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INDICES OF TREES WITH A PRESCRIBED DIAMETER

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The index of a graph is is the largest eigenvalue of its adjacency matrix. Let $\mathcal{T}_{n,d}$ be the class of trees with n vertices and diameter d. For all integers n and d with $4 \leq d \leq n-3$ we identify in $\mathcal{T}_{n,d}$ the tree with the k-th largest index for all k up to $\left\lfloor \frac{d}{2} \right\rfloor + 1$ if $d \leq n-4$, or for all k up to $\left\lfloor \frac{d}{2} \right\rfloor$ if d = n-3.

1. INTRODUCTION

Let G = (V(G), E(G)) be a simple graph, and let A be its adjacency matrix. The characteristic polynomial det(xI - A) of A is called the characteristic polynomial of G, and is denoted by $\phi(G, x)$. The eigenvalues of A (i.e. the zeros $\phi(G, x)$) are called the eigenvalues of G. The index of a graph G is the largest eigenvalue of G, denoted by $\rho(G)$. It has been studied extensively in the literature $[\mathbf{1}, \mathbf{3}]$; see also $[\mathbf{2}]$.

In the class of all trees with $n \ge 6$ vertices, M. HOFMEISTER [7] determined the trees whose indices are the k-th largest, for k = 1, 2, ..., 5.

Let $\mathcal{T}_{n,d}$ be the class of trees on n vertices and diameter d, with $2 \leq d \leq n-1$. Obviously, if $T \in \mathcal{T}_{n,2}$ then T is a star $(=K_{1,n-1})$, and if $T \in \mathcal{T}_{n,n-1}$ then T is a path $(=P_n)$. In addition, if d = 3 or d = n-2 then (as noted in Section 3) we can easily order all trees in non-increasing order with respect to the index. So we can assume further (as mentioned in the abstract) that $4 \leq d \leq n-3$.

The main purpose of this paper is to identify the trees in $\mathcal{T}_{n,d}$ having the k-th largest index, for all k up to $\left\lfloor \frac{d}{2} \right\rfloor + 1$, or $\left\lfloor \frac{d}{2} \right\rfloor$ if d = n - 3.

REMARK. The first determination of the graphs in $\mathcal{T}_{n,d}$ with the largest index can be found in [12] (see also [11]).

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2. BASIC TOOLS

Let G be a graph and u a vertex of G. Then G-u denotes the graph obtained from G by deleting vertex u and the edges incident to u. A *pendant vertex* is a vertex of degree 1; a *pendant edge* is an edge incident to a pendant vertex. A *bouquet* is a non-empty collection of pendant edges attached at the same vertex.

Lemma 1. [1] Let u be a pendant vertex of a graph G and v the neighbour of u. Then

$$\phi(G, x) = x\phi(G - u, x) - \phi(G - u - v, x),$$

where $\phi(G - u - v, x) = 1$ if $G = P_2$.

Lemma 2. [3, 8] Let G be a connected non-trivial graph and H a proper spanning subgraph. Then

$$\phi(H, x) > \phi(G, x)$$
 for $x \ge \rho(G)$.

A dot product (or coalescence) of two rooted graphs G_u and H_v (u and v are their roots, respectively) is the graph (denoted by $G_u \cdot H_v$) which is obtained by identifying their roots.

Lemma 3. [10] Let G be a connected non-trivial graph, and $H = K_{1,s}$ $(s \ge 2)$ a star. Let c be the central vertex of H, and let v be any other vertex. Let G_u , H_c and H_v be the graphs whose roots are u (any vertex of G), c and v, respectively. Then

$$\rho(G_u \cdot H_c) > \rho(G_u \cdot H_v).$$

Lemma 4. [3, 8] Let $G_{k,\ell}$ be a graph obtained from a connected non-trivial graph G by adding at some fixed vertex two hanging paths of lengths k and ℓ . If $k \ge \ell \ge 1$, then

$$\rho(G_{k,\ell}) > \rho(G_{k+1,\ell-1}).$$

Recall first that for a connected graph the positive unit eigenvector corresponding to its index is called a *principal eigenvector*. For a given graph G of order n, let $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ be its principal eigenvector. We next have:

Lemma 5. [3, 11] Let G be a connected graph in which r is a vertex adjacent to vertex s, but not to vertex t. Let G' be the graph obtained by rotating edge rs around r to the non-edge rt (i.e, by removing edge rs and adding edge rt). Also let \mathbf{x} be the principal eigenvector of G. Then the following holds:

if
$$x_t \ge x_s$$
 then $\rho(G') > \rho(G)$.

Lemma 6. [4, 11] Let G be a connected graph, and define r, s, t and G' as in Lemma 5. Assume G' is connected as well. Next, let \mathbf{x} and \mathbf{x}' be the principal eigenvectors of G and G', respectively. Then the following holds:

if $x_t \ge x_s$ then $x'_t > x'_s$.

To state the following result, we need more definitions. An *internal path* in some graph, say $v_0, v_1, \ldots, v_{k-1}, v_k$, is a path joining the vertices v_0 and v_k so that both v_0 and v_k (which need not be distinct) have degree greater than 2, while all other vertices (i.e. v_1, \ldots, v_{k-1}) are of degree equal to 2. A *double snake* T_n is a tree obtained from a path (on n - 4 vertices) by adding to each of its terminal vertices two pendant edges.

Lemma 7. [6, 3] Let G' be a graph obtained from a connected graph G by inserting a vertex of degree 2 in an edge e. Then the following holds:

- (i) If e belongs to an internal path and $G \neq T_n$, then $\rho(G') < \rho(G)$; for $G = T_n$ we have $\rho(G') = \rho(G) = 2$.
- (ii) If e does not belong to an internal path and $G \neq C_n$, then $\rho(G') > \rho(G)$; for $G = C_n$ we have $\rho(G') = \rho(G) = 2$.

3. MAIN RESULTS

Recall first that a tree of diameter three is usually called a *double star*. It consists of an edge and two (non-empty) bouquets added to the end-vertices of this edge. Denote by $D_{p,q}$ a double star with p, q pendant edges contained in the bouquets (see Fig. 1). Clearly, $D_{p,q} \in \mathcal{T}_{p+q+2,3}$ whenever $p, q \geq 1$.

Theorem 1. Let $D_{p,q}$ be a double star with 1 .Then

$$\rho(D_{p,q}) < \rho(D_{p-1,q+1}).$$



Proof. Let s and t be the vertices of $D_{p,q}$, of degrees Fig. 1: The graph $D_{p,q}$. p+1 and q+1, respectively. Note, as already assumed,

 $p \leq q$. Let $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ (n = p + q + 2) be the principal eigenvector of $D_{p,q}$. It is now easy to prove (using the eigenvalue equations) that $x_s \leq x_t$. Therefore, by making use of Lemma 5, the proof easily follows.

Let $P_{n,d,i}$ be the tree obtained from the path P_{d+1} by attaching a bouquet with n-d-1 pendant edges to the vertex *i* of the path (see Fig. 2). Clearly, $P_{n,d,i} \in \mathcal{T}_{n,d}$ for any $1 \leq i \leq d-1$. In particular, if i = 1 then $P_{n,d,1}$ is called a *palm tree*, and denoted by $P_{n,d}$.



Fig. 2: The graph $P_{n,d,i}$.

REMARK. Theorem 1 and Lemma 4 enable us to order (by indices) all trees from $\mathcal{T}_{n,3}$ and $\mathcal{T}_{n,n-2}$. Namely, for trees of diameter 3 we have:

(1)
$$\rho(D_{1,n-3}) > \rho(D_{2,n-4}) > \dots > \rho(D_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}).$$

For trees of diameter d = n - 2 we have:

(2)
$$\rho(P_{n,d,\lfloor\frac{d}{2}\rfloor}) > \rho(P_{n,d,\lfloor\frac{d}{2}\rfloor-1}) > \dots > \rho(P_{n,d,1}).$$

Recall also, that for $d \leq 2$ or d = n - 1 the corresponding sets of trees are singletons, and thus these cases are not of any interest. From now on, we will assume that $4 \leq d \leq n - 3$ (and thus $n \geq 7$).

A caterpillar is a tree in which the removal of all pendant vertices makes it a path. If C is a caterpillar, let P_C be a path (of C) of maximal length. So, if $C \in \mathcal{T}_{n,d}$ then P_C is a path of length d. If u is any non-pendant vertex of P_C , then a bouquet (possibly empty) is attached to u. So any caterpillar of diameter d is determined by a (d-1)-tuple $(n_1, n_2, \ldots, n_{d-1})$, where n_i is the number of edges in the *i*-th bouquet (it is assumed here that, as above, the vertices of P_C are labeled from 0 to d). We denote by $\mathcal{C}_{n,d}$ the set of caterpillars on n vertices with diameter d.

We will now find a tree in $\mathcal{T}_{n,d} \setminus \mathcal{C}_{n,d}$ with the largest index. Below we will prove that this tree, denoted by $N_{n,d}$, is unique. It can be constructed as follows: take a caterpillar from $\mathcal{C}_{n-1,d}$ with $n_i = 0$ for all i except $i = \left\lfloor \frac{d}{2} \right\rfloor$ (hence $n_i = n - d - 2$), and add to one pendant vertex from the latter bouquet a pendant edge (see Fig. 3). Clearly, if $d \ge 4$ then the new tree is of diameter d.



Fig. 3: The graph $N_{n,d}$.

Theorem 2. For any tree $T \in \mathcal{T}_{n,d} \setminus \mathcal{C}_{n,d}$ $(d \ge 4)$

$$\rho(T) \le \rho(N_{n,d}),$$

with equality if and only if $T = N_{n,d}$.

Proof. Let T be any tree from $\mathcal{T}_{n,d} \setminus \mathcal{C}_{n,d}$, and let P_T be the path (of T) of maximal length (and hence it has length d). We will next show that for any $T \neq N_{n,d}$ there is a tree T' from $\mathcal{T}_{n,d} \setminus \mathcal{C}_{n,d}$ having a larger index.

Assume first that T is a tree having a vertex at distance $h \ge 2$ from P_T . Let u be a vertex (of T) whose distance from P_T is maximal. Since it is at least two, let u, v and w be the first three vertices belonging to the shortest path from u to P_T . Consider now a star induced by the edges incident to v. As in Lemma 3 this star can be turned to a star with all its edges hanging at w. By the same lemma the resulting tree T' has a larger index. The only situation when this argument does not give raise to a tree T' as required is the case when T' is a caterpillar.

But then all hanging elements of T (with respect to P_T), but one, are bouquets; the exceptional element is a double star hanging at one of its central vertices, or in particular, a star hanging at one of its pendant vertices.

Assume next that T contains, besides an exceptional element hanging at some vertex, say u, a bouquet hanging at some other vertex, say v. We can now relocate the observed hanging elements in such a way so that the edges which were previously attached at u are now attached at v, or conversely. But then, one of the two trees just obtained (depending on x_u and x_v - see Lemma 5, and Lemma 6 if necessary) has a greater index than T. Again we find a required tree T'. The only situation when this argument does not give raise to a tree T' as required is the case when there are no bouquets in T.

Assume next that T contains just one exceptional element as a hanging element (attached at vertex u, of P_T). Let $k \ge 1$ be the number of pendant vertices at distance 2 from P_T . Let $l \ge 0$ the number of pendant vertices at distance 1 from P_T . Any such tree T can be denoted by $T_{k,l}$. Let m = k + l. Observe now the trees $T_{m,0}$ and $T_{1,m-1}$. They can be obtained by relocating hanging edges of the exceptional element of $T_{k,l}$, l from one side, or k - 1 from the other side, respectively. By Lemmas 5 and 6 (as above), we get that $\rho(T_{k,l}) \le \max\{\rho(T_{m,0}), \rho(T_{1,m-1})\}$. So to finish the proof, it is sufficient to prove that $\rho(T_{m,0}) < \rho(T_{1,m-1}) \le \rho(N_{n,d})$ for $m \ge 2$.

Let $\Delta_m(x) = \phi(T_{m,0}, x) - \phi(T_{1,m-1}, x)$. Applying Lemma 1 for these two graphs (at pendant vertices), we easily get

$$\Delta_m(x) = x \Delta_{m-1}(x) - x^{m-2} \big(x \phi(P_{d+1}, x) - \phi(P_2, x) \phi(P_{d+1} - u, x) \big).$$

Applying SCHWENK's formula at vertex u (see [1], p. 78) we get that $\phi(P_{d+1}, x) = x\phi(P_{d+1} - u, x) - \phi(P_{d+1} - u - u_1, x) - \phi(P_{d+1} - u - u_2, x)$, where $u_1 = u - 1$ and $u_2 = u + 1$. Therefore, since $\phi(P_2, x) = x^2 - 1$, we get

$$\Delta_m(x) = x \Delta_{m-1}(x) + x^{m-2} (x \phi(P_{d+1} - u - u_1, x) + x \phi(P_{d+1} - u - u_2, x) - \phi(P_{d+1} - u, x)).$$

If we prove that $\Delta_m(x) \geq 0$ for x > 2 we are done. Note first that $\Delta_1(x) = 0$. So it is sufficient to prove that $x\phi(P_{d+1}-u-u_1,x)+x\phi(P_{d+1}-u-u_2,x)-\phi(P_{d+1}-u,x)>0$ for x > 2. For this aim we will only prove that $x\phi(P_{d+1}-u-u_s,x)-\phi(P_{d+1}-u,x)>0$ (x,x)>0 for x > 2 (Here, s = 1 or 2. If s = 1 set $u_t = u - 2$, otherwise set $u_t = u + 2$. Note that $u_t \in V(P_T)$ since $d \geq 4$.) Let $H = P_{d+1} - u$. Then $x\phi(P_{d+1}-u-u_s,x)-\phi(P_{d+1}-u,x)$ is equal to $\phi(H-u_su_t,x)-\phi(H,x)$, and this expression is positive for x > 2 (follows by using Lemma 2), and consequently $\rho(T_{m,0}) < \rho(T_{1,m-1})$ for $m \geq 2$. Finally, by Lemma 4, we get that $\rho(T_{1,m-1}) \leq \rho(N_{n,d})$. The equality can hold only for $u = \left\lfloor \frac{d}{2} \right\rfloor$ (by Lemma 4). Note also that for $T_{k,l} \neq T_{1,m-1}$ we have $\rho(T_{m,0}) \leq \rho(T_{k,l}) < \rho(T_{1,m-1})$ (by Lemmas 5 and 6). So the equality statement follows.

This completes the proof.

We now focus our attention on caterpillars.

Theorem 3. For any caterpillar $C \in C_{n,d}$ $(d \ge 4)$ having $k \ge 2$ bouquets, there is a caterpillar $C' \in C_{n,d}$ having k - 1 bouquets such that $\rho(C') > \rho(C)$.

Proof. Let C be a caterpillar as stated above, and let t be a vertex of P_C with maximum weight (with respect to \mathbf{x} , the principal eigenvector of C) among the vertices of P_C with bouquets attached. Let s be any other vertex of P_C with a bouquet attached. Then, by applying Lemma 5 and, if necessary, Lemma 6, we can relocate (by a sequence of rotations) all edges from the bouquet at s to the bouquet at t, to get a caterpillar C' with a larger index.

Due to Theorem 3, it seems reasonable to consider further only the caterpillars with at most two bouquets. At the moment we will focus our attention on those caterpillars with exactly two bouquets. Let $M_{n,d}$ be a caterpillar (from $C_{n,d}$) satisfying the following conditions: it has only two bouquets which are of sizes 1 and k (= n - d - 2); the distance between the roots of these two bouquets is 1;

both bouquets if possible, but the larger one for sure, are "rooted" in the center of the tree in question (in fact, a center of P_C) - see Fig. 4. According to [11], this graph is an instance of an alternating caterpillars (cf. [11), i.e. a caterpillars with prescribed degrees, but with maximal index.



Theorem 4. For any caterpillar $C \in C_{n,d}$ $(d \ge 4)$ having exactly two bouquets, we have $\rho(C) \le \rho(M_{n,d})$, with equality if and only if $C = M_{n,d}$.

Proof. Let *C* be a caterpillar as mentioned above. Using the same argument as in the proof of Theorem 3, we can easily get that there exists a caterpillar *C'* in the class under considerations such that one of its bouquets has size 1, while the other one has size n - d - 2, and that in addition $\rho(C) \leq \rho(C')$ holds. The rest of the proof follows immediately from Theorem 3.8 [11].

Consider now the caterpillars (from $C_{n,d}$) with just one bouquet. By Lemma 4, they can be completely ordered by their indices. Namely we have:

$$\rho(P_{n,d,1}) < \rho(P_{n,d,2}) < \dots < \rho(P_{n,d,\lfloor \frac{d}{2} \rfloor}).$$

Theorem 5. For any n and $d \ge 4$, $\rho(N_{n,d}) < \rho(M_{n,d})$.

Proof. For short, put $T = N_{n,d}$ and $T' = M_{n,d}$. Let $u \in V(T)$ be a pendant vertex at distance 2 from P_T (by u' we denote its neighbor). Next, let $v \in V(T')$ be a pendant vertex belonging to a pendant edge in the bouquet of size 1 (by v' we denote its neighbour). Then, clearly, T - u = T' - v. By Lemma 1, we easily get $\phi(T', x) - \phi(T, x) = \phi(T - u - u', x) - \phi(T' - v - v', x)$. Therefrom, by Lemma 2 $\phi(T', x) - \phi(T, x) < 0$ for $x \ge \rho(T')$, since T' - v - v' is a spanning subgraph

of T - u - u' (note that the former graph can be obtained from the latter one by deleting one edge). So the proof follows easily.

Recall here that $P_{n,d}$ is a palm tree as already defined.

Theorem 6. If $4 \le d \le n - 4$ then $\rho(M_{n,d}) < \rho(P_{n,d})$.

Proof. For short, put $T_k = M_{n,d}$ and $T'_k = P_{n,d}$, where k = n - d - 2. Note that k is the number of pendant edges in the larger bouquet of T_k , while k+1 is the number of edges in the unique bouquet of T'. Clearly, $k \ge 2$ (by assumptions).

Assume first that d = 4. Let $\Delta_k(x) = \phi(T_k, x) - \phi(T'_k, x)$. By Lemma 1 (in both trees take u a pendant vertex taken from the bouquets of sizes k, or k + 1) we easily get

$$\Delta_k(x) = x \Delta_{k-1}(x) - x^{k-1} \big(\phi(P_2 \cup P_3, x) - x^2 \phi(P_3, x) \big).$$

Therefore, $\Delta_k(x) = x\Delta_{k-1}(x) + x^k(x^2 - 2)$. Since $\Delta_2(x) = 2x^2(x^2 - 4)$ (by direct calculations), we have that $\Delta_2(x) > 0$ for any x > 2. Consequently, $\Delta_k(x) > 0$ for any $k \geq 2$ whenever we take x > 2. Since the indices of the observed graphs are always greater than 2, we are done.

Assume next that $d \ge 5$. Consider first the graph $T_k + e$, where e is an edge joining the vertices in T_k which are at distance d. Clearly, $\rho(T_k) < \rho(T_k + e)$. We note also that the graph $T_k + e$ is a unicyclic graph containing a cycle of length d+1. Next, all vertices of this cycle but two are of degree 2. We can now remove (or suppress) d-4 vertices of degree 2 from the cycle to reduce its length to 5. The graph obtained in this way, extended by an isolated vertex, will be denoted by T_k . By Lemma 7, we have $\rho(T_k + e) < \rho(T_k)$, and thus $\rho(T_k) < \rho(T_k)$. Note that \hat{T}_k has k+7 vertices. Consider next the graph \hat{T}'_k obtained from $P_{n,d}$ by reducing its diameter to five, namely $\hat{T}'_k = P_{k+7,5}$. Note that \hat{T}'_k has also k+7 vertices. Clearly, we then we have that $\rho(\hat{T}'_k) < \rho(T'_k)$. To prove the theorem it is enough to prove that $\rho(\hat{T}_k) < \rho(\hat{T}'_k)$. Now, let $\Delta_k(x) = \phi(\hat{T}_k, x) - \phi(\hat{T}'_k, x)$. By Lemma 1 again (choosing u as above) we easily get

$$\Delta_k(x) = x \Delta_{k-1}(x) - x^k \big(\phi(P_5, x) - x \phi(P_4, x) \big).$$

From this we obtain $\Delta_k(x) = x \Delta_{k-1}(x) + x^k \phi(P_3, x)$. Since $\Delta_2(x) = 2x^3 (x^2 - x)^2 (x^2$ $x-\frac{5}{2}$ (by direct calculations) we have that $\Delta_2(x) > 0$ for any $x > \frac{1+\sqrt{11}}{2}$. Consequently, $\Delta_k(x) > 0$ for any $k \ge 2$ and $x > \frac{1+\sqrt{11}}{2}$. Since the indices of the observed graphs are always greater than $\frac{1+\sqrt{11}}{2}$ (as can be easily seen by the Interlacing theorem, and direct calculations on some subgraphs), we are done. \square

This completes the proof.

A more interesting situation appears when d = n - 3 (then k = 1, and $M_{n,d}$) has a very simple structure). Based on computer experiments we now have that for $7 \leq n \leq 9$ (then $4 \leq d \leq 6$) that $\rho(M_{n,d}) < \rho(P_{n,d})$. But for $n \geq 10$ (or

 $d \geq 7$) it was observed that $\rho(M_{n,d}) > \rho(P_{n,d})$. The following theorem resolves this situation.

Theorem 7. If d = n - 3 and $n \ge 10$, then $\rho(P_{n,d,1}) < \rho(M_{n,d}) < \rho(P_{n,d,2})$.

Proof. We first consider the left inequality. According to A. J. HOFFMAN (see [5], or [1], p. 78) we have that the limiting point for the index of G_n , where G_n is a graph obtained from a connected graph G by attaching to a vertex u a path of length n, is equal to the greatest positive root of the equation

$$\frac{1}{2}\left(x + \sqrt{x^2 - 4}\right)\phi(G, x) - \phi(G - u, x) = 0.$$

Of course, this holds only if the limiting point is greater than 2. Applying this fact to $G = K_{1,3}$, where u is the central vertex, we get that $\rho^* \approx 2.1213$ is the limit point. On the other hand, $\rho(M_{n,n-3}) \ge \rho(M_{10,7}) \approx 2.1268$. So we are done.

Consider next the right inequality. For n = 10, we have that $\rho(M_{10,7}) \approx 2.1268$, while $\rho(P_{10,7,2}) \approx 2.1679$ and we are done. Assume next that $n \geq 11$. We will now use the same argument as in the proof of the previous theorem. So, if we add an edge between two vertices at the greatest distance, and if we reduce the number of vertices of degree 2 on the cycle to 7, we get a graph whose index is approximately equal to 2.1634, and thus (by Lemma 7) $\rho(M_{n,d}) < 2.1634$. On the other hand $2.1692 \approx \rho(P_{11,8}) \leq \rho(P_{n,n-3})$ for any $n \geq 11$. So we are again done.

This completes the proof.

We will now summarize the main results of this paper. Let $\mathcal{T}_{n,d}$ be the set of trees on n vertices and diameter d. For a fixed n we will assume that $4 \le d \le n-3$ (cases $d \le 2$ or d = n-1 are trivial; case d = 3 is given in (1); case d = n-2 is given in (2)).

Theorem 8. If $4 \le d \le n-4$, or if $n \le 9$ and d = n-3, then

$$(3) \qquad \rho\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right) > \rho(P_{n,d,\lfloor\frac{d}{2}\rfloor-1}) > \dots > \rho(P_{n,d,2}) > \rho(P_{n,d,1}) > \rho(M_{n,d})$$

and $\rho(M_{n,d}) > \rho(T)$ for any other tree from $\mathcal{T}_{n,d}$. If d = n - 3 and $n \ge 10$, then

(4)
$$\rho\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right) > \rho(P_{n,d,\lfloor\frac{d}{2}\rfloor-1}) > \dots > \rho(P_{n,d,3}) > \rho(P_{n,d,2}) > \rho(M_{n,d})$$

and $\rho(M_{n,d}) > \rho(T)$ for any other tree from $\mathcal{T}_{n,d}$.

It is interesting to note that in (4) we have a slight change which can be interesting to explain. More on this phenomenon will appear elsewhere in the forthcoming papers by F. BELARDO, E. M. LI MARZI and S. K. SIMIĆ.

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