $x_1, x_2, \ldots, x_k$ the*

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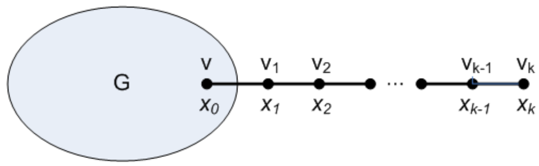

FIG. 3.1. *Principal eigenvector components in $G(v,k)$.*

components of x along P_k, starting with the vertex of P_k adjacent to v (see Figure 3.1). If s denotes the sum of components of x, then there exist constants $a_k = a(\varrho, s, x_0, k)$ and $b_k = b(\varrho, s, x_0, k)$ such that

$$x_i = a_k t_1^i + b_k t_2^i, \qquad 0 \le i \le k,$$

where $t_{1,2} = 1 + \frac{1}{\varrho} \pm \frac{\sqrt{2\varrho+1}}{\varrho}$.

Proof. Let D be the distance matrix of $G(v,k)$. From the eigenvalue equation $\varrho x = Dx$, written for components x_{j-1}, x_j and x_{j+1}, for $1 \le j \le k-1$,

$$\varrho x_{j-1} = x_j + 2x_{j+1} + \sum_{u \in G} (d_{uv} + j - 1)x_u + \sum_{i=0}^{j-2} (j-1-i)x_i + \sum_{i=j+2}^{k} (i-j+1)x_i,$$

$$\varrho x_j = x_{j-1} + x_{j+1} + \sum_{u \in G} (d_{uv} + j)x_u + \sum_{i=0}^{j-2} (j-i)x_i + \sum_{i=j+2}^{k} (i-j)x_i,$$

$$\varrho x_{j+1} = 2x_{j-1} + x_j + \sum_{u \in G} (d_{uv} + j + 1)x_u + \sum_{i=0}^{j-2} (j+1-i)x_i + \sum_{i=j+2}^{k} (i-j-1)x_i,$$

we obtain the recurrence equation

$$2\varrho x_j + 2x_j = \varrho x_{j-1} + \varrho x_{j+1}, \tag{3.1}$$

whose characteristic equation has roots

$$t_{1,2} = 1 + \frac{1}{\varrho} \pm \frac{\sqrt{2\varrho+1}}{\varrho}, \qquad 0 < t_2 < 1 < t_1.$$

On the other hand, the eigenvalue equation $\varrho x = Dx$ written for components x_{k-1} and x_k,

$$\varrho x_{k-1} = x_k + \sum_{u \in G} (d_{uv} + k - 1)x_u + \sum_{i=0}^{k-2} (k-1-i)x_i,$$

$$\varrho x_k = x_{k-1} + \sum_{u \in G} (d_{uv} + k)x_u + \sum_{i=0}^{k-2} (k-i)x_i,$$

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yields

$$\varrho x_k - \varrho x_{k-1} = s - 2x_k. \tag{3.2}$$

We may use the recurrence equation (3.1) to formally extend the sequence $x_0, x_1, \ldots, x_k$ with new terms $x_{k+1}, x_{k+2}, \ldots$, so that it represents a particular solution of (3.1). In such case, the equation in (3.2) may be rewritten as

$$\varrho x_{k+1} = s + \varrho x_k. \tag{3.3}$$

From the theory of linear recurrence equations, there exist constants a_k and b_k such that for $i \geq 0$ it holds

$$x_i = a_k t_1^i + b_k t_2^i.$$

The values of a_k and b_k may be obtained from the boundary conditions, i.e., the value of x_0 and the equation (3.3),

$$x_0 = a_k + b_k, \tag{3.4}$$

$$s/\varrho = a_k t_1^k (t_1 - 1) + b_k t_2^k (t_2 - 1). \tag{3.5}$$

Having in mind that $t_2 = \frac{1}{t_1}$, the equation (3.5) is further equivalent to

$$a_k - \frac{b_k}{t_1^{2k+1}} = \frac{s/\varrho}{(t_1 - 1)t_1^k}. \tag{3.6}$$

From (3.4) and (3.6) we finally get:

$$a_k = \frac{1}{1 + t_1^{2k+1}} \left(x_0 + \frac{s}{\varrho} \frac{t_1^{k+1}}{t_1 - 1} \right), \tag{3.7}$$

$$b_k = \frac{1}{1 + t_1^{2k+1}} \left(x_0 t_1^{2k+1} - \frac{s}{\varrho} \frac{t_1^{k+1}}{t_1 - 1} \right). \quad \square \tag{3.8}$$

The previous lemma allows us to compare the sum of components of the principal eigenvector along two pendent paths attached to the same vertex.

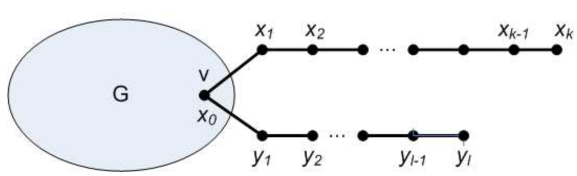

FIG. 3.2. *Principal eigenvector components in $G(v, k, l)$.*

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Lemma 3.2. *Let x be a positive eigenvector of $G(v,k,l)$, $k,l \geq 1$, corresponding to $\varrho = \varrho_{G(v,k,l)}$. Denote by x_0 the component of x at v, by $x_1, \dots, x_k$ the components of x along P_k, starting with the vertex of P_k adjacent to v, and by $y_1, \dots, y_l$ the components of x along P_l, starting with the vertex of P_l adjacent to v (see Figure 3.2). If $k \geq l$, then*

$$\sum_{i=0}^{k} x_i \geq \sum_{j=0}^{l} y_j.$$

Proof. Let s denote the sum of components of x, and let $t = 1 + \frac{1}{\varrho} + \frac{\sqrt{2\varrho+1}}{\varrho}$. From Lemma 3.1 we get

$$\begin{aligned} x_i &= a_k t^i + b_k / t^i, \qquad 1 \leq i \leq k, \\ y_j &= a_l t^i + b_l / t^i, \qquad 1 \leq j \leq l, \end{aligned}$$

where a_k, b_k, a_l and b_l are given by (3.7) and (3.8). Now, we have

$$\begin{aligned} \sum_{i=1}^{k} x_k &= \sum_{i=1}^{k} a_k t^i + b_k / t^i \\ &= a_k \frac{t(t^k - 1)}{t-1} + b_k \frac{t^k - 1}{t^k (t-1)} \\ &= \frac{1}{1 + t^{2k+1}} \left(x_0 \frac{t(t^{2k} - 1)}{t-1} + \frac{s}{\varrho} \, \frac{t(t^k - 1)(t^{k+1} - 1)}{(t-1)^2} \right), \\ &= x_0 f(k) + \frac{s}{\varrho} \, g(k), \end{aligned}$$

where

$$f(x) = \frac{t(t^{2x} - 1)}{(1 + t^{2x+1})(t-1)} \quad \text{and} \quad g(x) = \frac{t(t^x - 1)(t^{x+1} - 1)}{(1 + t^{2x+1})(t-1)^2}.$$

Similarly,

$$\sum_{j=1}^{l} y_l = x_0 f(l) + \frac{s}{\varrho} \, g(l).$$

Since $t > 1$, the functions $f(x)$ and $g(x)$ have positive first derivatives,

$$f'(x) = \frac{2t^{2x+1}(t+1) \ln t}{(t-1)(t^{2x+1} + 1)^2} \quad \text{and} \quad g'(x) = \frac{t^{x+1}(t+1)(t^{2x+1} - 1) \ln t}{(t-1)^2 (t^{2x+1} + 1)^2}.$$

Therefore, the function $f(x)$ and $g(x)$ are monotonically increasing in x, and from $k \geq l$, we get $f(k) \geq f(l)$ and $g(k) \geq g(l)$. Since x_0, s and ϱ are positive, we conclude

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that

$$\sum_{i=1}^{k} x_i = x_0 f(k) + \frac{s}{\varrho}\, g(k) \geq x_0 f(l) + \frac{s}{\varrho}\, g(l) = \sum_{j=1}^{l} y_j. \qquad \square$$

We are now in a position to prove the main lemma in this section.

LEMMA 3.3. *Let G be a simple graph and v one of its vertices. If $k \geq l \geq 1$, then*

$$\varrho_{G(v,k,l)} < \varrho_{G(v,k+1,l-1)}. \tag{3.9}$$

Proof. Let D be the distance matrix of $G(v,k,l)$ and D^* the distance matrix of $G(v,k+1,l-1)$. Let x be a positive eigenvector of D corresponding to $\varrho_{G(v,k,l)}$, let x_0 be the component of x at v, $x_1,\ldots,x_k$ the components of x along P_k, and $x_{-1},x_{-2},\ldots,x_{-l}$ the components of x along P_l, as illustrated in Figure 3.3.

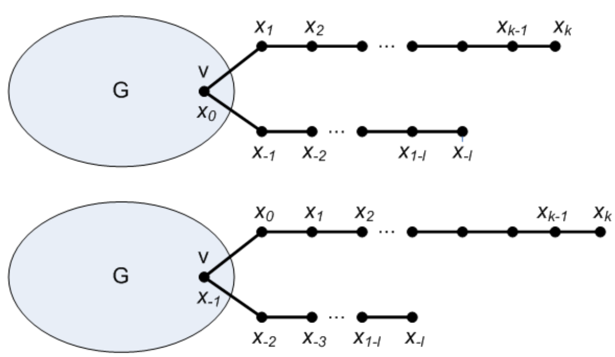

FIG. 3.3. *Graphs $G(v,k,l)$ and $G(v,k+1,l-1)$.*

We may suppose that the graph $G(v,k+1,l-1)$ is obtained from $G(v,k,l)$ by "shifting" the paths P_k and P_l for one position each over v. Suppose further that each vertex "carries" its own x-component during this transformation, and let x^* be the vector obtained in this way, as illustrated in Figure 3.3. It follows that $x^{*T}x^* = x^T x$. On the other hand, the product $x^T Dx$ can be partitioned into three sums

$$x^T Dx = \sum_{u,w\in G-v} d_{uw}x_u x_w + \sum_{i=-l}^{k}\sum_{j=-l}^{i-1} |i-j| x_i x_j + \sum_{u\in G-v}\sum_{i=-l}^{k} (d_{uv}+|i|) x_u x_i,$$

while the product $x^{*T}D^*x^*$ can be partitioned into four sums (the first two sums correspond to the first two sums in the product $x^T Dx$)

$$x^{*T}D^*x^* = \sum_{u,w\in G-v} d_{uw}x_u x_w + \sum_{i=-l}^{k}\sum_{j=-l}^{i-1} |i-j| x_i x_j$$

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$$+\sum_{u\in G-v}\sum_{i=0}^{k}(d_{uv}+|i|+1)x_ux_i+\sum_{u\in G-v}\sum_{i=-l}^{-1}(d_{uv}+|i|-1)x_ux_i$$
$$=x^TDx+\left(x_0+\sum_{i=1}^{k}x_i-\sum_{i=-l}^{-1}x_i\right)\sum_{u\in G-v}x_u.$$

Since $k\geq l\geq 1$, it follows from Lemma 3.2 that

$$\sum_{i=1}^{k}x_i\geq\sum_{i=-l}^{-1}x_i,$$

so that

$$x^{*T}D^*x^*\geq x^TDx+x_0\sum_{u\in G-v}x_u>x^TDx.$$

Since x is an eigenvector of D corresponding to $\varrho_{G(v,k,l)}$, from the Rayleigh quotient we get

$$\varrho_{G(v,k+1,l-1)}=\sup_{z\neq 0}\frac{z^TD^*z}{z^Tz}\geq\frac{x^{*T}D^*x^*}{x^{*T}x^*}>\frac{x^TDx}{x^Tx}=\varrho_{G(v,k,l)}.\qquad\square$$

Therefore, we showed that for $k\geq l\geq 1$,

$$\varrho_{G(v,k,l)}<\varrho_{G(v,k+1,l-1)}<\varrho_{G(v,k+2,l-2)}<\cdots<\varrho_{G(v,k+l,0)}. \tag{3.10}$$

Let T be a tree with the maximum distance spectral radius among trees on n vertices. Suppose that the maximum vertex degree in T is at least three. Let v be at the largest distance from the center of T among the vertices of T having degree at least three. Then T can be represented as $G(v,k,l)$ for some subgraph G, k and l, with $k\geq l\geq 1$. For the tree $T'=G(v,k+l,0)$, we have $\varrho_T<\varrho_{T'}$ by (3.10), which is a contradiction with the choice of T.

Thus, T has maximum vertex degree two, i.e., the tree with the maximum distance spectral radius is a path P_n.

4. Trees with the fixed maximum degree. The path is a unique tree with $\Delta=2$, while the star S_n is the unique tree with $\Delta=n-1$. Therefore, we can assume that $3\leq\Delta\leq n-2$.

THEOREM 4.1. *Let $T\ncong B_{n,\Delta}$ be an arbitrary tree on n vertices with the maximum vertex degree Δ. Then*

$$\varrho(B_{n,\Delta})<\varrho(T).$$

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Proof. Fix a vertex v of degree Δ as a root. Let $T_1, T_2, \dots, T_\Delta$ be maximal disjoint trees attached at v. We can repeatedly apply the transformation from Lemma 3.3 at any vertex of degree at least three with the largest eccentricity from the root in every tree T_i, as long as T_i does not become a path. By Lemma 3.3, it follows that each application of this transformation strictly decreases its distance spectral radius.

When all trees $T_1, T_2, \dots, T_\Delta$ turn into paths, we can again apply the inequalities (3.10) at the vertex v as long as there exist at least two paths of length at least two, further decreasing the distance spectral radius. At the end of this process, we arrive at the broom $B_{n,\Delta}$. ∎

Next, for $\Delta > 2$, we can apply the transformation of Lemma 3.3 at the vertex of degree Δ in $B_{n,\Delta}$ and obtain $B_{n,\Delta-1}$. Thus, $\varrho(B_{n,\Delta}) < \varrho(B_{n,\Delta-1})$ for $\Delta > 2$, which shows the chain of inequalities

$$\varrho(S_n) = \varrho(B_{n,n-1}) < \varrho(B_{n,n-2}) < \cdots < \varrho(B_{n,3}) < \varrho(B_{n,2}) = \varrho(P_n).$$

From the proof of Theorem 4.1, it follows that $B_{n,3}$ has the second maximum distance spectral radius among trees on n vertices.

A complete Δ-ary tree is defined as follows. Start with the root having Δ children. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. While in the last level all nodes need not exist, those that do fill the level consecutively (see Figure 4.1). Thus, at most one vertex on the level before the last has its degree different from Δ and 1.

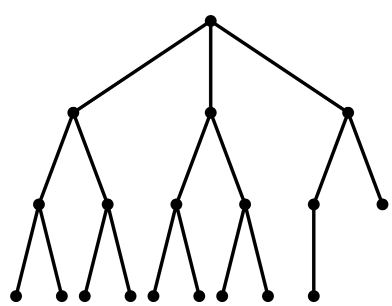

FIG. 4.1. *The complete 3-ary tree of order* 19.

These trees are also called *Volkmann trees*, as they represent alkanes with the minimal Wiener index [10]. Volkmann trees also have the maximal greatest eigenvalue among trees with maximum degree Δ, as shown in [20]. For more details, see [12] and references therein.

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A computer search among trees with up to 24 vertices revealed that complete Δ-ary trees attain the minimum values of the distance spectral radius among the trees with the minimum vertex degree Δ. Based on this argument and the above-mentioned empirical observations, we pose the following.

CONJECTURE 4.2. *A complete Δ-ary tree has the minimum distance spectral radius $\varrho(T)$ among trees on n vertices with maximum degree Δ.*

While we do not have the proof of the above conjecture at the moment, we make a humble step forward by characterizing starlike trees which minimize the distance spectral radius. A Δ-starlike tree $T(n_1, n_2, \ldots, n_\Delta)$ is a tree composed of the root vertex v, and the paths $P_1, P_2, \ldots, P_\Delta$ of lengths $n_1, n_2, \ldots, n_\Delta$ attached at v. Therefore, the number of vertices of $T(n_1, n_2, \ldots, n_\Delta)$ equals $n = n_1 + n_2 + \ldots + n_\Delta + 1$. The Δ-starlike tree is *balanced* if all paths have almost equal lengths, i.e., $|n_i - n_j| \leq 1$ for every $1 \leq i \leq j \leq \Delta$. Notice that the broom $B_{n,\Delta} = T(1, 1, \ldots, 1, n - \Delta - 1)$ is a Δ-starlike tree.

THEOREM 4.3. *The balanced Δ-starlike tree has minimum distance spectral radius among Δ-starlike trees of order n.*

Proof. Let $T = T(n_1, \ldots, n_\Delta)$ be an arbitrary Δ-starlike tree. If there exists i and j, $1 \leq i, j \leq \Delta$, such that $|n_i - n_j| > 1$, then we can strictly increase its even spectral moments by applying Lemma 3.3 repeatedly until we obtain Δ-starlike trees with paths of lengths $\lfloor \frac{n_i+n_j}{2} \rfloor$ and $\lceil \frac{n_i+n_j}{2} \rceil$ instead of n_i and n_j. The minimality of the distance spectral radius in such trees is shown analogously using Theorem 4.1. $\square$

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