On the zero forcing number
and spectral radius of graphs

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Abstract

In this paper, we determine the graphs (respectively, trees) with maximum spectral radius among all graphs (respectively, trees) with zero forcing number at most k. As an application, we give a sharp lower bound for the zero forcing number of graphs involving the spectral radius.

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1 Introduction

All graphs consider here are simple, finite and undirected. For any notation and terminology used but not defined, one may refer to [9, 15]. Let $G = (V(G), E(G))$ be such a graph with order $n = |V(G)|$. The *color-change rule* on G is defined as follows. Originally, color the vertices in $V(G)$ and its subset S to be white and blue respectively. For each of the

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steps, a blue vertex u in S with exactly one white neighbor v will force v to turn into blue. At this time, we say u *forces* v. The set S is said to be a *zero forcing set* if all vertices of $V(G)$ become blue by applying the color-change rule. And this process is called the *forcing process* of S in G. The *zero forcing number* of G is the minimum cardinality of zero forcing sets of G, denoted by $Z(G)$.

As pointed in [20, 26], the forcing process is an instance of a propagation process on graphs, and it has many applications to other branches of mathematics, computer science and physics, such as the linear and quantum controllability for systems that stem from networks [11, 12] and the power domination [34]. Moreover, diverse graph processes are employed to model technical or societal processes in other fields. For more details and an overview of the different models and applications, refer to the book [5] and the papers [20, 26] with the references therein.

Notice that the zero forcing process was proposed in [13]. Independently, the zero forcing number was introduced in [1] as a bound for the minimum rank or, equivalently, the maximum nullity $M(G)$ of a graph G. Recall, the *minimum rank* of G is defined to be the smallest possible rank over all symmetric real matrices whose ij-th entry (for $i \neq j$) is nonzero whenever $ij \in E(G)$ in G and is zero otherwise. Then, the minimum rank of G is $n - M(G)$. In [2], it was shown that $Z(G) \geqslant M(G)$ for any graph G. This parameter has been extensively studied in over half a century, largely due to its connection to inverse eigenvalue problems for graphs, singular graphs, biclique partitions, as well as its applications to other problems and disciplines. For more results on this topic, refer to [1, 22, 35].

Recently, it has attracted great concern about the relations between the zero forcing number and other graph parameters, such as the connected domination number [3], the tree-width [4], the degree sequence [14, 24], the perfect dominating set [19], the path cover number [23], the girth and minimum degree [26], the Grundy (total) domination number [8, 29] and the chromatic number [32]. Up to now, a mass of papers about the zero forcing number have been published. We here tend not to list all, but we focus primarily on those related to the lower bounds for the zero forcing number. Let δ and g be the minimum degree and the girth of a graph G. Recall that the *girth* is the length of the shortest cycle in a graph. Easily to see that a trivial but tight one is $Z(G) \geqslant \delta$. Whereas, if $g \geqslant 3$ and $\delta \geqslant 2$, Davila, Kalinowski, and Stephen [17] showed that $Z(G) \geqslant \delta + (\delta - 2)(g - 3)$, confirming the earlier conjecture from [18]. Kalinowski, Kamčev and Sudakov [26] essentially improved this bound with few exception of very small values of δ and $g = 3, 4$, whose bound is stated as follows:

$$ Z(G) \geqslant \begin{cases} e^{-1} \left(\frac{\delta^k}{k+1} - \delta^{k-1} \right) & \text{if } g = 2k + 1, \\ 2e^{-1} \left(\frac{\delta^k}{k+1} - \delta^{k-1} \right) & \text{if } g = 2k + 1. \end{cases} \tag{1} $$

Further, Inq. (1) was extended to H-free graphs by their method based on the Turán numbers [26]. When it comes to our interests, we prefer to their spectral bounds on the zero forcing number of a graph. Some jargon from spectral graph theory are now introduced. The *adjacency matrix* $A(G) = (a_{ij})$ of a graph G with order n is an $n \times n$
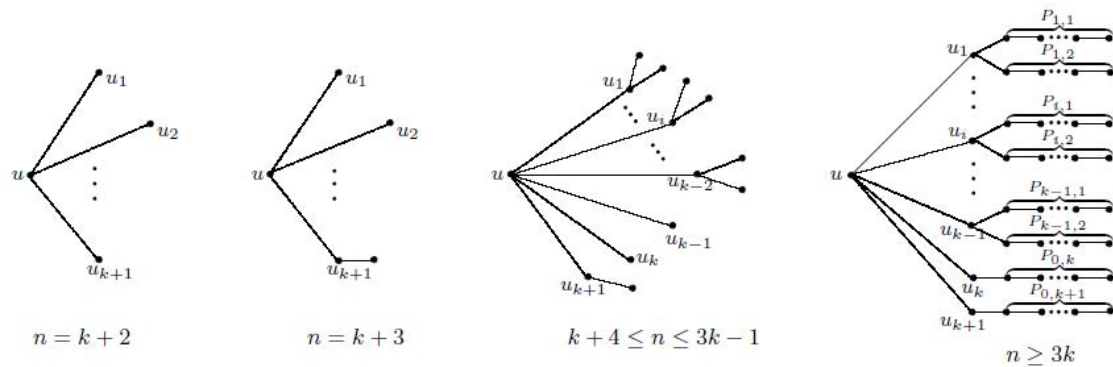
Figure 1: The tree $T_{n,k}$.

matrix whose entry a_{ij} is 1 if $ij \in E(G)$, and 0 otherwise. The *eigenvalues* of G are those of its adjacency matrix. An (n, d, λ)-*graph* is a d-regular graph with order n in which all eigenvalues but the largest one are at most λ in absolute value. Using the well-known estimate on the edge distribution of a graph in terms of its eigenvalues (eg, [27]), Kalinowski, Kamčev and Sudakov [26] provided the following spectral bounds for the (n, d, λ)-graphs G:

$$Z(G) \geqslant n \left(1 + \frac{2\lambda_{\min}}{d - \lambda_{\min}}\right), \qquad (2)$$

where $\lambda_{\min}$ is the smallest eigenvalue of G, and the bound is tight. Remember that the *spectral radius*, denoted by $\rho(G) = \lambda_{\max}$, of G is its largest eigenvalue. In the paper, we will investigate the relations between the zero forcing number and the spectral radius of a graph.

Let $\mathscr{S}_{n,k}$ be the set of all graphs with order n and zero forcing number at most k ($1 \leqslant k \leqslant n - 1$). The first goal of this paper is about to determine the extremal graphs with maximum spectral radius in $\mathscr{S}_{n,k}$. This is the type of Brualdi-Solheid Problem [10] that determining the maximal spectral radius of graphs in a given family, with a considerable number of results having been published (see [7, 16, 21] for examples).

Let $G\nabla H$ be the *join* obtained from two disjoint graphs G and H by connecting each vertex of G to each vertex of H. As usual, let K_n and P_n be the *complete graph* and the *path* with order n respectively. It is the time to state the first main result in the paper.

Theorem 1. *In $\mathscr{S}_{n,k}$, the maximum spectral radius is attained by the following unique graph:*

(i) P_n *if $k = 1$;*

(ii) $G_{n,k} = K_{k-1}\nabla P_{n-k+1}$ *if $2 \leqslant k \leqslant n - 2$;*

(iii) K_n *if $k = n - 1$.*

We next consider the same problem for the trees. Let $\mathscr{T}_{n,k}$ be the set of all trees with order n and zero forcing number at most k, where $k \geqslant 1$ and $n \geqslant k + 2$.

Theorem 2. *In $\mathscr{T}_{n,k}$, the maximum spectral radius is attained by the following unique tree:*

(i) *P_n if $k = 1$;*

(ii) *$T_{n,k}$ if $2 \leqslant k \leqslant n - 2$,*

where $T_{n,k}$ is shown in Fig. 1 and minutely defined in Definition 13.

Note, in the tree $T_{n,k}$ with $n \geqslant 3k$, that the pendant paths attached at the vertices u_i's $(1 \leqslant i \leqslant k+1)$ are of almost equal length, and $\min\{|P_{i,1}|, |P_{i,2}|\} \geqslant \max\{|P_{0,k}|, |P_{0,k-1}|\}$ $(1 \leqslant i \leqslant k-1)$ as well as $\min\{|P_{i,1}|, |P_{i,2}|\} \geqslant \max\{|P_{j,1}|, |P_{j,2}|\}$ $(1 \leqslant i < j \leqslant k-1)$, where $|P_{i,j}|$ means the length of pendant path $P_{i,j}$.

In the end, on the basis of Theorem 1, we can provide the following lower bound for the zero forcing number of a graph by means of its spectral radius.

Theorem 3. *Let G be a graph with order n and spectral radius $\lambda_{\max}$. Then*

$$Z(G) \geqslant 1 + \left\lfloor \frac{n + \lambda_{\max} - \sqrt{n^2 + 2(\lambda_{\max} - 2)n - 3\lambda_{\max}^2 + 12}}{2} \right\rfloor. \tag{3}$$

Moreover, this bound is sharp.

Here is the remainder of the paper. In Section 2 we give a proof of Theorem 1 by employing the k-trees. In Section 3, to show Theorem 2, we mainly use several old and new grafting transformations on the spectral radius of graphs. In Section 4, we provide a proof of Theorem 3, which is based on Theorem 1 and some spectral techniques including the equitable partition.

2 Proof of Theorem 1

The following lemma follows from the well-know Perron–Frobenius Theorem, referring to Theorem 2.2.1 in [9].

Lemma 4. *Let G be a connected graph, and H be a subgraph of G. Then $\rho(H) \leqslant \rho(G)$, and equality holds if and only if $H = G$.*

A column vector $\mathbf{x}$ indexed by the vertices of G can be denoted by $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$, where x_i is the component of $\mathbf{x}$ corresponding to the vertex i for any $1 \leqslant i \leqslant n$, and the sign t means the transpose of the vector. If G is connected, from Perron–Frobenius Theorem it follows that $\rho(G)$ is simple and its associated eigenvector, named as *Perron vector*, is positive.

The following lemma is a generalization of Theorem 8.1.3 in [15].

Lemma 5. *Let G be a connected graph with Perron vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$. Let u, v, be any two vertices, and W be a set of vertices which are adjacent to u but not adjacent to v. Let G' be the graph obtained from G by deleting the edges between u and W, and adding the edges between v and W. If $x_v \geqslant x_u$, then $\rho(G') > \rho(G)$.*

For an integer $r \geqslant 1$, a subset $V' \subseteq V(G)$ is called a *r-clique* of a graph G if $G[V']$, the subgraph of G induced by V', is a compete graph on r vertices. A *k-tree* is a chordal graph which has an inductive definition that extends the definition of a tree, which was introduced by Beineke and Pippert in [6].

Definition 6. [6] For an integer $k \geqslant 1$, a k-tree can be inductively defined as follows:

(i) Every complete graph with $k + 1$ vertices is a k-tree;

(ii) If G is a k-tree, $v \notin V(G)$ and $V' \subseteq V(G)$ induces a k-clique of G, then $G' = (V(G) \cup \{v\}, E(G) \cup (v, w) \mid w \in V')$ is also a k-tree;

(iii) Nothing else is a k-tree.

Let $\mathscr{K}_{n,k}$ be the family of all the k-trees with order n and zero forcing number k. Let G be a graph on n vertices with $Z(G) = k$. Clearly, $k = 1$ iff $G = P_n$. If $k = n - 1$, then $\rho(G) \leqslant \rho(K_n)$ and equality holds iff $G = K_n$. In what follows we set $2 \leqslant k \leqslant n - 2$.

Mitchell [30] showed the following useful result.

Proposition 7. [30] *Let G be a graph in $\mathscr{S}_{n,k}$ with $2 \leqslant k \leqslant n-2$. Then G is a spanning subgraph of some graph in $\mathscr{K}_{n,k}$.*

Note, any k-tree with order n has precisely $\frac{k(k-1)}{2} + k(n - k)$ edges. For any graph $G \in \mathscr{K}_{n,k}$, every vertex has degree at least k. Since $Z(G) = k$, for any minimum zero forcing set $Z \subseteq V(G)$, the first forcing vertex must have degree k, and its neighbourhood must induce a k-clique (since each vertex of a k-tree is contained in a $(k + 1)$-clique). Recall, a vertex $u \in V(G)$ is called a *leaf* if its degree $d(u) = 1$.

Proposition 8. *Let $2 \leqslant k \leqslant n - 2$. Then the graph $G_{n,k} = K_{k-1} \nabla P_{n-k+1}$ is the unique graph maximizing the spectral radius in $\mathscr{K}_{n,k}$.*

Proof: Clearly, $G_{n,k} = K_{k-1} \nabla P_{n-k+1}$ is a k-tree with zero forcing number k, since the set of vertices in K_{k-1} and a leaf of P_{n-k+1} is a zero forcing set with k vertices.

Let G be a k-tree in $\mathscr{K}_{n,k}$ with maximum spectral radius. Set $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ to be its Perron vector. Due to $Z(G) = k$, suppose that $Z = \{u_1, u_2, \ldots, u_k\}$ is a zero forcing set of G. As mentioned above, $G[Z]$, the induced subgraph by Z, is a k-clique of G. Let the vertices of Z be initially blue in G. Then by color-change rule, without loss of generality, we can denote the other vertices (not in Z) of G which are forced blue in order by $u_{k+1}, u_{k+2}, \ldots, u_n$. In detail, let the zero forcing process starting with Z be described as $v_1 \to u_{k+1}, v_2 \to u_{k+2}, \ldots, v_{n-k} \to u_n$, where $v \to u$ indicates that vertex v forces vertex u.

Notice that for any $i < j$, if u_i forces u_j, by color-change rule we know that u_i is adjacent to u_j but not adjacent to any vertex u_ℓ for $\ell \geqslant j + 1$. For any $t \geqslant k$, set $Z_t = \{u_1, u_2, \ldots, u_t\}$. For any vertex u of G, let $N_G(u)$ denote the neighbourhood of u. Then the following claims are easy to establish:

(i) $G[Z_{k+1}]$ is a $(k + 1)$-clique, and $N_G(v_1) = Z_{k+1} - \{v_1\}$;

(ii) $N_G(v_j) \bigcap \{u_{k+j}, u_{k+j+1}, \ldots, u_n\} = \{u_{k+j}\}$ for all $j \in \{1, 2, \ldots, n-k\}$;

(iii) $N_G(u_j) \bigcap Z_{j-1} = Z_{j-1} - \{v_1, v_2, \ldots, v_{j-1-k}\}$ for all $j \in \{k+2, k+3, \ldots, n\}$.

Notice that for $k+1 \leqslant j \leqslant n$, the vertex u_j has precisely k neighbors in Z_{j-1}. Moreover, for any $k+1 \leqslant j \leqslant n-1$, u_j is adjacent to the vertex u_{j+1}, and v_{j-k} is the unique vertex in Z_{j-1} which is adjacent to u_j but not adjacent to u_{j+1} (This fact will be used repeatedly in the following paragraph, which is denoted by Fact*).

Let $Z' = V(G) - (\{v_1, v_2, \ldots, v_{n-1-k}\} \cup \{u_{n-1}\})$. We shall prove Z' is another zero forcing set of G with k vertices, and the forcing process starting from Z' is $u_n \to u_{n-1}, u_{n-1} \to v_{n-1-k}, u_{n-2} \to v_{n-2-k}, \ldots, u_{k+1} \to v_1$ (Note, Z' is actually the *reversal* of Z, which is also a zero forcing set by [2]. But for the completeness of the proof, we give the details here). Clearly, $G[Z']$ is a k-clique containing u_n as a vertex. Now color the vertices in Z' to be blue initially. By letting $j = n$ in (iii), we have that u_{n-1} is the unique neighbor with white color of u_n. Then by the color-change rule, the vertex u_n forces the vertex u_{n-1}. Hence, the vertex u_n and its neighbors are all forced blue. By Fact*, v_{n-1-k} is the unique vertex except the neighbors of u_n, which is adjacent to u_{n-1}. Then, u_{n-1} forces v_{n-1-k}, and hence the vertex u_{n-1} and its neighbors are all forced blue. Again by Fact*, v_{n-2-k} is the unique vertex except the neighbors of u_{n-1}, which is adjacent to u_{n-2}. Then, u_{n-2} forces v_{n-2-k}, and hence the vertex u_{n-2} and its neighbors are all forced blue. Continue the process until the vertex u_{k+1} and its neighbors are all forced blue. Consequently, all the vertices of G are forced blue. Therefore, Z' is a zero forcing set of G.

Let $p_1, p_2, \ldots, p_{k-1}$ be $k-1$ vertices of G such that their corresponding components $x_{p_1}, \ldots, x_{p_{k-1}}$ in $\mathbf{x}$ are the first $k-1$ largest ones among all the vertices of G. For $1 \leqslant i \leqslant k-1$, we shall prove $d_G(p_i) = n-1$, where $d_G(p_i)$ is the degree of vertex p_i in G. Assume by contradiction that $d_G(p_j) \leqslant n-2$ for some $1 \leqslant j \leqslant k-1$. We next distinguish into the following two cases.

Case 1. The vertex $p_j \in Z \bigcup \{u_{k+1}\}$. In the forcing process starting from Z, let u_ℓ be the first vertex which is not adjacent to vertex p_j, where $\ell \geqslant k+2$. (Then we must have $p_j \to u_{\ell-1}$.) Since the vertex u_ℓ has exactly k neighbors in $Z_{\ell-1}$, then there is a neighbor (say, u_b) of u_ℓ in $Z_{\ell-1}$ such that $u_b \notin \{u_{\ell-1}, p_1, p_2, \ldots, p_{k-1}\}$, and thus $x_{u_b} \leqslant x_{p_j}$. For $\ell \leqslant i \leqslant n$, if u_i is adjacent to u_b (notice that u_i is not adjacent to p_j), after deleting the edge $u_b u_i$ and adding the edge $p_j u_i$ to G, we obtain the graph G_1. For any $\ell \leqslant i \leqslant n$, since p_j is adjacent to all other vertices in $G_1[Z_{i-1}]$, then the neighbors within Z_{i-1} of u_i in G_1 induces a k-clique of $G_1[Z_{i-1}]$. Thus G_1 is a k-tree on n vertices. Furthermore, Z is also a zero forcing set in G_1 (we just change $p_j \to u_{\ell-1}$ to $u_b \to u_{\ell-1}$ in the forcing process of Z, and change $u_b \to v$ to $p_j \to v$ in G_1 if $u_b \to v$ in G for some vertex v). Hence G_1 is a k-tree on n vertices with zero forcing number $Z(G_1) = k$. Thereby, $G_1 \in \mathscr{K}_{n,k}$. By Lemma 5 we get $\rho(G) < \rho(G_1)$, a contradiction.

Case 2. The vertex $p_j \notin Z \bigcup \{u_{k+1}\}$. Then we have $p_j = u_m$ for some $k+2 \leqslant m \leqslant n$. In the forcing process starting from Z, if there exists a vertex u_i ($i \geqslant m+1$) which is not adjacent to u_m, then we can assume that u_ℓ is such a vertex with $\ell(\geqslant m+1)$ being minimum. Since the vertex u_ℓ has precisely k neighbors in $Z_{\ell-1}$, there is a neighbor (say, u_c) of u_ℓ in $Z_{\ell-1}$ such that $u_c \notin \{u_{\ell-1}, p_1, p_2, \ldots, p_{k-1}\}$, and thus $x_{u_c} \leqslant x_{u_m}$. For $\ell \leqslant i \leqslant n$,

if u_i is adjacent to u_c (notice that u_i is not adjacent to u_m), by deleting the edge $u_c u_i$ and adding the edge $u_m u_i$ in G, we obtain the graph G_2. But G_2 is a k-tree on n vertices with zero forcing number $Z(G_2) = k$, with a similar discussion in Case 1. Hence, $G_2 \in \mathscr{K}_{n,k}$. From Lemma 5 it follows that $\rho(G) < \rho(G_2)$, a contradiction again.

Consequently, we have that, for any $i \geqslant m+1$, the vertex u_i is adjacent to the vertex u_m. In particular, u_m is adjacent to u_n. Since $d_G(u_n) = k$, thus u_m is contained in the (unique) $(k+1)$-clique containing u_n in G. Recall, $u_m = p_j$. Then $p_j \in Z' \bigcup \{u_{n-1}\}$. Considering the forcing process starting from Z', we will have a contradiction by a similar way to Case 1.

As proved above, $d_G(p_i) = n-1$ for any $1 \leqslant i \leqslant k-1$. Then, for $1 \leqslant i \leqslant k-1$, p_i must be in $Z \cup \{u_{k+1}\}$, and thus $G[V(G)\backslash\{p_1, p_2, \ldots, p_{k-1}\}]$ is a tree on $n+1-k$ vertices with zero forcing number 1, and thus $G[V(G)\backslash\{p_1, p_2, \ldots, p_{k-1}\}]$ is the path on $n+1-k$ vertices. As a consequence, G is the graph $G_{n,k} = K_{k-1}\nabla P_{n+1-k}$, as required.

This completes the proof. $\qquad\square$

Proof of Theorem 1: Let G be a graph G in $\mathscr{S}_{n,k}$ with $2 \leqslant k \leqslant n-2$. By Proposition 7 there exists a graph $H \in \mathscr{K}_{n,k}$ such that G is a spanning subgraph of H. From Lemma 4 and Proposition 8, it follows that $\rho(G) \leqslant \rho(H) \leqslant \rho(G_{n,k})$, where $\rho(G) = \rho(G_{n,k})$ iff $G = G_{n,k}$.

This ends the proof. $\qquad\square$

3   Proof of Theorem 3

The study of spectral radius and its relation to other graph parameters is a hot area of research with many different techniques and applications, surveyed in the monographs of, eg., [9, 15, 25]. Due to Theorem 1, we are now in the stage to show Theorem 3.

Proof of Theorem 3: If G is edgeless, then $\rho(G) = 0$, and thus the inequality (3) holds as $Z(G) \geqslant 1$. Since $Z(P_n) = 1$ and $\rho(P_n) < 2$, the inequality (3) holds for $G = P_n$. We next assume that $G \neq P_n$ contains at least one edge. Let $Z(G) = k$. Then $k \geqslant 2$ and $1 \leqslant \rho(G) \leqslant n-1$.

For convenience, set $\rho(G) = \lambda_{\max} = \rho$. We prove Ineq. (3) by contradiction. Assume that

$$k = Z(G) \leqslant \left\lfloor \frac{1}{2}\left(n + \rho - \sqrt{n^2 + 2(\rho-2)n - 3\rho^2 + 12}\right) \right\rfloor. \tag{4}$$

Due to $\rho \geqslant 1$, a direct calculation shows that

$$\frac{1}{2}\left(n + \rho - \sqrt{n^2 + 2(\rho-2)n - 3\rho^2 + 12}\right) \leqslant 2\rho,$$

which together with (4) results in $2\rho - k \geqslant 0$. On the other hand, it is routine to verify

$$\left\lfloor \frac{1}{2}\left(n + \rho - \sqrt{n^2 + 2(\rho-2)n - 3\rho^2 + 12}\right) \right\rfloor \leqslant n-2.$$

Hence $2 \leqslant k \leqslant n - 2$. By Theorem 1 we get $\rho \leqslant \rho(G_{n,k})$. From Lemma 4 it follows that $\rho(G_{n,k}) < \rho(K_{k-1}\nabla C_{n+1-k})$, where C_{n+1-k} is the cycle with order $n + 1 - k$. By the obvious equitable partition of the graph $K_{k-1}\nabla C_{n+1-k}$ (see [9, Chapter 2], or [15, Theorem 2.1.8]), it is easy to obtain that

$$\rho(K_{k-1}\nabla C_{n+1-k}) = \frac{k + \sqrt{4(k-1)n - 3k^2 + 12}}{2}.$$

Then

$$\rho < \frac{k + \sqrt{4(k-1)n - 3k^2 + 12}}{2}, \text{ and thus } 2\rho - k < \sqrt{4(k-1)n - 3k^2 + 12}.$$

Squaring both sides of the above inequality, we get $4k^2 - 4k(\rho + n) + 4(\rho^2 + n - 3) < 0$. Hence,

$$k > \frac{1}{2}(n + \rho - \sqrt{n^2 + 2(\rho - 2)n - 3\rho^2 + 12}),$$

which is contradictive to the assumption (4).

We next show that this bound is sharp. Note that $\rho(P_n) = 2\cos\frac{\pi}{n+1}$ and $Z(P_n) = 1$ and $\rho(K_n) = Z(K_n) = n - 1$. Easily to verify that P_n and K_n satisfy the equality in Theorem 3.

In fact, the graph $G_{n,k}$ also satisfies the equality in Theorem 3. Otherwise, from Theorem 3 it follows that

$$Z(G_{n,k}) = k \geqslant 2 + \left\lfloor \frac{1}{2}(n + \rho(G_{n,k}) - \sqrt{n^2 + 2(\rho(G_{n,k}) - 2)n - 3\rho^2(G_{n,k}) + 12}) \right\rfloor,$$

which results in

$$k - 1 > \frac{1}{2}(n + \rho(G_{n,k}) - \sqrt{n^2 + 2(\rho(G_{n,k}) - 2)n - 3\rho^2(G_{n,k}) + 12}).$$

Since $G_{n,k}$ contains K_{k+1} as a subgraph, then $\rho(G_{n,k}) \geqslant k$. Along with the above inequality we obtain

$$\rho(G_{n,k}) < \frac{k - 1 + \sqrt{4(k-2)n - 3(k-1)^2 + 12}}{2}. \tag{5}$$

Note $Z(G_{n,k}) = k$. As proved above, $\rho(H) = \frac{k + \sqrt{4(k-1)n - 3k^2 + 12}}{2}$ with $H = K_{k-1}\nabla C_{n+1-k}$. Let $\mathbf{x} = (x_i)$ be the Perron vector of H corresponding to $\rho(H)$. By the symmetry, we can set $x_u = a$ if u is in $V(K_{k-1})$, and $x_u = b$ if u is in $V(C_{n+1-k})$. Hence, $(k-1)a^2 + (n + 1 - k)b^2 = 1$. Clearly, $a \geqslant b$, and thus $b^2 \leqslant \frac{1}{n}$. Then

$$\rho(G_{n,k}) \geqslant \mathbf{x}^{\mathbf{t}} A(G_{n,k})\mathbf{x} = \rho(H) - 2b^2 \geqslant \rho(H) - \frac{2}{n}. \tag{6}$$

Combining (5) and (6) we get

$$\frac{k + \sqrt{4(k-1)n - 3k^2 + 12}}{2} - \frac{2}{n} < \frac{k - 1 + \sqrt{4(k-2)n - 3(k-1)^2 + 12}}{2},$$

which is equivalent to

$$1 - \frac{4}{n} < \frac{6k - 4n - 3}{\sqrt{4(k-1)n - 3k^2 + 12} + \sqrt{4(k-2)n - 3(k-1)^2 + 12}}.$$

Then by $k \geqslant 2$ and $n \geqslant k+2$ we have

$$1 - \frac{4}{k+2} < \frac{2k - 11}{2k + 3},$$

which yields $3k + 8 < 0$, a contradiction.

This finishes the proof. $\qquad\square$

4 Proof of Theorem 2

In this section, to show Theorem 2 we firstly introduce two grafting transformations on the spectral radius of graphs, which stem from [28] and can be found in the monograph [15, Theorem 8.1.20] and [15, Theoem 8.1.22].

Lemma 9. [28] *Let G be a connected graph on $n \geqslant 2$ vertices, and $v \in V(G)$. Let $G(k, \ell)$ ($k \geqslant \ell \geqslant 1$) be the graph obtained from G by attaching two pendant paths of length k and ℓ at the same vertex v. Then $\rho(G(k, \ell)) > \rho(G(k+1, \ell-1))$.*

Lemma 10. [28] *Let u, v be adjacent vertices of a connected graph G, both of degree at least 2. Let $G(k, \ell)$ ($k \geqslant \ell \geqslant 1$) be the graph obtained from G by attaching two pendant paths of length k and ℓ at u and v respectively. Then $\rho(G(k, \ell)) > \rho(G(k+1, \ell-1))$.*

Besides the above two ones, we need the following grafting transformation also.

Lemma 11. *Let G be a connected graph and $\mathbf{x} = (x_u, x_v, \cdots, x_w)^t$ be its Perron vector whose components indexed by the vertices of G. Suppose $uu_1 \cdots u_s$ and $vv_1 \cdots v_t$ are two pendant paths attached at u and v, respectively, where $s > t \geqslant 0$. Let H be the graph obtained from G by deleting edges uu_1 and vv_1 (for $t \geqslant 1$), and adding edges uv_1 and vu_1. If $x_v \geqslant x_u$, then $\rho(H) > \rho(G)$.*

Proof. We prove the lemma by induction on t. For $t = 0$ (i.e., $v_0 = v$), the result follows from Lemma 5. Suppose the lemma is true for $t = k - 1$, where $k \geqslant 1$. For $t = k$, we prove the lemma by the following two cases.

Case 1. $x_{u_1} \leqslant x_{v_1}$. Note that $u_1 u_2 \cdots u_s$ and $v_1 v_2 \cdots v_t$ are two pendant paths attached at u_1 and v_1, respectively. Clearly, H is also the graph obtained from G by deleting edges $u_1 u_2$ and $v_1 v_2$, and adding edges $u_1 v_2$ and $v_1 u_2$. Notice that the length of $v_1 v_2 \cdots v_t$ is equal to $t - 1 = k - 1$. Along with the induction hypothesis, we have $\rho(H) > \rho(G)$.

Case 2. $x_{u_1} > x_{v_1}$. From the well-known Rayleigh Theorem it follows that

$$\begin{aligned}
\rho(H) &\geqslant \mathbf{x}^t A(H) \mathbf{x} \\
&= \mathbf{x}^t A(G) \mathbf{x} + 2(x_u x_{v_1} + x_v x_{u_1}) - 2(x_u x_{u_1} + x_v x_{v_1}) \\
&= \rho(G) + 2(x_u - x_v)(x_{v_1} - x_{u_1}) \\
&\geqslant \rho(G).
\end{aligned} \tag{7}$$

If equality holds, then $x_u = x_v$, and $\mathbf{x}$ is also the Perron vector of H. Hence, $\rho(G)x_u - \rho(H)x_u = x_{u_1} - x_{v_1} > 0$, and then $\rho(G) > \rho(H)$, a contradiction. $\qquad\square$

A vertex $u \in V(G)$ is called a *major vertex* if $d(u) \geqslant 3$, and a *branch vertex* if it is a major vertex attached $d(u) - 1$ pendant paths. $T_{l_1, l_2, \ldots, l_k}$ stands for the *starlike tree* with a major vertex u of degree k satisfying $T_{l_1, l_2, \ldots, l_k} - u = P_{l_1} \cup P_{l_2} \cup \cdots \cup P_{l_k}$. The following conclusion follows from [33, Lemma 2.6] or [31, Theorem 3.8].

Lemma 12. *Let T be a tree on n vertices with at least two major vertices, and u be a branch vertex of T. The subtree T_1 is obtained from T by deleting u and the all vertices in its pendant paths. Then*

$$Z(T) = Z(T_1) + d(u) - 2. \tag{8}$$

We now introduce the tree $T_{n,k}$ on n vertices with zero forcing number k.

Definition 13. Let n and k be two integers with $n \geqslant k + 2 \geqslant 4$. Set $K_{1,k+1}$ to be a star with center u and leaves $u_1, u_2, \ldots, u_{k+1}$. Then $T_{n,k}$ is defined as follows (See Fig. 1):

- For $n \in \{k+2, k+3\}$, let $T_{k+2,k} = K_{1,k+1}$ and $T_{k+3,k}$ be the tree obtained from $K_{1,k+1}$ by attaching a pendant edge at a leaf of $K_{1,k+1}$.

- For $k+4 \leqslant n \leqslant 3k-1$, let $T_{n,k}$ be the tree obtained from $K_{1,k+1}$ by attaching two pendant edges at the vertex u_i for $1 \leqslant i \leqslant \lfloor \frac{n-k}{2} \rfloor - 1$, and attaching $(n-k) - 2\lfloor \frac{n-k}{2} \rfloor$ (equal to 0 or 1) pendant edge at the vertex u_{k+1}.

- For $n \geqslant 3k$, $T_{n,k}$ denotes the tree obtained from $K_{1,k+1}$ by attaching two pendant paths at each u_i for $1 \leqslant i \leqslant k-1$ and attaching one pendant path at u_j for $j = k, k+1$, such that the pendant paths attached at the vertices $u_1, u_2, \cdots, u_{k+1}$ are almost equal length; moreover, the lengths of the pendant paths attached at u_k and u_{k+1} are not greater than those of pendant paths attached at $u_1, u_2, \ldots, u_{k-1}$; for any $1 \leqslant i < j \leqslant k-1$, the lengths of the pendant paths attached at u_i are not less than those of pendant paths attached at u_j.

Let $\mathscr{T}'_{n,k}$ is the set of all trees with order n and zero forcing number k, where $k \geqslant 2$ and $n \geqslant k + 2$.

Theorem 14. *Let n and k be two integers with $k \geqslant 2$ and $n \geqslant k + 2$, and let $T \in \mathscr{T}'_{n,k}$. Then $\rho(T) \leqslant \rho(T_{n,k})$ with equality if and only if $T \cong T_{n,k}$.*

Proof. Suppose that $T \in \mathscr{T}'_{n,k}$ has the maximum spectral radius. Clearly, it is sufficient to prove $T \cong T_{n,k}$. If $n \in \{k+2, k+3\}$, by $Z(T) = k$ we arrive at $T \in \{T_{k+2,k}, T_{k+3,k}\}$ easily.

We next consider $n \geqslant k + 4$. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ be the Perron vector of T. Assume that T has a unique major vertex. Then T is a starlike tree with major vertex u of degree $k+1$, due to $Z(T) = k$. Let $u_1, u_2, \ldots, u_{k+1}$ be the neighbors of u. Without loss of generality, set $x_{u_1} \geqslant x_{u_i}$ for any $2 \leqslant i \leqslant k+1$. Since $n \geqslant k+4$, there is a leaf, say v, which

is not the neighbor of u or u_1. Note that $\rho(T) > 2$. Then we can deduced that $x_{u_1} \geqslant x_{v'}$, where v' is the unique neighbor of v. Let T_1 be the tree obtained from T by deleting the edge vv' and connecting v to u_1. Using Lemma 12, we get $Z(T_1) = Z(T) = k$. However, by Lemma 5 we obtain $\rho(T_1) > \rho(T)$, which contradicts the choice of T. Thereby, the tree T owns at least two major vertices.

Let w be the vertex of T with $x_w = \max\{x_i \mid 1 \leqslant i \leqslant n\}$. By $\rho(T) > 2$ we get that w is a major vertex of T. Let $w_1 \neq w$ be any branch vertex of T, and h be the (unique) neighbor of w_1 which does not lie in the pendant paths attached at w_1. If $h \neq w$, then $x_h \leqslant x_w$ by the hypothesis. We denote by T_2 the tree obtained from T by deleting the edge $w_1 h$ and adding the edge $w_1 w$. Then by Lemma 12 we deduce that $Z(T_2) = Z(T) = k$. From Lemma 5 it follows that $\rho(T) < \rho(T_2)$, a contradiction. Therefore, $h = w$ and w_1 is adjacent to w. Consequently, each major vertex other than w is a branch vertex of T which is a neighbor of w.

Claim 1. The vertex w possesses at least two pendant paths. If not, then w owns i pendant paths ($i = 0, 1$). Let w_2 be a branch vertex of T. Construct the tree T_3 obtained from T by deleting $d(w_2) - 1 - i$ pendant paths and attaching them to w. Using Lemma 12, we get $Z(T_3) = Z(T) = k$. In terms of Lemma 5, by $x_w \geqslant x_{w_2}$ we get $\rho(T) < \rho(T_3)$, a contradiction. Hence, there are at least two pendant paths attached at w. $\square$

Claim 2. All branch vertices except w of T have degree 3. Otherwise, there exists a branch vertex w_3 with $d(w_3) \geqslant 4$. Construct a new tree T_4 obtained from T by grafting one pendant path of w_3 to w. Applying Lemma 12 to T_4 and T, we get $Z(T_4) = Z(T) = k$. Since $x_w \geqslant x_{w_3}$, by Lemma 5 we have $\rho(T) < \rho(T_4)$, a contradiction. $\square$

Using Claims 1 and 2, by Lemma 12 we have $d(w) = k + 1$ as $Z(T) = k$. In order to get $T \cong T_{n,k}$, we next distinguish the following two cases.

Case 1. $k + 4 \leqslant n \leqslant 3k - 1$. Along with $d(w) = k + 1$ we know that w possesses at least three pendant paths.

Claim 3. All the pendant paths attached at w have length one, except possibly one of length two. Assume that there exits a pendant path P of w with length at least three. Construct a new tree T' from T by removing the leaf of P and connecting it to the unique neighbor of w in this path P. By Lemma 12, we get $Z(T') = k$, and so $\rho(T') > \rho(T)$ by Lemma 5, a contradiction. Suppose that w has two pendant paths P and P' with length two. Let T'' be the tree from T by transferring one leaf in P to the unique neighbor of w in P'. By Lemmas 12 and 5 we get $Z(T'') = k$ and $\rho(T) < \rho(T'')$, a contradiction. $\square$

Claim 4. For any branch vertex $u \neq w$, any pendant path attached at u has length one. In fact, if there is a pendant path P attached at u has length at least two, then let T_5 be the tree obtained from T by interchanging P with a pendant path of length one attached at w. By Lemma 12 we have $Z(T_5) = Z(T)$. But $\rho(T_5) > \rho(T)$ by Lemma 11, a contradiction. $\square$

From Claims 2, 3 and 4 it follows that $T \cong T_{n,k}$ defined in Definition 13(ii).

Case 2. $n \geqslant 3k$. We claim that w possesses exactly two pendant paths. If not, assume that there are at least three pendant paths attached at w. Similarly, Claims 3 and 4 are still true. But then $n \leqslant 3k - 1$, contradicting the condition $n \geqslant 3k$.

Recall $d(w) = k + 1$. Label the $k + 1$ neighbors of w as $w_1, w_2, \ldots, w_{k+1}$. Without

loss of generality, From Claims 2 and the above discussion we can suppose that $d_{w_i} = 3$ for $1 \leqslant i \leqslant k - 1$, and $d_{w_{k+1}} \leqslant d_{w_k} \leqslant 2$. By symmetry, we can assume $x_{w_i} \geqslant x_{w_j}$ for $1 \leqslant i < j \leqslant k - 1$. Using the similar methods as Claim 4, by Lemma 11 we get that the length of each pendant path attached at w is not less than that of each pendant path attached at $w_1, w_2, \ldots, w_{k-1}$, and for any $1 \leqslant i < j \leqslant k - 1$ the length of each pendant path attached at w_i is not less than that of each pendant path attached at w_j. Then by Lemmas 9 and 10, we see that all the pendant paths of T are of almost equal length. Hence, $T \cong T_{n,k}$ defined in Definition 13(iii). □

Lemma 15. *Let n be an integer with $n \geqslant 4$. Then $\rho(P_n) < \rho(T_{n,2}) < \rho(T_{n,3}) < \cdots < \rho(T_{n,n-2})$.*

Proof. Let $\mathbf{x} = (x_1, \cdots, x_n)$ be the Perron vector of P_n. Choose $u \in V(P_n)$ with $x_u = \max\{x_i \mid 1 \leqslant i \leqslant n\}$. Then $d(u) = 2$ by $\rho(P_n) > 1$. For $n \geqslant 4$, there exists a leaf, say v, which is not adjacent to u. Let T_1 be the tree obtained from P_n by removing v and connecting it to u. By Lemma 5 we get $\rho(P_n) < \rho(T_1)$. Clearly, $Z(T_1) = 2$, and $\rho(T_1) \leqslant \rho(T_{n,2})$ by Theorem 14.

We now prove $\rho(T_{n,k}) < \rho(T_{n,k+1})$ for $2 \leqslant k \leqslant n - 3$. Similarly above, let $\mathbf{x} = (x_i)$ be the Perron vector of $T_{n,k}$ and u be the vertex satisfying $x_u = \max\{x_i \mid 1 \leqslant i \leqslant n\}$. By $k \leqslant n - 3$, there exists a leaf of $T_{n,k}$, say v, which is not adjacent to u. Let T_2 be the tree obtained from $T_{n,k}$ by removing v from one pendant path and connecting to u. By Lemma 5 we get $\rho(T_{n,k}) < \rho(T_2)$. From Lemma 12 it follows that $Z(T_2) = k + 1$. In view of Theorem 14, we arrive at $\rho(T_2) \leqslant \rho(T_{n,k+1})$, and thus $\rho(T_{n,k}) < \rho(T_2) \leqslant \rho(T_{n,k+1})$. Consequently, $\rho(P_n) < \rho(T_{n,2}) < \rho(T_{n,3}) < \cdots < \rho(T_{n,n-2})$.

This completes the proof. □

Proof of Theorem 2: The theorem follows from Theorem 14 and Lemma 15 immediately. □

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