

## Article

# The First Zagreb Index and Some Hamiltonian Properties of Graphs

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**Abstract:** Let  $G = (V, E)$  be a graph. The first Zagreb index of a graph  $G$  is defined as  $\sum_{u \in V} d_G^2(u)$ , where  $d_G(u)$  is the degree of vertex  $u$  in  $G$ . A graph  $G$  is called Hamiltonian (resp. traceable) if  $G$  has a cycle (resp. path) containing all the vertices of  $G$ . Using two established inequalities, in this paper, we present sufficient conditions involving the first Zagreb index for Hamiltonian graphs and traceable graphs. We also present upper bounds for the first Zagreb index of a graph and characterize the graphs achieving the upper bounds.

**Keywords:** the first Zagreb index; Hamiltonian graph, traceable graph; upper bound

**MSC:** 05C45; 05C09

## 1. Introduction

We consider only finite undirected graphs without loops or multiple edges. Notation and terminology not defined in this paper follow those in [1]. Let  $G = (V(G), E(G))$  be a graph. We use  $n$  and  $e$  to denote the number of vertices and the number of edges in  $G$ , respectively. The degree of a vertex  $u$  is represented by  $d_G(u)$ . The minimum and maximum degrees of a graph  $G$  are represented, respectively, by  $\delta(G)$  and  $\Delta(G)$ . A subset of  $V(G)$  in a graph  $G$  is an independent set if any two vertices in the subset are not adjacent. An independent set in a graph  $G$  is called a maximum independent set if its size is as large as possible. The independence number, denoted  $\beta(G)$ , of a graph  $G$  is defined as the size of a maximum independent set in  $G$ . For two disjoint vertex subsets,  $A$  and  $B$ , of  $V(G)$ , we define  $E(A, B)$  as the set of all the edges in  $E(G)$  such that one end vertex of each edge is in  $A$  and another end vertex of the edge is in  $B$ . Namely,  $E(A, B) := \{e : e = ab \in E, a \in A, b \in B\}$ . We use  $K_{r,s}$  to denote a complete bipartite graph with two partition sets  $X$  and  $Y$  such that  $|X| = r$  and  $|Y| = s$ . A cycle  $C$  in a graph  $G$  is a Hamiltonian cycle of  $G$  if all the vertices of  $G$  are on  $C$ . A graph  $G$  is called Hamiltonian if  $G$  contains a Hamiltonian cycle. A path  $P$  in a graph  $G$  is a Hamiltonian path of  $G$  if all the vertices of  $G$  are on  $P$ . A graph  $G$  is called traceable if  $G$  contains a Hamiltonian path.

The first Zagreb index of a graph was introduced by Gutman and Trinajstić in [2]. For a graph  $G$ , its first Zagreb index, denoted  $Z_1(G)$ , is defined as  $\sum_{u \in V(G)} d_G^2(u)$ . The first Zagreb index is one of the most important topological indices of a graph. It has been intensively investigated since its introduction. Many results on the first Zagreb index of a graph have been obtained. The survey paper [3] and the references therein are good resources for these results. Using the first Zagreb index and its variants, researchers, in recent years, have obtained sufficient conditions for the Hamiltonian properties of graphs. Some of these sufficient conditions appeared in [4–10]. Using two established inequalities, we, in this paper, present new sufficient conditions involving the first Zagreb index for Hamiltonian and traceable graphs. We also present new upper bounds for the first Zagreb index of a graph and characterize graphs achieving the upper bounds. The main results of this paper are as follows.



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**Theorem 1.** Let  $G$  be a  $k$ -connected ( $k \geq 2$ ) graph with  $n \geq 3$  vertices and  $e$  edges.

(1) If

$$Z_1(G) \geq (n - k - 1)\Delta^2 + \frac{e^2}{k+1} + \left(\sqrt{n - k - 1} - \sqrt{\delta}\right)^2 e,$$

then  $G$  is Hamiltonian or  $G$  is  $K_{k,k+1}$ .

(2) If

$$Z_1(G) \geq (n - k - 1)\Delta^2 + \frac{1}{k+1} \left( \frac{(k+1)(n - k - 1 - \delta)^2}{4(\delta + n - k - 1)} + e \right)^2,$$

then  $G$  is Hamiltonian or  $G$  is  $K_{k,k+1}$ .

**Theorem 2.** Let  $G$  be a  $k$ -connected ( $k \geq 1$ ) graph with  $n \geq 9$  vertices and  $e$  edges.

(1) If

$$Z_1(G) \geq (n - k - 2)\Delta^2 + \frac{e^2}{k+2} + \left(\sqrt{n - k - 2} - \sqrt{\delta}\right)^2 e,$$

then  $G$  is traceable or  $G$  is  $K_{k,k+2}$ .

(2) If

$$Z_1(G) \geq (n - k - 2)\Delta^2 + \frac{1}{k+2} \left( \frac{(k+2)(n - k - 2 - \delta)^2}{4(\delta + n - k - 2)} + e \right)^2,$$

then  $G$  is traceable or  $G$  is  $K_{k,k+2}$ .

**Theorem 3.** Let  $G$  be a graph with  $n$  vertices,  $e$  edges, and  $\delta \geq 1$ . Then,

(1)

$$Z_1(G) \leq (n - \beta)\Delta^2 + \frac{e^2}{\beta} + \left(\sqrt{n - \beta} - \sqrt{\delta}\right)^2 e$$

with equality if and only if  $G$  is  $K_{\beta, n-\beta}$  or  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$  such that  $|I| = \beta$ ,  $\delta < n - \beta$ , and  $d(v) = \Delta$  for each vertex  $v$  in  $v - I$  and  $I = P \cup Q$ , where  $P = \{x : x \in I, d(x) = n - \beta\}$ ,  $Q = \{y : y \in I, d(y) = \delta\}$ , and

$$\frac{\beta}{|P|} = 1 + \left(\frac{n - \beta}{\delta}\right)^{\frac{1}{2}},$$

where  $|P|$  is an integer.

(2)

$$Z_1(G) \leq (n - \beta)\Delta^2 + \frac{1}{\beta} \left( \frac{\beta(n - \beta - \delta)}{4(\delta + n - \beta)} + e \right)^2$$

with equality if and only if  $G$  is  $K_{\beta, n-\beta}$  or  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$  such that  $|I| = \beta$ ,  $\delta < n - \beta$ , and  $d(v) = \Delta$  for each vertex  $v$  in  $v - I$  and  $I = P \cup Q$ , where  $P = \{x : x \in I, d(x) = n - \beta\}$ ,  $Q = \{y : y \in I, d(y) = \delta\}$ ,  $P \cap Q = \emptyset$ , and

$$|P| = \frac{n - \beta + 3\delta}{4(n - \beta + \delta)}$$

is an integer.

## 2. Preliminaries

We will use the following results as our lemmas. The first two are from [11].

**Lemma 1** ([11]). Let  $G$  be a  $k$ -connected graph of order  $n \geq 3$ . If  $\beta \leq k$ , then  $G$  is Hamiltonian.

**Lemma 2** ([11]). Let  $G$  be a  $k$ -connected graph of order  $n$ . If  $\beta \leq k + 1$ , then  $G$  is traceable.

Lemma 3 is an inequality given on Page 303 in [12].

**Lemma 3 ([12]).** Let the real numbers  $a_k$  and  $b_k$  ( $k = 1, 2, \dots, s$ ) satisfy  $0 < m_1 \leq a_k \leq M_1$  and  $0 < m_2 \leq b_k \leq M_2$ . Then,

$$\sum_{k=1}^s a_k^2 \sum_{k=1}^s b_k^2 - \left( \sum_{k=1}^s a_k b_k \right)^2 \leq \left( \sqrt{\frac{M_1}{m_2}} - \sqrt{\frac{m_1}{M_2}} \right)^2 \sum_{k=1}^s a_k b_k \sum_{k=1}^s b_k^2,$$

with equality holding if and only if there exists a subsequence  $(k_1, k_2, \dots, k_t)$  of  $(1, 2, \dots, s)$  such that

$$\frac{n}{t} = 1 + \left( \frac{M_1}{m_1} \right)^{\frac{1}{2}} \left( \frac{m_2}{M_2} \right)^{\frac{3}{2}},$$

$a_{k_\mu} = M_1, b_{k_\mu} = m_2$  ( $\mu = 1, 2, \dots, t$ ), and  $a_k = m_1, b_k = M_2$  for every  $k$  distinct from all  $k_\mu$ .

Lemma 4 is Theorem 5.21 on Page 82 and Page 83 in [13].

**Lemma 4 ([13]).** Suppose  $a_k$  and  $b_k$  ( $k = 1, 2, \dots, s$ ) are positive real numbers satisfying  $0 < \gamma \leq \frac{a_k}{b_k} \leq \Gamma < \infty$  for any  $k \in \{1, 2, \dots, s\}$ . Then,

$$0 \leq \left( \sum_{k=1}^s a_k^2 \sum_{k=1}^s b_k^2 \right)^{\frac{1}{2}} - \sum_{k=1}^s a_k b_k \leq \frac{(\Gamma - \gamma)^2}{4(\gamma + \Gamma)} \sum_{k=1}^s b_k^2.$$

Equality holds in the above inequality if and only if there exists a subsequence  $(k_1, k_2, \dots, k_t)$  of  $(1, 2, \dots, s)$  such that

$$\sum_{m=1}^t b_{k_m}^2 = \frac{\Gamma + 3\gamma}{4(\Gamma + \gamma)} \sum_{j=1}^s b_j^2,$$

$\frac{a_{k_m}}{b_{k_m}} = \Gamma$  ( $m = 1, 2, \dots, t$ ), and  $\frac{a_k}{b_k} = \gamma$  for every  $k$  distinct from all  $k_m$ .

**Lemma 5 ([14]).** Let  $G$  be a balanced bipartite graph of order  $2n$  with the bipartition  $(A, B)$ . If  $d(x) + d(y) \geq n + 1$  for any  $x \in A$  and any  $y \in B$  with  $xy \notin E$ , then  $G$  is Hamiltonian.

**Lemma 6 ([15]).** Let  $G$  be a two-connected bipartite graph with the bipartition  $(A, B)$ , where  $|A| \geq |B|$ . If each vertex in  $A$  has a degree of at least  $s$  and each vertex in  $B$  has a degree of at least  $t$ , then  $G$  contains a cycle with a length of at least  $2 \min(|B|, s + t - 1, 2s - 2)$ .

### 3. Proofs of the Main Results

**Proof of Theorem 1.** Let  $G$  be a  $k$ -connected ( $k \geq 2$ ) graph with  $n \geq 3$  vertices and  $e$  edges satisfying the conditions in Theorem 1. Suppose  $G$  is not Hamiltonian. Then, Lemma 1 implies that  $\beta \geq k + 1$ . Also, we have that  $n \geq 2\delta + 1 \geq 2k + 1$ ; otherwise,  $\delta \geq k \geq n/2$  and  $G$  is Hamiltonian. Let  $I_1 := \{u_1, u_2, \dots, u_\beta\}$  be a maximum independent set in  $G$ . Then,  $I := \{u_1, u_2, \dots, u_{k+1}\}$  is an independent set in  $G$ . Thus,

$$\sum_{u \in I} d(u) = |E(I, V - I)| \leq \sum_{v \in V - I} d(v).$$

Since  $\sum_{u \in I} d(u) + \sum_{v \in V - I} d(v) = 2e$ , we have that

$$\sum_{u \in I} d(u) \leq e \leq \sum_{v \in V - I} d(v).$$

Notice that  $0 < \delta \leq d(u) \leq n - k - 1$  for each  $u \in I$ .

(1). Applying Lemma 3 with  $s = k + 1$ ,  $a_i = d(u_i)$ , and  $b_i = 1$ , with  $i = 1, 2, \dots, (k + 1)$ ,  $m_1 = \delta > 0$ ,  $M_1 = n - k - 1$ ,  $m_2 = 1 > 0$ , and  $M_2 = 1$ , we have

$$\sum_{i=1}^{k+1} d^2(u_i) \sum_{i=1}^{k+1} 1^2 - \left( \sum_{i=1}^{k+1} d(u_i) \right)^2 \leq \left( \sqrt{n-k-1} - \sqrt{\delta} \right)^2 \sum_{i=1}^{k+1} d(u_i) \sum_{i=1}^{k+1} 1^2.$$

Thus,

$$\begin{aligned} \sum_{i=1}^{k+1} d^2(u_i) &\leq \frac{\left( \sum_{i=1}^{k+1} d(u_i) \right)^2}{k+1} + \left( \sqrt{n-k-1} - \sqrt{\delta} \right)^2 \sum_{i=1}^{k+1} d(u_i) \\ &\leq \frac{e^2}{k+1} + \left( \sqrt{n-k-1} - \sqrt{\delta} \right)^2 e. \end{aligned}$$

Therefore,

$$\begin{aligned} (n-k-1)\Delta^2 + \frac{e^2}{k+1} + \left( \sqrt{n-k-1} - \sqrt{\delta} \right)^2 e \\ \leq Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ \leq (n-k-1)\Delta^2 + \frac{e^2}{k+1} + \left( \sqrt{n-k-1} - \sqrt{\delta} \right)^2 e. \end{aligned}$$

Hence,  $d(v) = \Delta$  for each  $v \in V - I$ ,

$$\sum_{i=1}^{k+1} d^2(u_i) \sum_{i=1}^{k+1} 1^2 - \left( \sum_{i=1}^{k+1} d(u_i) \right)^2 = \left( \sqrt{n-k-1} - \sqrt{\delta} \right)^2 \sum_{i=1}^{k+1} d(u_i) \sum_{i=1}^{k+1} 1^2,$$

and  $\sum_{i=1}^{k+1} d(u_i) = e$ , which implies that  $\sum_{v \in V-I} d(v) = e$  and  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$ .

For the characterization of the extremal graphs, we divide the remaining proofs into two cases.

**Case 1.**  $\delta = n - k - 1$ .

In this case, we have  $d(u) = \delta$  for each  $u$  in  $I$  and thereby  $\delta(k+1) = |E(I, V-I)| = \Delta(n-k-1) \geq \delta(n-k-1)$ . Thus,  $n \leq 2k+2$ . Since  $n \geq 2k+1$ , we have  $n = 2k+2$  or  $n = 2k+1$ . If  $n = 2k+2$ , then Lemma 5 implies that  $G$  is Hamiltonian, which is a contradiction. If  $n = 2k+1$ , then  $G$  is  $K_{k,k+1}$ .

**Case 2.**  $\delta < n - k - 1$ .

In this case, set  $P = \{x : x \in I, d(x) = n - k - 1\}$  and  $Q = \{y : y \in I, d(y) = \delta\}$ . From Lemma 3, we have

$$\frac{k+1}{|P|} = 1 + \left( \frac{n-k-1}{\delta} \right)^{\frac{1}{2}}.$$

Choose one vertex  $x$  in  $P$  and one vertex  $w$  in  $V - I$ . Then,  $n - k - 1 = d(x) \leq \Delta = d(w) \leq k + 1$ . Thus,  $n \leq 2k + 2$ . Since  $n \geq 2k + 1$ , we have  $n = 2k + 2$  or  $n = 2k + 1$ . If  $n = 2k + 2$ , then Lemma 5 implies that  $G$  is Hamiltonian, which is a contradiction. If  $n = 2k + 1$ , then  $G$  is  $K_{k,k+1}$ , which implies that  $n - k - 1 = \delta$ , which is a contradiction.

(2). Applying Lemma 4 with  $s = k + 1$ ,  $a_i = d(u_i)$ , and  $b_i = 1$ , with  $i = 1, 2, \dots, (k + 1)$ ,  $\gamma = \delta > 0$ , and  $\Gamma = n - k - 1$ , we have

$$\left( \sum_{i=1}^{k+1} d^2(u_i) \sum_{i=1}^{k+1} 1^2 \right)^{\frac{1}{2}} - \sum_{k=1}^{k+1} d(u_i) \leq \frac{(n-k-1-\delta)^2}{4(\delta+n-k-1)} \sum_{i=1}^{k+1} 1^2.$$

Thus,

$$\begin{aligned} \sum_{i=1}^{k+1} d^2(u_i) &\leq \frac{1}{k+1} \left( \frac{(k+1)(n-k-1-\delta)^2}{4(\delta+n-k-1)} + \sum_{k=1}^{k+1} d(u_i) \right)^2 \\ &\leq \frac{1}{k+1} \left( \frac{(k+1)(n-k-1-\delta)^2}{4(\delta+n-k-1)} + e \right)^2. \end{aligned}$$

Therefore,

$$\begin{aligned} (n-k-1)\Delta^2 + \frac{1}{k+1} \left( \frac{(k+1)(n-k-1-\delta)^2}{4(\delta+n-k-1)} + e \right)^2 \\ \leq Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ \leq (n-k-1)\Delta^2 + \frac{1}{k+1} \left( \frac{(k+1)(n-k-1-\delta)^2}{4(\delta+n-k-1)} + e \right)^2. \end{aligned}$$

Hence,  $d(v) = \Delta$  for each  $v \in V - I$ ,

$$\left( \sum_{i=1}^{k+1} d^2(u_i) \sum_{i=1}^{k+1} 1^2 \right)^{\frac{1}{2}} - \sum_{k=1}^{k+1} d(u_i) = \frac{(n-k-1-\delta)^2}{4(\delta+n-k-1)} \sum_{i=1}^{k+1} 1^2,$$

and  $\sum_{i=1}^{k+1} d(u_i) = e$ , which implies that  $\sum_{v \in V-I} d(v) = e$  and  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$ .

For the characterization of the extremal graphs, we divide the remaining proofs into two cases.

**Case 1.**  $\delta = n - k - 1$ .

In this case, we have  $d(u) = \delta$  for each  $u$  in  $I$ , and thereby  $\delta(k+1) = |E(I, V-I)| = \Delta(n-k-1) \geq \delta(n-k-1)$ . Thus,  $n \leq 2k+2$ . Since  $n \geq 2k+1$ , we have  $n = 2k+2$  or  $n = 2k+1$ . If  $n = 2k+2$ , then Lemma 5 implies that  $G$  is Hamiltonian, which is a contradiction. If  $n = 2k+1$ , then  $G$  is  $K_{k,k+1}$ .

**Case 2.**  $\delta < n - k - 1$ .

In this case, set  $P = \{x : x \in I, d(x) = n - k - 1\}$  and  $Q = \{y : y \in I, d(y) = \delta\}$ . From Lemma 4, we have

$$|P| = \frac{(k+1)(n-k-1+3\delta)}{4(\delta+n-k-1)}.$$

Choose one vertex  $x$  in  $P$  and one vertex  $w$  in  $V - I$ . Then,  $n - k - 1 = d(x) \leq \Delta = d(w) \leq k + 1$ . Thus,  $n \leq 2k + 2$ . Since  $n \geq 2k + 1$ , we have  $n = 2k + 2$  or  $n = 2k + 1$ . If  $n = 2k + 2$ , then Lemma 5 implies that  $G$  is Hamiltonian, which is a contradiction. If  $n = 2k + 1$ , then  $G$  is  $K_{k,k+1}$ , which implies that  $n - k - 1 = \delta$ , which is a contradiction.

This completes the proof of Theorem 1.  $\square$

The proof of Theorem 2 is similar to the proof of Theorem 1. For the sake of completeness, we still present a full proof of Theorem 2 below.

**Proof of Theorem 2.** Let  $G$  be a  $k$ -connected ( $k \geq 1$ ) graph with  $n \geq 9$  vertices and  $e$  edges satisfying the conditions in Theorem 2. Suppose  $G$  is not traceable. Then, Lemma 2 implies that  $\beta \geq k + 2$ . Also, we have that  $n \geq 2\delta + 2 \geq 2k + 2$ ; otherwise,  $\delta \geq k \geq (n - 1)/2$  and  $G$  is traceable. Let  $I_1 := \{u_1, u_2, \dots, u_\beta\}$  be a maximum independent set in  $G$ . Then,  $I := \{u_1, u_2, \dots, u_{k+2}\}$  is an independent set in  $G$ . Thus,

$$\sum_{u \in I} d(u) = |E(I, V - I)| \leq \sum_{v \in V - I} d(v).$$

Since  $\sum_{u \in I} d(u) + \sum_{v \in V - I} d(v) = 2e$ , we have that

$$\sum_{u \in I} d(u) \leq e \leq \sum_{v \in V - I} d(v).$$

Notice that  $0 < \delta \leq d(u) \leq n - k - 2$  for each  $u \in I$ .

(1). Applying Lemma 3 with  $s = k + 2$ ,  $a_i = d(u_i)$ , and  $b_i = 1$ , with  $i = 1, 2, \dots, (k + 2)$ ,  $m_1 = \delta > 0$ ,  $M_1 = n - k - 2$ ,  $m_2 = 1 > 0$ , and  $M_2 = 1$ , we have

$$\sum_{i=1}^{k+2} d^2(u_i) \sum_{i=1}^{k+2} 1^2 - \left( \sum_{k=1}^{k+2} d(u_i) \right)^2 \leq \left( \sqrt{n - k - 2} - \sqrt{\delta} \right)^2 \sum_{k=1}^{k+2} d(u_i) \sum_{i=1}^{k+2} 1^2.$$

Thus,

$$\begin{aligned} \sum_{i=1}^{k+2} d^2(u_i) &\leq \frac{\left( \sum_{k=1}^{k+2} d(u_i) \right)^2}{k + 2} + \left( \sqrt{n - k - 2} - \sqrt{\delta} \right)^2 \sum_{k=1}^{k+2} d(u_i) \\ &\leq \frac{e^2}{k + 2} + \left( \sqrt{n - k - 2} - \sqrt{\delta} \right)^2 e. \end{aligned}$$

Therefore,

$$\begin{aligned} (n - k - 2)\Delta^2 + \frac{e^2}{k + 2} + \left( \sqrt{n - k - 2} - \sqrt{\delta} \right)^2 e \\ \leq Z_1 = \sum_{v \in V - I} d^2(v) + \sum_{u \in I} d^2(u) \\ \leq (n - k - 2)\Delta^2 + \frac{e^2}{k + 2} + \left( \sqrt{n - k - 2} - \sqrt{\delta} \right)^2 e. \end{aligned}$$

Hence,  $d(v) = \Delta$  for each  $v \in V - I$ ,

$$\sum_{i=1}^{k+2} d^2(u_i) \sum_{i=1}^{k+2} 1^2 - \left( \sum_{k=1}^{k+2} d(u_i) \right)^2 = \left( \sqrt{n - k - 2} - \sqrt{\delta} \right)^2 \sum_{k=1}^{k+2} d(u_i) \sum_{i=1}^{k+2} 1^2,$$

and  $\sum_{i=1}^{k+2} d(u_i) = e$ , which implies that  $\sum_{v \in V - I} d(v) = e$  and  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$ .

For the characterization of the extremal graphs, we divide the remaining proofs into two cases.

**Case 1.**  $\delta = n - k - 2$ .

In this case, we have  $d(u) = \delta$  for each  $u$  in  $I$ , and thereby  $\delta(k + 2) = |E(I, V - I)| = \Delta(n - k - 2) \geq \delta(n - k - 2)$ . Thus,  $n \leq 2k + 4$ . Since  $n \geq 2k + 2$ , we have  $n = 2k + 4$ ,  $n = 2k + 3$ , or  $n = 2k + 2$ . If  $n = 2k + 4$ , then Lemma 5 implies that  $G$  is Hamiltonian and thereby  $G$  is traceable. If  $n = 2k + 3$ , then  $k \geq 3$  since  $n \geq 9$ . Thus, Lemma 6 implies that  $G$  has a cycle with a length of at least  $(n - 1)$  and thereby  $G$  is traceable, which is a contradiction. If  $n = 2k + 2$ , then  $G$  is  $K_{k, k+2}$ .

**Case 2.**  $\delta < n - k - 2$ .

In this case, set  $P = \{x : x \in I, d(x) = n - k - 2\}$  and  $Q = \{y : y \in I, d(y) = \delta\}$ . From Lemma 3, we have

$$\frac{k+2}{|P|} = 1 + \left(\frac{n-k-2}{\delta}\right)^{\frac{1}{2}}.$$

Choose one vertex  $x$  in  $P$  and one vertex  $w$  in  $V - I$ . Then,  $n - k - 2 = d(x) \leq \Delta = d(w) \leq k + 2$ . Thus,  $n \leq 2k + 4$ . Since  $n \geq 2k + 2$ , we have  $n = 2k + 4$ ,  $n = 2k + 3$ , or  $n = 2k + 2$ . If  $n = 2k + 4$ , then Lemma 5 implies that  $G$  is Hamiltonian and thereby  $G$  is traceable, which is a contradiction. If  $n = 2k + 3$ , then  $k \geq 3$  since  $n \geq 9$ . Then, Lemma 6 implies that  $G$  has a cycle with a length of at least  $(n - 1)$  and thereby  $G$  is traceable, which is a contradiction. If  $n = 2k + 2$ , then  $G$  is  $K_{k,k+2}$  and  $n - k - 2 = \delta$ , which is a contradiction.

(2). Applying Lemma 4 with  $s = k + 2$ ,  $a_i = d(u_i)$ , and  $b_i = 1$ , with  $i = 1, 2, \dots, (k + 2)$ ,  $\gamma = \delta > 0$ , and  $\Gamma = n - k - 2$ , we have

$$\left(\sum_{i=1}^{k+2} d^2(u_i) \sum_{i=1}^{k+2} 1^2\right)^{\frac{1}{2}} - \sum_{k=1}^{k+2} d(u_i) \leq \frac{(n-k-2-\delta)^2}{4(\delta+n-k-2)} \sum_{i=1}^{k+2} 1^2.$$

Thus,

$$\begin{aligned} \sum_{i=1}^{k+2} d^2(u_i) &\leq \frac{1}{k+2} \left( \frac{(k+2)(n-k-2-\delta)^2}{4(\delta+n-k-2)} + \sum_{k=1}^{k+2} d(u_i) \right)^2 \\ &\leq \frac{1}{k+2} \left( \frac{(k+2)(n-k-2-\delta)^2}{4(\delta+n-k-2)} + e \right)^2. \end{aligned}$$

Therefore,

$$\begin{aligned} (n-k-2)\Delta^2 + \frac{1}{k+2} \left( \frac{(k+2)(n-k-2-\delta)^2}{4(\delta+n-k-2)} + e \right)^2 \\ \leq Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ \leq (n-k-2)\Delta^2 + \frac{1}{k+2} \left( \frac{(k+2)(n-k-2-\delta)^2}{4(\delta+n-k-2)} + e \right)^2. \end{aligned}$$

Hence,  $d(v) = \Delta$  for each  $v \in V - I$ ,

$$\left(\sum_{i=1}^{k+2} d^2(u_i) \sum_{i=1}^{k+2} 1^2\right)^{\frac{1}{2}} - \sum_{k=1}^{k+2} d(u_i) = \frac{(n-k-2-\delta)^2}{4(\delta+n-k-2)} \sum_{i=1}^{k+2} 1^2,$$

and  $\sum_{i=1}^{k+2} d(u_i) = e$ , which implies that  $\sum_{v \in V-I} d(v) = e$  and  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$ .

For the characterization of the extremal graphs, we divide the remaining proofs into two cases.

**Case 1.**  $\delta = n - k - 2$ .

In this case, we have  $d(u) = \delta$  for each  $u$  in  $I$ , and thereby  $\delta(k + 2) = |E(I, V - I)| = \Delta(n - k - 2) \geq \delta(n - k - 2)$ . Thus,  $n \leq 2k + 4$ . Since  $n \geq 2k + 2$ , we have  $n = 2k + 4$ ,  $n = 2k + 3$ , or  $n = 2k + 2$ . If  $n = 2k + 4$ , then Lemma 5 implies that  $G$  is Hamiltonian and thereby  $G$  is traceable. If  $n = 2k + 3$ , then  $k \geq 3$  since  $n \geq 9$ . Then, Lemma 6 implies

that  $G$  has a cycle with a length of at least  $(n - 1)$  and thereby  $G$  is traceable, which is a contradiction. If  $n = 2k + 2$ , then  $G$  is  $K_{k,k+2}$ .

**Case 2.**  $\delta < n - k - 2$ .

In this case, set  $P = \{x : x \in I, d(x) = n - k - 2\}$  and  $Q = \{y : y \in I, d(y) = \delta\}$ . From Lemma 4, we have

$$|P| = \frac{(k+2)(n-k-2+3\delta)}{4(\delta+n-k-2)}.$$

Choose one vertex  $x$  in  $P$  and one vertex  $w$  in  $V - I$ . Then,  $n - k - 2 = d(x) \leq \Delta = d(w) \leq k + 2$ . Thus,  $n \leq 2k + 4$ . Since  $n \geq 2k + 2$ , we have  $n = 2k + 4$ ,  $n = 2k + 3$ , or  $n = 2k + 2$ . If  $n = 2k + 4$ , then Lemma 5 implies that  $G$  is Hamiltonian and thereby  $G$  is traceable. If  $n = 2k + 3$ , then  $k \geq 3$  since  $n \geq 9$ . Then, Lemma 6 implies that  $G$  has a cycle with a length of at least  $(n - 1)$  and thereby  $G$  is traceable, which is a contradiction. If  $n = 2k + 2$ , then  $G$  is  $K_{k,k+2}$  and  $n - k - 2 = \delta$ , which is a contradiction.

This completes the proof of Theorem 2.  $\square$

**Proof of Theorem 3.** Let  $G$  be a graph with  $n$  vertices,  $e$  edges, and  $\delta \geq 1$ . Clearly,  $\beta < n$ . Let  $I := \{u_1, u_2, \dots, u_\beta\}$  be a maximum independent set in  $G$ . Then,

$$\sum_{u \in I} d(u) = |E(I, V - I)| \leq \sum_{v \in V - I} d(v).$$

Since  $\sum_{u \in I} d(u) + \sum_{v \in V - I} d(v) = 2e$ , we have that

$$\sum_{u \in I} d(u) \leq e \leq \sum_{v \in V - I} d(v).$$

Notice that  $0 < \delta \leq d(u) \leq n - \beta$  for each  $u \in I$ .

(1). Applying Lemma 3 with  $s = \beta$ ,  $a_i = d(u_i)$ , and  $b_i = 1$ , with  $i = 1, 2, \dots, \beta$ ,  $m_1 = \delta > 0$ ,  $M_1 = n - \beta$ ,  $m_2 = 1 > 0$ , and  $M_2 = 1$ , we have

$$\sum_{i=1}^{\beta} d^2(u_i) \sum_{i=1}^{\beta} 1^2 - \left( \sum_{k=1}^{\beta} d(u_i) \right)^2 \leq \left( \sqrt{n - \beta} - \sqrt{\delta} \right)^2 \sum_{k=1}^{\beta} d(u_i) \sum_{i=1}^{\beta} 1^2.$$

Thus,

$$\begin{aligned} \sum_{i=1}^{\beta} d^2(u_i) &\leq \frac{\left( \sum_{k=1}^{\beta} d(u_i) \right)^2}{\beta} + \left( \sqrt{n - \beta} - \sqrt{\delta} \right)^2 \sum_{k=1}^{\beta} d(u_i) \\ &\leq \frac{e^2}{\beta} + \left( \sqrt{n - \beta} - \sqrt{\delta} \right)^2 e. \end{aligned}$$

Therefore,

$$\begin{aligned} Z_1 &= \sum_{v \in V - I} d^2(v) + \sum_{u \in I} d^2(u) \\ &\leq (n - \beta)\Delta^2 + \frac{e^2}{\beta} + \left( \sqrt{n - \beta} - \sqrt{\delta} \right)^2 e. \end{aligned}$$

If

$$Z_1 = (n - \beta)\Delta^2 + \frac{e^2}{\beta} + \left( \sqrt{n - \beta} - \sqrt{\delta} \right)^2 e,$$

then  $d(v) = \Delta$  for each  $v \in V - I$ , so

$$\sum_{i=1}^{\beta} d^2(u_i) \sum_{i=1}^{\beta} 1^2 - \left( \sum_{k=1}^{\beta} d(u_i) \right)^2 = \left( \sqrt{n - \beta} - \sqrt{\delta} \right)^2 \sum_{k=1}^{\beta} d(u_i) \sum_{i=1}^{\beta} 1^2,$$

and  $\sum_{i=1}^{k+1} d(u_i) = e$ , which implies that  $\sum_{v \in V-I} d(v) = e$  and  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$ .

For the characterization of the extremal graphs, we divide the remaining proofs into two cases.

**Case 1.**  $\delta = n - \beta$ .

In this case, we have  $d(u) = \delta$  for each  $u$  in  $I$ , and thereby  $G$  is  $K_{\beta, n-\beta}$ .

**Case 2.**  $\delta < n - \beta$ .

In this case, set  $P = \{x : x \in I, d(x) = n - \beta\}$  and  $Q = \{y : y \in I, d(y) = \delta\}$ . From Lemma 3, we have that  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$  such that  $|I| = \beta$ ,  $\delta < n - \beta$  and  $d(v) = \Delta$  for each vertex  $v$  in  $v - I$  and  $I = P \cup Q$ :

$$\frac{\beta}{|P|} = 1 + \left(\frac{n - \beta}{\delta}\right)^{\frac{1}{2}},$$

where  $|P|$  is an integer.

Suppose  $G$  is  $K_{\beta, n-\beta}$ . Since  $V - I$  is independent,  $n - \beta = |V - I| \leq \beta$ . Thus,  $\delta = n - \beta$ ,  $\Delta = \beta$ , and  $e = \beta(n - \beta)$ . A simple computation can verify that

$$Z_1 = (n - \beta)\Delta^2 + \beta\delta^2 = (n - \beta)\Delta^2 + \frac{e^2}{\beta} + (\sqrt{n - \beta} - \sqrt{\delta})^2 e.$$

Suppose  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$  such that  $|I| = \beta$ ,  $\delta < n - \beta$ , and  $d(v) = \Delta$  for each vertex  $v$  in  $v - I$ , and  $I = P \cup Q$ , where  $P = \{x : x \in I, d(x) = n - \beta\}$ ,  $Q = \{y : y \in I, d(y) = \delta\}$ , and

$$\frac{\beta}{|P|} = 1 + \left(\frac{n - \beta}{\delta}\right)^{\frac{1}{2}},$$

where  $|P|$  is an integer.

Then,  $|P| = \frac{\beta\sqrt{\delta}}{\sqrt{n-\beta}+\sqrt{\delta}}$ ,  $|Q| = \beta - |P| = \frac{\beta\sqrt{n-\beta}}{\sqrt{n-\beta}+\sqrt{\delta}}$ , and

$$\begin{aligned} e &= |P|(n - \beta) + |Q|\delta = \frac{\beta(n - \beta)\sqrt{\delta}}{\sqrt{n - \beta} + \sqrt{\delta}} + \frac{\beta\delta\sqrt{n - \beta}}{\sqrt{n - \beta} + \sqrt{\delta}} \\ &= \frac{\beta\sqrt{\delta(n - \beta)}(\sqrt{n - \beta} + \sqrt{\delta})}{\sqrt{n - \beta} + \sqrt{\delta}} = \beta\sqrt{\delta(n - \beta)}. \end{aligned}$$

Thus,

$$\begin{aligned} |P|(n - \beta)^2 + |Q|\delta^2 &= \frac{\beta(n - \beta)^2\sqrt{\delta}}{\sqrt{n - \beta} + \sqrt{\delta}} + \frac{\beta\delta^2\sqrt{n - \beta}}{\sqrt{n - \beta} + \sqrt{\delta}} \\ &= \beta\sqrt{\delta(n - \beta)} \frac{(n - \beta)^{\frac{3}{2}} + \delta^{\frac{3}{2}}}{(n - \beta)^{\frac{1}{2}} + \delta^{\frac{1}{2}}} \\ &= \beta\sqrt{\delta(n - \beta)} \left( n - \beta - \sqrt{\delta(n - \beta)} + \delta \right). \end{aligned}$$

Note that

$$\frac{e^2}{\beta} + (\sqrt{n - \beta} - \sqrt{\delta})^2 e = e \left( \frac{e}{\beta} + (\sqrt{n - \beta} - \sqrt{\delta})^2 \right)$$

$$\begin{aligned}
&= \beta \sqrt{\delta(n-\beta)} \left( \sqrt{\delta(n-\beta)} + (n-\beta-2\sqrt{\delta(n-\beta)} + \delta) \right) \\
&= \beta \sqrt{\delta(n-\beta)} \left( n-\beta - \sqrt{\delta(n-\beta)} + \delta \right).
\end{aligned}$$

Therefore,

$$\begin{aligned}
Z_1 &= \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) = (n-\beta)\Delta^2 + |P|(n-\beta)^2 + |Q|\delta^2 \\
&= (n-\beta)\Delta^2 + \beta \sqrt{\delta(n-\beta)} \left( n-\beta - \sqrt{\delta(n-\beta)} + \delta \right) \\
&= (n-\beta)\Delta^2 + \frac{e^2}{\beta} + \left( \sqrt{n-\beta} - \sqrt{\delta} \right)^2 e.
\end{aligned}$$

(2). Applying Lemma 4 with  $s = \beta$ ,  $a_i = d(u_i)$ , and  $b_i = 1$ , with  $i = 1, 2, \dots, \beta$ ,  $\gamma = \delta > 0$ , and  $\Gamma = n - \beta$ , we have

$$\left( \sum_{i=1}^{\beta} d^2(u_i) \sum_{i=1}^{\beta} 1^2 \right)^{\frac{1}{2}} - \sum_{k=1}^{\beta} d(u_i) \leq \frac{(n-\beta-\delta)^2}{4(\delta+n-\beta)} \sum_{i=1}^{\beta} 1^2.$$

Thus,

$$\begin{aligned}
\sum_{i=1}^{\beta} d^2(u_i) &\leq \frac{1}{\beta} \left( \frac{\beta(n-\beta-\delta)^2}{4(\delta+n-\beta)} + \sum_{k=1}^{\beta} d(u_i) \right)^2 \\
&\leq \frac{1}{\beta} \left( \frac{\beta(n-\beta-\delta)^2}{4(\delta+n-\beta)} + e \right)^2.
\end{aligned}$$

Therefore,

$$\begin{aligned}
Z_1 &= \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\
&\leq (n-\beta)\Delta^2 + \frac{1}{\beta} \left( \frac{\beta(n-\beta-\delta)^2}{4(\delta+n-\beta)} + e \right)^2.
\end{aligned}$$

If

$$Z_1 = (n-\beta)\Delta^2 + \frac{1}{\beta} \left( \frac{\beta(n-\beta-\delta)^2}{4(\delta+n-\beta)} + e \right)^2,$$

then  $d(v) = \Delta$  for each  $v \in V - I$ , so

$$\left( \sum_{i=1}^{\beta} d^2(u_i) \sum_{i=1}^{\beta} 1^2 \right)^{\frac{1}{2}} - \sum_{k=1}^{\beta} d(u_i) = \frac{(n-\beta-\delta)^2}{4(\delta+n-\beta)} \sum_{i=1}^{\beta} 1^2,$$

and  $\sum_{i=1}^{k+1} d(u_i) = e$ , which implies that  $\sum_{v \in V-I} d(v) = e$  and  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$ .

For the characterization of the extremal graphs, we divide the remaining proofs into two cases.

**Case 1.**  $\delta = n - \beta$ .

In this case, we have  $d(u) = \delta$  for each  $u$  in  $I$ , and thereby  $G$  is  $K_{\beta, n-\beta}$ .

**Case 2.**  $\delta < n - \beta$ .

In this case, set  $P = \{x : x \in I, d(x) = n - \beta\}$  and  $Q = \{y : y \in I, d(y) = \delta\}$ . From Lemma 4,  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$  such that  $|I| = \beta$ ,  $\delta < n - \beta$ , and  $d(v) = \Delta$  for each vertex  $v$  in  $v - I$  and  $I = P \cup Q$ , where  $P = \{x : x \in I, d(x) = n - \beta\}$ ,  $Q = \{y : y \in I, d(y) = \delta\}$ ,  $P \cap Q = \emptyset$ , and

$$|P| = \frac{n - \beta + 3\delta}{4(n - \beta + \delta)}$$

is an integer.

Suppose  $G$  is  $K_{\beta, n-\beta}$ . Since  $V - I$  is independent,  $n - \beta = |V - I| \leq \beta$ . Thus,  $\delta = n - \beta$ ,  $\Delta = \beta$ , and  $e = \beta(n - \beta)$ . A simple computation can verify that

$$Z_1 = (n - \beta)\Delta^2 + \beta\delta^2 = (n - \beta)\Delta^2 + \frac{1}{\beta} \left( \frac{\beta(n - \beta - \delta)^2}{4(\delta + n - \beta)} + e \right)^2.$$

Suppose  $G$  is a bipartite graph with partition sets of  $I$  and  $V - I$  such that  $|I| = \beta$ ,  $\delta < n - \beta$ , and  $d(v) = \Delta$  for each vertex  $v$  in  $v - I$  and  $I = P \cup Q$ , where  $P = \{x : x \in I, d(x) = n - \beta\}$ ,  $Q = \{y : y \in I, d(y) = \delta\}$ , and

$$|P| = \frac{\beta(n - \beta + 3\delta)}{4(n - \beta + \delta)}$$

is an integer.

Then,

$$|Q| = \beta - |P| = \frac{\beta(3(n - \beta) + \delta)}{4(n - \beta + \delta)}$$

is also an integer and

$$e = |P|(n - \beta) + |Q|\delta = \frac{\beta((n - \beta)^2 + 6\delta(n - \beta) + \delta^2)}{4(n - \beta + \delta)}.$$

Thus,

$$\begin{aligned} & \frac{1}{\beta} \left( \frac{\beta(n - \beta - \delta)^2}{4(n - \beta + \delta)} + e \right)^2 \\ &= \frac{1}{\beta} \left( \frac{\beta(n - \beta - \delta)^2}{4(n - \beta + \delta)} + \frac{\beta((n - \beta)^2 + 6\delta(n - \beta) + \delta^2)}{4(n - \beta + \delta)} \right)^2 \\ &= \frac{1}{\beta} \left( \frac{\beta((n - \beta)^2 - 2\delta(n - \beta) + \delta^2)}{4(n - \beta + \delta)} + \frac{\beta((n - \beta)^2 + 6\delta(n - \beta) + \delta^2)}{4(n - \beta + \delta)} \right)^2 \\ &= \frac{1}{\beta} \left( \frac{\beta(n - \beta + \delta)}{2} \right)^2 = \frac{\beta(n - \beta + \delta)^2}{4}. \end{aligned}$$

We also have

$$\begin{aligned} \sum_{u \in I} d^2(u) &= |P|(n - \beta)^2 + |Q|\delta^2 \\ &= \frac{\beta(n - \beta)^2(n - \beta + 3\delta)}{4(n - \beta + \delta)} + \frac{\beta\delta^2(3(n - \beta) + \delta)}{4(n - \beta + \delta)} \\ &= \frac{\beta((n - \beta)^3 + 3(n - \beta)^2\delta + 3(n - \beta)\delta^2 + \delta^3)}{4(n - \beta + \delta)} \\ &= \frac{\beta(n - \beta + \delta)^3}{4(n - \beta + \delta)} = \frac{\beta(n - \beta + \delta)^2}{4}. \end{aligned}$$

Therefore,

$$\begin{aligned} Z_1 &= \sum_{v \in V-I} d^2(v) + \sum_{u \in V} d^2(u) \\ &= (n - \beta)\Delta^2 + \frac{\beta(n - \beta + \delta)^2}{4} \\ &= (n - \beta)\Delta^2 + \frac{1}{\beta} \left( \frac{\beta(n - \beta - \delta)^2}{4(n - \beta + \delta)} + e \right)^2. \end{aligned}$$

This completes the proof of Theorem 3.  $\square$

#### 4. Conclusions

In this paper, we, utilizing the two established inequalities, obtain new sufficient conditions based on the Zagreb index for the Hamiltonian graphs and traceable graphs and new upper bounds for the Zagreb index of a graph. In the future, we will adopt the methodology exhibited in this paper to investigate sufficient conditions based on other topological indices for the Hamiltonian graphs and traceable graphs and upper bounds for the corresponding topological indices of a graph.

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