

Article

The first Zagreb index conditions for Hamiltonian and traceable graphs

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Communicated by: Muhammad Kamran Jamil

Received: 27 August 2024; Accepted: 01 October 2024; Published: 24 June 2025

Abstract: The first Zagreb index of a graph is one of the most important topological indices in chemical graph theory. It is also an important invariant of general graphs. The first Zagreb index of a graph is defined as the sum of the squares of the degrees of the vertices in the graph. The research on the Hamiltonian properties of a graph is an important topic in graph theory. Use the Diaz-Metcalf inequality, we in this paper present new sufficient conditions based on the first Zagreb index for the Hamiltonian and traceable graphs. In addition, using the ideas of obtaining the sufficient conditions, we also present an upper bound for the first Zagreb index of a graph. The graphs achieving the upper bound are also characterized.

Keywords: the first Zagreb index, Hamiltonian graph, traceable graph

MSC: 05C45, 05C09.

1. Introduction

We consider only finite undirected graphs without loops or multiple edges. We use [1] as a reference for the notation and terminology not defined here. Let $G = (V(G), E(G))$ be a graph. An independent set in G is a set of vertices in G such that for every two vertices in the set there is no edge connecting them. The independence number of a graph G , denoted $\beta(G)$, is the cardinality of a largest independent set. Suppose X and Y are two disjoint subsets of $V(G)$, we define $E(X, Y) := \{e : e = xy \in E, x \in X, y \in Y\}$.

A graph G is Hamiltonian if G has a cycle containing all the vertices of G . A graph G is traceable if G has a path containing all the vertices of G . The Hamiltonian problem, determining when a graph is Hamiltonian, is a major unsolved problem in graph theory. While investigating the Hamiltonian problem, researchers often focus on finding the sufficient conditions for the Hamiltonian properties such as the Hamiltonicity or traceability of a graph. The readers are referred to see the survey papers [2–4] and references therein on the research of Hamiltonian problem in graph theory.

In 1972, Gutman and Trinajstić introduced the concept of the first Zagreb index of a graph in [5], see also [6]. The first Zagreb index of a graph G , denoted $Z_1(G)$, is defined as $\sum_{u \in V(G)} d_G^2(u)$, where $d_G(u)$ is the degree of the vertex u in G . After its introduction, the first Zagreb index has been intensively investigated and it is one of the important topological indices in chemical graph theory. The first Zagreb index is also an important invariant of general graphs. Researchers have obtained a lot of results on the first Zagreb index of a graph. The readers are referred to see the survey papers [7–9], and the references therein on the research of the first Zagreb index of a graph.

In recent years, researchers have utilized the first Zagreb index and its variants to obtain sufficient conditions for the Hamiltonian and traceable graphs. Some results on this research can be found in [10–18]. In this paper, we still work along this direction. In particular, using the Diaz-Metcalf inequality in [19], we present the first Zagreb index conditions for the Hamiltonian and traceable graphs. In addition, using the ideas of obtaining the sufficient conditions, we also present an upper bound for the first Zagreb index of a graph and characterize the graphs achieving the upper bound. The main results of this paper are as follows.

Theorem 1. Suppose G is a graph with $n \geq 3$ vertices and e edges. If G is k -connected with $k \geq 2$ and

$$Z_1(G) \geq (n - k - 1)\Delta^2 + e(\delta + n - k - 1) - \delta(k + 1)(n - k - 1),$$

then G is Hamiltonian or G is $K_{k,k+1}$, where δ and Δ are respectively the minimum and maximum degrees of the graph G .

Theorem 2. Suppose G is a with $n \geq 9$ vertices and e edges. If G is k -connected with $k \geq 1$ and

$$Z_1(G) \geq (n - k - 2)\Delta^2 + e(\delta + n - k - 2) - \delta(k + 2)(n - k - 2),$$

then G is traceable or G is $K_{k,k+2}$, where δ and Δ are respectively the minimum and maximum degrees of the graph G .

Theorem 3. Suppose G is a graph with n vertices and e edges. If the minimum degree δ of G is at least 1, then

$$Z_1(G) \leq (n - \beta)\Delta^2 + e(\delta + n - \beta) - \delta\beta(n - \beta),$$

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 $|I| = \beta$, $\delta < n - \beta$, $d(v) = \Delta$ for each vertex v in $V - I$, and $I = P \cup Q$, where $P = \{x : x \in I, d(x) = n - \beta\}$, $Q = \{y : y \in I, d(y) = \delta\}$, where Δ is the maximum degree of G .

2. Lemmas

The following existing results will be used as our lemmas.

Lemma 1. [20] Suppose G is a k -connected graph of order $n \geq 3$ with independence number β . If $\beta \leq k$, then G is Hamiltonian.

Lemma 2. [20] Suppose G is a k -connected graph of order n with independence number β . If $\beta \leq k + 1$, then G is traceable.

Lemma 3 follows from Theorem 1 on Page 61 and Page 62 in [19].

Lemma 3. [19] Let the real numbers a_k and b_k ($k = 1, 2, \dots, s$) satisfy $0 \leq m_1 \leq a_k \leq M_1$ and $0 \leq m_2 \leq b_k \leq M_2$. Then

$$m_1 M_1 \sum_{k=1}^s b_k^2 + m_2 M_2 \sum_{k=1}^s a_k^2 \leq (M_1 M_2 + m_1 m_2) \sum_{k=1}^s a_k b_k.$$

If $0 < m_1$ and $0 < m_2$, then the equality holds if and only if for each k one has either $(a_k, b_k) = (m_1, M_2)$ or $(a_k, b_k) = (M_1, m_2)$.

Lemma 4. [21] Suppose G is a bipartite graph of order $2n$ with partition sets X and Y such that $|X| = |Y| = n$. If $d(x) + d(y) \geq n + 1$ for each $xy \notin E$, where $x \in X$ and $y \in Y$, then G is Hamiltonian.

Lemma 5. [22] Let G be a 2-connected bipartite graph with partition sets X and Y such that $|X| \geq |Y|$. If $d(x) \geq s$, where x is any vertex in X , and $d(y) \geq t$, where y is any vertex in Y , then G has a cycle of length at least $2 \min(|Y|, s + t - 1, 2s - 2)$.

3. Proofs

Before we present the proof of Theorem 1, let us recall Theorem 1.

Suppose G is a graph with $n \geq 3$ vertices and e edges. If G is k -connected with $k \geq 2$ and

$$Z_1(G) \geq (n - k - 1)\Delta^2 + e(\delta + n - k - 1) - \delta(k + 1)(n - k - 1),$$

then G is Hamiltonian or G is $K_{k,k+1}$, where δ and Δ are respectively the minimum and maximum degrees of the graph G .

Proof of Theorem 1. Let G be a graph with $n \geq 3$ vertices and e edges. Suppose G satisfies the conditions in Theorem 1 and G is not Hamiltonian. Since G is not Hamiltonian, then from Lemma 1 we have that $k+1 \leq \beta$. Furthermore, we have that $n \geq 2\delta + 1$ otherwise G is Hamiltonian since $\delta \geq n/2$. Since $\delta \geq k$, we have $n \geq 2k+1$. Let $S := \{u_1, u_2, \dots, u_\beta\}$ be an independent set of maximum cardinality in G . Since $\beta \geq k+1$, we have that $I := \{u_1, u_2, \dots, u_{k+1}\}$ is an independent set in G . Clearly,

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

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

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

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

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

Thus

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

From the conditions in Theorem 1, we have that

$$(n-k-1)\Delta^2 + e(\delta + n - k - 1) - \delta(k+1)(n-k-1) \leq Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ \leq (n-k-1)\Delta^2 + e(\delta + n - k - 1) - \delta(k+1)(n-k-1).$$

Therefore

$$(n-k-1)\Delta^2 + e(\delta + n - k - 1) - \delta(k+1)(n-k-1) = Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ = (n-k-1)\Delta^2 + e(\delta + n - k - 1) - \delta(k+1)(n-k-1).$$

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

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

and $\sum_{i=1}^{k+1} d(u_i) = e$. Thus $\sum_{v \in V-I} d(v) = e$ and G is a bipartite graph with partition sets of I and $V-I$ and $\Delta = d(v) \leq k+1$, where v is any vertex in $V-I$.

The remaining proofs are divided into two cases.

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

In this case, we have $d(u) = \delta$ for each u in I . Thus $\delta(k+1) = |E(I, V-I)| = \Delta(n-k-1) \geq \delta(n-k-1)$. Therefore $n \leq 2k+2$. Since $n \geq 2k+1$, we have $n = 2k+2$ or $n = 2k+1$. If $n = 2k+2$, we, from Lemma 4, have that G is Hamiltonian, a contradiction. If $n = 2k+1$, then G is $K_{k,k+1}$.

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

In this case, we, from Lemma 3, have that $I = P \cup Q$, where $P = \{x : x \in I, d(x) = n-k-1\}$ and $Q = \{y : y \in I, d(y) = \delta\}$. If $|P| > 0$, then there exists a vertex z in I such that $d(z) = n-k-1$. Thus $n-k-1 = d(z) \leq \Delta \leq k+1$. Thus $n \leq 2k+2$. Since $n \geq 2k+1$, we have $n = 2k+2$ or $n = 2k+1$. If $n = 2k+2$, we, from Lemma 4, have that G is Hamiltonian, a contradiction. If $n = 2k+1$, then G is $K_{k,k+1}$. Thus $n-k-1 = k = \delta$, a contradiction again. If $|P| = 0$, then all the vertices in I have a degree of δ . Therefore $\delta(k+1) = |E(I, V-I)| = \Delta(n-k-1) \geq \delta(n-k-1)$. Thus $n \leq 2k+2$. Since $n \geq 2k+1$, we have $n = 2k+2$ or $n = 2k+1$. If $n = 2k+2$, we, from Lemma 4, have that G is Hamiltonian, a contradiction. If $n = 2k+1$, then G is $K_{k,k+1}$. Thus $n-k-1 = k = \delta$, 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 here. Before we present the proof of Theorem 2, let us recall Theorem 2.

Suppose G is a with $n \geq 9$ vertices and e edges. If G is k -connected with $k \geq 1$ and

$$Z_1(G) \geq (n - k - 2)\Delta^2 + e(\delta + n - k - 2) - \delta(k + 2)(n - k - 2),$$

then G is traceable or G is $K_{k,k+2}$, where δ and Δ are respectively the minimum and maximum degrees of the graph G .

Proof of Theorem 2. Let G be a graph with $n \geq 9$ vertices and e edges. Suppose G satisfies the conditions in Theorem 2 and G is not traceable. Since G is not traceable, then from Lemma 2 we have that $k + 2 \leq \beta$. Furthermore, we have that $n \geq 2\delta + 2$ otherwise G is traceable since $\delta \geq (n - 1)/2$. Since $\delta \geq k$, we have $n \geq 2k + 2$. Let $T := \{u_1, u_2, \dots, u_\beta\}$ be an independent set of maximum cardinality in G . Since $\beta \geq k + 2$, we have that $I := \{u_1, u_2, \dots, u_{k+2}\}$ is an independent set in G . Clearly,

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

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

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

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

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

Thus

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

From the conditions in Theorem 2, we have that

$$(n - k - 2)\Delta^2 + e(\delta + n - k - 2) - \delta(k + 2)(n - k - 2) \leq Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ \leq (n - k - 2)\Delta^2 + e(\delta + n - k - 2) - \delta(k + 2)(n - k - 2).$$

Therefore

$$(n - k - 2)\Delta^2 + e(\delta + n - k - 2) - \delta(k + 2)(n - k - 2) = Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \\ = (n - k - 2)\Delta^2 + e(\delta + n - k - 2) - \delta(k + 2)(n - k - 2).$$

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

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

and $\sum_{i=1}^{k+2} d(u_i) = e$. Thus $\sum_{v \in V-I} d(v) = e$ and G is a bipartite graph with partition sets of I and $V - I$ and $\Delta = d(v) \leq k + 2$, where v is any vertex in $V - I$.

The remaining proofs are divided into two cases.

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

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

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

In this case, we, from Lemma 3, have that $I = P \cup Q$, where $P = \{x : x \in I, d(x) = n-k-2\}$ and $Q = \{y : y \in I, d(y) = \delta\}$. If $|P| > 0$, then there exists a vertex z in I such that $d(z) = n-k-2$. Thus $n-k-2 = d(z) \leq \Delta \leq k+2$. 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 $k \geq 3$ since $n \geq 9$. Notice now that $|I| = |V-I| = k+2$. We, from Lemma 4, have that G is Hamiltonian and thereby G is traceable, a contradiction. If $n = 2k+3$, then $k \geq 3$ since $n \geq 9$. We, from Lemma 5, have that G has a cycle of length at least $(n-1)$ and thereby G is traceable, a contradiction. If $n = 2k+2$, then G is $K_{k,k+2}$. Thus $n-k-2 = k = \delta$, a contradiction again. If $|P| = 0$, then all the vertices in I have a degree of δ . Therefore $\delta(k+2) = |E(I, V-I)| = \Delta(n-k-2) \geq \delta(n-k-2)$. Thus $n \leq 2k+4$. Since $n \geq 2k+2$, we have $n = 2k+4$, $n = 2k+3$, or $n = 2k+2$. Repeating the arguments above, we can reach a contradiction for each of the three cases of $n = 2k+4$, $n = 2k+3$, or $n = 2k+2$.

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

Before we present the proof of Theorem 3, let us recall Theorem 3.

Suppose G is a graph with n vertices and e edges. If the minimum degree δ of G is at least 1, then

$$Z_1(G) \leq (n-\beta)\Delta^2 + e(\delta+n-\beta) - \delta\beta(n-\beta)$$

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 $|I| = \beta$, $\delta < n-\beta$, $d(v) = \Delta$ for each vertex v in $V-I$, and $I = P \cup Q$, where $P = \{x : x \in I, d(x) = n-\beta\}$, $Q = \{y : y \in I, d(y) = \delta\}$, where Δ is the maximum degree of G .

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 . Clearly,

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

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

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

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

$$\sum_{i=1}^{\beta} d^2(u_i) + \delta(n-\beta) \sum_{i=1}^{\beta} 1^2 \leq (\delta+n-\beta) \sum_{i=1}^{\beta} d(u_i) \leq (\delta+n-\beta)e.$$

Thus

$$\sum_{i=1}^{\beta} d^2(u_i) \leq e(\delta+n-\beta) - \delta(n-\beta)\beta.$$

Therefore

$$Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) \leq (n-\beta)\Delta^2 + e(\delta+n-\beta) - \delta\beta(n-\beta).$$

If

$$Z_1 = \sum_{v \in V-I} d^2(v) + \sum_{u \in I} d^2(u) = (n-\beta)\Delta^2 + e(\delta+n-\beta) - \delta\beta(n-\beta),$$

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

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

and $\sum_{i=1}^{\beta} d(u_i) = e$. Thus $\sum_{v \in V-I} d(v) = e$ and G is a bipartite graph with partition sets of I and $V - I$ and $\Delta = d(v) \leq \beta$, where v is any vertex in $V - I$.

The remaining proofs are divided into two cases.

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

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

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

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

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

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

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

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

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

Acknowledgments: The author would like to thank the anonymous referees for their constructive suggestions and comments, which helped to improve on the initial version of this note.

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