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Note

Extremal values and bounds for the zero forcing number

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ABSTRACT

A set Z of vertices of a graph G is a zero forcing set of G if iteratively adding to Z vertices from $V(G) \setminus Z$ that are the unique neighbor in $V(G) \setminus Z$ of some vertex in Z, results in the entire vertex set V(G) of G. The zero forcing number Z(G) of G is the minimum cardinality of a zero forcing set of G.

Amos et al. (2015) proved $Z(G) \le ((\Delta - 2)n + 2)/(\Delta - 1)$ for a connected graph G of order n and maximum degree $\Delta \ge 2$. Verifying their conjecture, we show that C_n , K_n , and $K_{\Delta,\Delta}$ are the only extremal graphs for this inequality. Confirming a conjecture of Davila and Kenter [5], we show that $Z(G) \ge 2\delta - 2$ for every triangle-free graph G of minimum degree $\delta \ge 2$. It is known that $Z(G) \ge P(G)$ for every graph G where G(G) is the minimum number of induced paths in G whose vertex sets partition G(G). We study the class of graphs G(G) which every induced subgraph G(G) of G(G) are subgraph G(G).

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1. Introduction

We consider graphs that are finite, simple, and undirected, and use standard terminology.

Let G be a graph. A set Z of vertices of G is a zero forcing set of G if every proper subset \overline{Z} of the vertex set V(G) of G with $Z \subseteq \overline{Z}$ contains a vertex that has exactly one neighbor in $V(G) \setminus \overline{Z}$. Equivalently, Z is zero forcing set of G if there is a linear ordering u_1, \ldots, u_k of the vertices in $V(G) \setminus Z$ such that for every index $i \in [k]$, there is a vertex v_i in $Z \cup \{u_1, \ldots, u_{i-1}\}$ such that u_i is the unique neighbor of v_i in $\{u_i, \ldots, u_k\}$. In this case we say that v_i forces u_i and denote this by $v_i \to u_i$. The sequence $v_1 \to u_1, v_2 \to u_2, \ldots, v_k \to u_k$ is called a forcing sequence for Z. Note that a forcing sequence specifies a linear order in which the vertices in $V(G) \setminus Z$ can be forced one after the other, and that neither the choice of the v_i nor of the forcing sequence is necessarily unique. The zero forcing number Z(G) of G is the minimum cardinality of a zero forcing set of G.

This parameter was introduced independently by the AIM Minimum Rank—Special Graphs Work Group [1] with an algebraic motivation in mind, and by Burgarth and Giovannetti [3] with a physical motivation in mind. It has already been studied in a number of papers, for instance [2,4–8,10–13].

Our contributions are as follows. In Section 2 we confirm a conjecture of Amos et al. [2] concerning the extremal graphs for some upper bound on the zero forcing number. In Section 3 we prove a lower bound on the zero forcing number of triangle-free graphs, which was conjectured by Davila and Kenter [5]. Finally, in Section 4, we extend a result of Row [11] concerning the graphs for which the zero forcing number equals a path cover number.

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2. Extremal graphs for two upper bounds

In [2] Amos et al. prove the following upper bounds on the zero forcing number.

Theorem 1 (Amos et al. [2]). Let G be a graph of order n, maximum degree Δ , and minimum degree at least 1.

- (i) $Z(G) \leq \frac{\Delta n}{\Lambda + 1}$.
- (ii) If G is connected and Δ is at least 2, then $Z(G) \leq \frac{(\Delta-2)n+2}{\Delta-1}$.

They conjecture (cf. Conjecture 6.1 in [2]) that the only extremal graphs for Theorem 1(ii) are the cycle C_n , the complete graph K_n , and the balanced complete bipartite graph $K_{\Delta,\Delta}$.

Our first goal is to prove this conjecture.

The following is a variant of Lemma 4.1 in [2].

Lemma 2. Let G be a connected graph of order n at least 2. If Z_0 is a zero forcing set of G such that $|Z_0| < n$ and $G - Z_0$ is connected, then there is a zero forcing set Z of G such that $Z \subseteq Z_0$, G-Z is connected, and every vertex in Z has a neighbor in $V(G) \setminus Z$.

Proof. Choose a zero forcing set *Z* of *G* such that $Z \subseteq Z_0$, G - Z is connected, and, subject to these conditions, *Z* is minimal with respect to inclusion. For a contradiction, we assume that some vertex in Z has no neighbor in $V(G) \setminus Z$. Since G is connected and has order at least 2, there is a path uvw such that $u, v \in Z, w \notin Z$, and u has no neighbor in $V(G) \setminus Z$. If $Z' = Z \setminus \{v\}$, then G - Z' is connected. Furthermore, since v is the unique neighbor of u in $V(G) \setminus Z'$, the set Z' is a zero forcing set of *G*, which is a contradiction.

We proceed to the proof of the conjecture of Amos et al. concerning the extremal graphs for Theorem 1(ii).

Theorem 3. If G is a connected graph of order n and maximum degree Δ at least 2, then

$$Z(G) \le \frac{(\Delta - 2)n + 2}{\Delta - 1} \tag{1}$$

with equality if and only if G is either C_n , or K_n , or $K_{\Delta,\Delta}$.

Proof. Let *G* be a connected graph of order *n* and maximum degree Δ .

Let Z_0 be an arbitrary zero forcing set of G such that $|Z_0| < n$ and $G - Z_0$ is connected. Note that such a set exists; in fact, every set of order n-1 has these properties. Let Z be as in Lemma 2. Let m be the number of edges between Z and $V(G) \setminus Z$, and let m' be the number of edges of G - Z. By Lemma 2,

$$m > |Z|. (2)$$

Since G - Z is connected

$$m' \ge n - |Z| - 1. \tag{3}$$

Since the maximum degree is Δ ,

$$m \le \Delta(n - |Z|) - 2m'. \tag{4}$$

This implies

$$|Z| \stackrel{(2)}{\leq} m \stackrel{(4)}{\leq} \Delta(n - |Z|) - 2m' \stackrel{(3)}{\leq} \Delta(n - |Z|) - 2(n - |Z| - 1),$$
 (5)

which is equivalent to (1).

We proceed to the characterization of the extremal graphs.

If
$$G = C_n$$
, then $Z(G) = 2$ and $\frac{(\Delta - 2)n + 2}{\Delta - 1} = \frac{(2 - 2)n + 2}{2 - 1} = 2$.

If
$$G = K_n$$
, then $Z(G) = n - 1$ and $\frac{(\Delta - 2)n + 2}{\Delta - 1} = \frac{(n - 3)n + 2}{n - 2} = n - 1$.

If
$$G = C_n$$
, then $Z(G) = 2$ and $\frac{(\Delta - 2)n + 2}{\Delta - 1} = \frac{(2 - 2)n + 2}{2 - 1} = 2$.
If $G = K_n$, then $Z(G) = n - 1$ and $\frac{(\Delta - 2)n + 2}{\Delta - 1} = \frac{(n - 3)n + 2}{n - 2} = n - 1$.
If $G = K_{\Delta, \Delta}$, then $Z(G) = 2\Delta - 2$ and $\frac{(\Delta - 2)n + 2}{\Delta - 1} = \frac{(\Delta - 2)2\Delta + 2}{\Delta - 1} = 2\Delta - 2$.
Therefore, if G is either C_n , or K_n , or $K_{\Delta, \Delta}$, then (1) holds with equality.

Now let (1) hold with equality. It remains to show that G is either C_n , or K_n , or $K_{\Delta,\Delta}$. In view of (5), equality in (1) implies that for every choice of Z_0 and every choice of Z, the inequalities (2), (3), and (4) hold with equality. Equality in (2) implies that

every vertex in *Z* has exactly one neighbor in $V(G) \setminus Z$. (6)

Equality in (3) implies that

$$G-Z$$
 is a tree. (7)

Finally, equality in (4) implies that

every vertex in
$$V(G) \setminus Z$$
 has degree Δ . (8)

Let u be an arbitrary vertex of G. The set $Z_0 = V(G) \setminus \{u\}$ is a zero forcing set such that $|Z_0| < n$ and $G - Z_0$ is connected. Since $u \notin Z$, (8) implies that u has degree Δ . Since u is an arbitrary vertex of G, this implies that

G is
$$\Delta$$
-regular. (9)

If $\Delta = 2$, then $G = C_n$. Hence, we may assume that $\Delta \geq 3$.

Let C be a shortest cycle of G. Let ℓ be the length of C.

First, we assume that $\ell \geq 5$. Since $\Delta \geq 3$, every vertex of C has a neighbor in $V(G) \setminus V(C)$. By the choice of C as a shortest cycle, no vertex in $V(G) \setminus V(C)$ has two neighbors on C, that is, every vertex of C is the unique neighbor in V(C) of some vertex in $V(G) \setminus V(C)$. Therefore, the set $Z_0 = V(G) \setminus V(C)$ is a zero forcing set such that $|Z_0| < n$ and $G - Z_0$ is connected. Since G - Z contains the cycle C, this yields a contradiction to C(T). Hence, $C(T) \in C(T)$.

Next, we assume that $\ell=4$. Let H be a complete bipartite subgraph of G such that each of the two partite sets A and B of H contains at least two vertices, and H has as many vertices as possible. In view of $C=K_{2,2}$, the graph H is well-defined. Since $\ell>3$, the graph G is triangle-free. Hence, H is an induced subgraph of G. Let $|A|\geq |B|$. If $|A|<\Delta$, then (9) and the choice of H imply the existence of vertices $a_1, a_2\in A$, $b_1, b_2\in B$, and $a_3, b_3\in V(G)\setminus V(H)$ such that $a_1b_3, b_1a_3\in E(G)$ and $a_2b_3, b_2a_3\not\in E(G)$. Since G is triangle-free, $a_3\neq b_3$, and $a_1a_3, a_2a_3, b_1b_3, b_2b_3\not\in E(G)$, that is, a_1 is the unique neighbor of b_3 in $\{a_1, a_2, b_1, b_2\}$, and b_1 is the unique neighbor of a_3 in $\{a_1, a_2, b_1, b_2\}$. Therefore, the set $Z_0=V(G)\setminus \{a_1, a_2, b_1, b_2\}$ is a zero forcing set such that $|Z_0|< n$ and $G-Z_0$ is connected. Since G-Z contains the cycle $a_1b_1a_2b_2a_1$, this yields a contradiction to (7). Hence, $|A|=\Delta$. By (9), we have $N_G(b)=A$ for every b in B. If $|B|=\Delta$, then $G=K_{\Delta,\Delta}$. Hence, we may assume that $|B|<\Delta$. Let $b\in B$. Now (9) and the choice of H imply the existence of vertices $a_1, a_2\in A$ and $c_1, c_2\in V(G)\setminus V(H)$ such that $a_1c_1, a_2c_2\in E(G)$ and $a_1c_2, a_2c_1\not\in E(G)$. Since G is triangle-free, G is the unique neighbor of G in G is connected. Let G be as above. If there is some G is the unique neighbor of G in G

Let K be a maximal clique in G. Since $\ell=3$, we have $n(K)\geq 3$. If $n(K)=\Delta+1$, then $G=K_n$. Hence, we may assume that $n(K)\leq \Delta$. By the choice of K, every vertex in $V(G)\setminus V(K)$ is non-adjacent to some vertex in V(K). By (9), this implies the existence of vertices $u_1,u_2\in V(K)$ and $v_1,v_2\in V(G)\setminus V(K)$ such that $u_1v_1,u_2v_2\in E(G)$ and $u_1v_2,u_2v_1\not\in E(G)$, that is, u_1 is the unique neighbor of v_1 in $\{u_1,u_2\}$, and u_2 is the unique neighbor of v_2 in $\{u_1,u_2\}$. The set $Z_0=V(G)\setminus \{u_1,u_2\}$ is a zero forcing set such that $|Z_0|< n$ and $G-Z_0$ is connected. Let Z be as above. Let $u_3\in V(K)\setminus \{u_1,u_2\}$. If $u_3\in Z$, then u_3 has the two neighbors u_1 and u_2 in $V(G)\setminus Z$, which contradicts (6). If $u_3\not\in Z$, then $u_1u_2u_3u_3$ is a cycle in G-Z, which contradicts (7). These final contradictions complete the proof.

Theorem 3 allows to determine the extremal graphs for Theorem 1(i) as well.

Corollary 4. If G is a graph of order n, maximum degree Δ , and minimum degree at least 1, then $Z(G) \leq \frac{\Delta n}{\Delta + 1}$ with equality if and only if every component of G is $K_{\Delta + 1}$.

Proof. Let G be a graph of order n, maximum degree Δ , and minimum degree at least 1. Let G be a zero forcing set of G that is minimal with respect to inclusion. A similar exchange argument as in the proof of Lemma 2 implies that every vertex in G has a neighbor in G ha

If $G = K_{\Delta+1}$, then $Z(G) = \Delta = \Delta n/(\Delta+1)$. Now let $Z(G) = \Delta n/(\Delta+1)$. If $\Delta = 1$, then $G = K_2$. Hence, we may assume that $\Delta \geq 2$. Since G is connected, Theorem 3 implies $\Delta n/(\Delta+1) \leq ((\Delta-2)n+2)/(\Delta-1)$, which is equivalent to $n \leq \Delta+1$. Since G has order G and maximum degree G, we obtain G implies that G is G has order G and maximum degree G we obtain G implies that G is G implies that G implies that G is G implies that G implies that G is G implies that G imp

3. A lower bound for triangle-free graphs

Our next result confirms a conjecture of Davila and Kenter (cf. Conjecture 2 in [5]).

Theorem 5. If G is a triangle-free graph of minimum degree δ at least 2, then $Z(G) \geq 2\delta - 2$.

Proof. Suppose for a contradiction that *G* is a triangle-free graph of minimum degree $\delta \geq 2$ such that *G* has a zero forcing set *Z* with $|Z| \leq 2\delta - 3$. Clearly, *Z* is a proper subset of V(G).

Let u_1, \ldots, u_ℓ be a maximal sequence of distinct vertices in $V(G) \setminus Z$ such that for every index $i \in [\ell]$, there is a vertex v_i in Z such that u_i is the unique neighbor of v_i in $V(G) \setminus (Z \cup \{u_1, \ldots, u_{i-1}\})$. Note that the vertices $u_i \in V(G) \setminus Z$ and $v_i \in Z$ are chosen in such a way that $v_1 \to u_1, v_2 \to u_2, \ldots, v_\ell \to u_\ell$ is part of a forcing sequence. Clearly, the vertices v_1, \ldots, v_ℓ

3

4

are all distinct. Since we require that v_i belongs to Z, the sequence u_1, \ldots, u_ℓ does not necessarily contain all vertices in $V(G) \setminus Z$.

Let
$$Z' = Z \cup \{u_1, \dots, u_\ell\}$$
 and $R = V(G) \setminus Z'$.

Claim 1. There are two distinct indices i and j in $[\ell]$ such that v_i and v_j are adjacent.

Proof of the claim. If $R \neq \emptyset$, then, since Z is a zero forcing set, the choice of the sequence u_1, \ldots, u_ℓ implies the existence of some index $i \in [\ell]$ such that u_i has a unique neighbor in R. On the other hand, if $R = \emptyset$, then let i = 1.

Note that in both cases, the vertex u_i has at most one neighbor in R and the vertex v_i has no neighbor in R. Since u_i and v_i are adjacent, this implies that there are at least $(\delta - 2) + (\delta - 1) = 2\delta - 3$ edges between $\{u_i, v_i\}$ and $Z' \setminus \{u_i, v_i\}$. By the pigeonhole principle, we obtain that there are at least 2 edges between $\{u_i, v_i\}$ and one of the $|Z| - 1 \le 2\delta - 4$ many sets in

$$\left\{ \{u_j, v_j\} : j \in [\ell] \setminus \{i\} \right\} \cup \left\{ \{v\} : v \in Z \setminus \{v_1, \dots, v_\ell\} \right\}.$$

Since G is triangle-free, the vertices u_i and v_i have no common neighbor, which implies the existence of some index $j \in [\ell] \setminus \{i\}$ such that there are 2 disjoint edges between $\{u_i, v_i\}$ and $\{u_j, v_j\}$. If v_i is adjacent to u_j and v_j is adjacent to u_i , we obtain a contradiction to the choice of the sequence u_1, \ldots, u_ℓ . Hence, the vertices v_i and v_j are adjacent, which completes the proof of the claim. \square

Let the pair (i,j) of distinct indices in $[\ell]$ be chosen lexicographically minimal such that v_i and v_j are adjacent. Note that the claim implies that (i,j) is well defined and that neither v_i nor v_j has a neighbor in R. Since v_i and v_j are adjacent, this implies that there are at least $(\delta-2)+(\delta-2)=2\delta-4$ edges between $\{v_i,v_j\}$ and $Z'\setminus\{v_i,v_j,u_i,u_j\}$. By the pigeonhole principle, we obtain that there are at least 2 edges between $\{v_i,v_j\}$ and one of the $|Z|-2\leq 2\delta-5$ many sets in

$$\Big\{\{u_r,v_r\}:r\in[\ell]\setminus\{i,j\}\Big\}\cup\Big\{\{v\}:v\in Z\setminus\{v_1,\ldots,v_\ell\}\Big\}.$$

Since G is triangle-free, the vertices v_i and v_j have no common neighbor, which implies the existence of some index $r \in [\ell] \setminus \{i, j\}$ such that there are 2 disjoint edges between $\{v_i, v_j\}$ and $\{u_r, v_r\}$.

If v_i is adjacent to v_r and, consequently, v_j is adjacent to u_r , then the choice of the sequence u_1, \ldots, u_ℓ implies r < j, and the pair (i, r) of distinct indices in $[\ell]$ is such that v_i and v_r are adjacent. Since (i, r) is lexicographically smaller than (i, j), we obtain a contradiction to the choice of (i, j). If v_i is adjacent to u_r and, consequently, v_j is adjacent to v_r , then the choice of the sequence u_1, \ldots, u_ℓ implies r < i, and the pair (r, j) of distinct indices in $[\ell]$ is such that v_r and v_j are adjacent. Since (r, j) is lexicographically smaller than (i, j), we obtain a contradiction to the choice of (i, j). Since both cases lead to a contradiction, the proof is complete. \square

4. Equality with a path cover number

In this section we consider a natural well known lower bound on the zero forcing number.

If Z is a zero forcing set of a graph G, and $v_1 \to u_1, v_2 \to u_2, \ldots, v_k \to u_k$ is a forcing sequence for Z, then a maximal sequence of the form $x_0, x_0 \to x_1, x_1, x_1 \to x_2, x_2, \ldots, x_{\ell-1} \to x_\ell, x_\ell$ for $\ell \geq 0$ defines an induced path $x_0 x_1 \ldots x_\ell$ in G with $x_0 \in Z$. Such a path is called a *forcing path* of the forcing sequence. Since Z is a zero forcing set, every vertex of G lies exactly on one forcing path, that is, the forcing paths of a forcing sequence form a set of induced paths in G such that every vertex of G lies on exactly one of these paths. If the *path cover number* P(G) is the minimum number of induced paths such that every vertex of G lies on exactly one of these paths, then the above observations imply

$$Z(G) > P(G). (10)$$

The AIM group [1] observed that (10) holds with equality for forests. This was extended by Row [11] who showed that (10) holds with equality for cacti, that is, for graphs in which every two distinct cycles are edge-disjoint. Since forests and cacti form hereditary classes of graphs, these results motivate the study of the hereditary class of graphs

$$\mathbb{Z}\mathcal{P} = \{G : G \text{ is a graph and } Z(H) = P(H) \text{ for every induced subgraph } H \text{ of } G\}.$$

For positive integers ℓ_1 , ℓ_2 , and ℓ_3 with ℓ_2 , $\ell_3 \geq 2$, let $\Theta(\ell_1, \ell_2, \ell_3)$ be the graph that has two vertices of degree 3 that are linked by three paths of lengths ℓ_1 , ℓ_2 , and ℓ_3 , respectively, whose internal vertices are all of degree 2.

The following is a folklore result; we include a proof for the sake of completeness.

Proposition 6. A graph is a cactus if and only if it is $\{K_4\} \cup \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_2, \ell_3 \geq 2\}$ -free.

Proof. If *G* is a cactus, then *G* is clearly $\{K_4\} \cup \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_2, \ell_3 \geq 2\}$ -free. Now let *G* be a $\{K_4\} \cup \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_2, \ell_3 \geq 2\}$ -free graph. Let *B* be a block of *G*. For a contradiction, we assume that *B* is neither K_2 nor an induced cycle. Let *C* be a shortest induced cycle of *B*. Let $u \in V(B) \setminus V(C)$ have a neighbor on *C*. If *u* has at least three neighbors on *C*, then the choice of *C* implies that *C* is a triangle, and $G[\{u\} \cup C]$ is K_4 , which is a contradiction. Hence, *u* has at most two neighbors on *C*. If *u* has two neighbors on *C*, then $G[\{u\} \cup C] \in \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_2, \ell_3 \geq 2\}$, which is a contradiction. Hence, *u* has exactly one neighbor *v* on *C*. By symmetry, we may assume that every vertex in $V(B) \setminus V(C)$ has at most one neighbor on *C*. Now, if *P* is a shortest path in B - v between *u* and a vertex of *C*, then $G[V(P) \cup V(C)] \in \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_2, \ell_3 \geq 2\}$, which is a contradiction, and completes the proof. \Box

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Note that $P(K_4) = 2 < 3 = Z(K_4)$. Furthermore, for $\ell_1, \ell_2, \ell_3 \ge 2$, we have $P(\Theta(\ell_1, \ell_2, \ell_3)) = 2 < 3 = Z(\Theta(\ell_1, \ell_2, \ell_3))$. Since every proper induced subgraph of K_4 or $\Theta(\ell_1, \ell_2, \ell_3)$ is a cactus, this implies that all graphs in $\{K_4\} \cup \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_1, \ell_2, \ell_3 \ge 2\}$ are minimal forbidden induced subgraphs for $\mathbb{Z}\mathcal{P}$. Our next result extends the result of Row [11] mentioned above.

Theorem 7. If G is a graph such that every cycle of G is induced, then the following statements are equivalent.

- (i) $G \in \mathbb{ZP}$.
- (ii) G is a cactus.
- (iii) G is $\{K_4\} \cup \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_1, \ell_2, \ell_3 \geq 2\}$ -free.

Proof. Let *G* be a graph such that every cycle of *G* is induced. Since $\Theta(1, \ell_2, \ell_3)$ contains a cycle that is not induced for every $\ell_2, \ell_3 \geq 2$, Proposition 6 implies the equivalence of (ii) and (iii). Since the class of cacti is hereditary, Row's result from [11] implies that (ii) implies (i). Finally, as observed just before the statement of Theorem 7, all graphs in $\{K_4\} \cup \{\Theta(\ell_1, \ell_2, \ell_3) : \ell_1, \ell_2, \ell_3 \in \mathbb{N} \text{ and } \ell_1, \ell_2, \ell_3 \geq 2\}$ are minimal forbidden induced subgraphs for $\mathbb{Z}\mathcal{P}$, which implies that (i) implies (iii), and completes the proof. \square

Note that the class of graphs such that every cycle is induced is still a relatively large class; for every graph, a suitable subdivision belongs to this class. We leave it as an open problem to determine the complete list of minimal forbidden induced subgraphs for $\mathbb{Z}P$.

Note that the complexities of Z(G) and P(G) differ drastically. For every fixed integer k, one can decide in $O(n^k)$ time whether a given graph G of order n satisfies $Z(G) \le k$ by considering all sets of k vertices of G and checking whether one of them is a zero forcing set. In contrast to that, Le et al. [9] showed that it is NP-complete to decide whether a given graph G satisfies $P(G) \le 2$.

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