Open Journal of Discrete Mathematics, 2025, 15(4), 92-99
https://www.scirp.org/journal/ojdm
ISSN Online: 2161-7643
ISSN Print: 2161-7635

The First Zagreb Index, the Independence Number and Some Hamiltonian Properties of Graphs

Rao Li

Department of Computer Science, Engineering and Mathematics, University of South Carolina Aiken, Aiken, SC 29801, USA
Email: raol@usca.edu

How to cite this paper: Li, R. (2025) The First Zagreb Index, the Independence Number and Some Hamiltonian Properties of Graphs. *Open Journal of Discrete Mathematics*, **15**, 92-99.
https://doi.org/10.4236/ojdm.2025.154007

Received: July 15, 2025
Accepted: September 2, 2025
Published: September 5, 2025

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. In this paper, we obtain two lower bounds involving the independence number for the first Zagreb index of a graph. We also characterize the graphs achieving the bounds. We further present sufficient conditions based on the first Zagreb index for Hamiltonian graphs and traceable graphs.

Keywords

The First Zagreb Index, The Independence Number, Hamiltonian Graph, Traceable Graph

1. Introduction

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

Gutman and Trinajstić [2] introduced the concept of the first Zagreb index of a graph in 1972. Also see [3]. Let $G = (V(G), E(G))$ be a graph. Its first Zagreb index is defined as $Z_1(G) := \sum_{u \in V(G)} d_G^2(u)$. As one of the most important topological indices of a graph, the first Zagreb index of a graph has been intensively investigated. A lot of results on the first Zagreb index of a graph have been obtained. The readers are referred to the survey paper [4] and the references therein. Finding the bounds for the first Zagreb index of a graph is one of the important topics. In this paper, using two established inequalities, we obtain two lower bounds involving the independence number for the first Zagreb index of a graph. We also characterize the graphs achieving the bounds. It is noticed that in recent years, using the first Zagreb index of a graph and its variants, researchers have presented sufficient conditions for the Hamiltonian properties of graphs. Some of the conditions can be found in [5]-[15]. In this paper, we present new sufficient conditions based on the first Zagreb index for Hamiltonian graphs and traceable graphs. The main results of this paper are as follows.

Theorem 1. Let G be a graph with n vertices, e edges, minimum degree $\delta \ge 1$, and maximum degree Δ. Then

(1)

$$Z_1(G) \ge \beta\delta^2 + \frac{\delta^2(2e + n - \beta)}{2\delta + 1}.$$

with equality if and only if G is a regular bipartite graph.

(2)

$$Z_1(G) \ge \beta\delta^2 + \frac{e^2(\Delta^2 + 1)}{(n - \beta)\Delta^2} - (n - \beta).$$

with equality if and only if G is a bipartite graph with partition sets of I and $V - I$ such that $|I| = \beta$, $d(u) = \delta$ for each $u \in I$, and $d(v) = \Delta$ for each $v \in V - I$.

Theorem 2. Let G be a k-connected ($k \ge 2$) graph with $n \ge 3$ vertices, e edges, minimum degree δ, and maximum degree Δ.

(1) If

$$Z_1(G) \le (k + 1)\delta^2 + \frac{\delta^2(2e + n - k - 1)}{2\delta + 1},$$

then G is Hamiltonian.

(2) If

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

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

Theorem 3. Let G be a k-connected ($k \ge 1$) with $n \ge 9$ vertices, e edges, minimum degree δ, and maximum degree Δ.

(1) If

$$Z_1(G) \le (k+2)\delta^2 + \frac{\delta^2(2e+n-k-2)}{2\delta+1}$$

then G is traceable.

(2) If

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

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

2. Lemmas

We will use the following results as our lemmas.

Lemma 1 [16]. Let G be a k-connected graph of order $n \ge 3$. If $\beta \le k$, then G is Hamiltonian.

Lemma 2 [16]. Let G be a k-connected graph of order n. If $\beta \le k+1$, then G is traceable.

Lemma 3 ([17], Theorem 6 on Page 9). Let $p \ge 1$ and a_i, $b_i \ge 0$ ($1 \le i \le s$). Then

$$\left(\sum_{i=1}^{s} a_i^p\right)\left(\sum_{i=1}^{s} b_i^p\right) \ge \sum_{i=1}^{s}(a_i+b_i)^p \sum_{i=1}^{s}\left(\frac{a_i b_i}{a_i+b_i}\right)^p$$

with the convention $0 \cdot 0/(0+0) = 0$. The equality is attained if and only if there exist constants λ, μ with $\lambda+\mu > 0$ and $\lambda a_i = \mu b_i$ for every $1 \le i \le s$.

Lemma 4 ([18], Theorem 3.20 on Page 37). Suppose p_k and q_k $(k = 1,2,\cdots,s)$ are real numbers with $|p_k|+|q_k| \ne 0$ $(k = 1,2,\cdots,s)$. One has the inequality

$$\left(\sum_{k=1}^{s} p_k q_k\right)^2 \le \sum_{k=1}^{s}\left(p_k^2+q_k^2\right)\sum_{k=1}^{s}\frac{p_k^2 q_k^2}{p_k^2+q_k^2}.$$

Lemma 5 [19]. Let G be a balanced bipartite graph of order $2n$ with bipartition (A, B). If $d(x)+d(y) \ge n+1$ for any $x \in A$ and any $y \in B$ with $xy \notin E$, then G is Hamiltonian.

Lemma 6 [20]. Let G be a 2-connected bipartite graph with bipartition (A, B), where $|A| \ge |B|$. If each vertex in A has degree at least s and each vertex in B has degree at least t, then G contains a cycle of length at least $2\min(|B|, s+t-1, 2s-2)$.

3. Proofs

Proof of Theorem 1. Let G be a graph with n vertices, e edges, and $\delta \ge 1$. Clearly, $\beta < n$. Let $I := \{u_1, u_2, \cdots, u_\beta\}$ be a maximum independent set in G and $V - I := \{v_1, v_2, \cdots, v_{n-\beta}\}$. Then

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

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

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

(1) Applying Lemma 3 with $p = 2$, $s = n - \beta$, $a_i = d(v_i)$, and $b_i = 1$, where $i = 1, 2, \cdots, n - \beta$, we have

$$\left(\sum_{i=1}^{n-\beta} d^2(v_i)\right)\left(\sum_{i=1}^{n-\beta} 1^2\right) \ge \left(\sum_{i=1}^{n-\beta} (d(v_i)+1)^2\right) \sum_{i=1}^{n-\beta} \left(\frac{d(v_i) \cdot 1}{d(v_i)+1}\right)^2.$$

Thus

$$\left(\sum_{i=1}^{n-\beta} d^2(v_i)\right)(n-\beta) \ge \left(\sum_{i=1}^{n-\beta} \left(d^2(v_i) + 2d(v_i) + 1\right)\right) \sum_{i=1}^{n-\beta} \left(\frac{\delta}{\delta+1}\right)^2.$$

Therefore

$$\left(\sum_{i=1}^{n-\beta} d^2(v_i)\right)(n-\beta) \ge \left(\sum_{i=1}^{n-\beta} d^2(v_i) + 2e + n - \beta\right)(n-\beta)\left(\frac{\delta}{\delta+1}\right)^2.$$

Hence

$$\left(\sum_{i=1}^{n-\beta} d^2(v_i)\right) \ge \frac{\delta^2(2e+n-\beta)}{2\delta+1}.$$

So

$$Z_1(G) = \sum_{w \in V(G)} d^2(w) = \sum_{i=1}^{\beta} d^2(u_i) + \sum_{i=1}^{n-\beta} d^2(v_i) \ge \beta\delta^2 + \frac{\delta^2(2e+n-\beta)}{2\delta+1}.$$

Suppose that

$$Z_1(G) = \beta\delta^2 + \frac{\delta^2(2e+n-\beta)}{2\delta+1}.$$

In review of all the proofs above, we have $\sum_{i=1}^{n-\beta} d(v_i) = e$ which implies that $\sum_{i=1}^{\beta} d(u_i) = e$ and G is a bipartite graph with partition sets of I and $V - I$. In addition, $d(u) = \delta$ for each $u \in I$ and $d(v) = \delta$ for each $v \in V - I$. Therefore G is a regular bipartite graph.

If G is a regular bipartite graph, then a simple computation yields that

$$Z_1(G) = \beta\delta^2 + \frac{\delta^2(2e+n-\beta)}{2\delta+1}.$$

This completes the proof of (1) in Theorem 1.

(2) Applying Lemma 4 with $s = n - \beta$, $p_i = d(v_i)$ and $q_i = 1$, where $i = 1, 2, \cdots, n - \beta$, we have

$$\left(\sum_{i=1}^{n-\beta} d(v_i)\cdot 1\right)^2 \le \sum_{i=1}^{n-\beta}\left(d^2(v_i)+1^2\right)\sum_{i=1}^{n-\beta}\frac{d^2(v_i)\cdot 1^2}{d^2(v_i)+1^2}.$$

Thus

$$e^2 \le \left(\sum_{i=1}^{n-\beta} d^2(v_i)+n-\beta\right)\sum_{i=1}^{n-\beta}\frac{\Delta^2}{\Delta^2+1}.$$

Therefore

$$e^2 \le \left(\sum_{i=1}^{n-\beta} d^2(v_i)+n-\beta\right)(n-\beta)\frac{\Delta^2}{\Delta^2+1}.$$

Hence

$$\sum_{i=1}^{n-\beta} d^2(v_i) \ge \frac{e^2\left(\Delta^2+1\right)}{(n-\beta)\Delta^2}-(n-\beta).$$

So

$$Z_1(G)=\sum_{w\in V(G)} d^2(w)=\sum_{i=1}^{\beta} d^2(u_i)+\sum_{i=1}^{n-\beta} d^2(v_i)\ge \beta\delta^2+\frac{e^2\left(\Delta^2+1\right)}{(n-\beta)\Delta^2}-(n-\beta).$$

Suppose that

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

In review of all the proofs above, we have $\sum_{i=1}^{n-\beta} d(v_i)=e$ which implies that $\sum_{i=1}^{\beta} d(u_i)=e$ and G is a bipartite graph with partition sets of I and $V-I$. In addition, $|I|=\beta$, $d(u)=\delta$ for each $u\in I$, and $d(v)=\Delta$ for each $v\in V-I$.

If G is a bipartite graph with partition sets of I and $V-I$ such that $|I|=\beta$, $d(u)=\delta$ for each $u\in I$, and $d(v)=\Delta$ for each $v\in V-I$, then $\delta\beta=e=\Delta(n-\beta)$. A simple computation yields that

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

This completes the proof of (2) in Theorem 1.

Proof of Theorem 2. Let G be a k-connected ($k\ge 2$) graph with $n\ge 3$ vertices and e edges satisfying exactly one of two conditions in Theorem 2. Suppose G is not Hamiltonian. Then Lemma 1 implies that $\beta\ge k+1$. Let $I_1:=\{u_1,u_2,\cdots,u_\beta\}$ be a maximum independent set in G. Then $I:=\{u_1,u_2,\cdots,u_{k+1}\}$ is an independent set in G. Set $V-I=\{v_1,v_2,\cdots,v_{n-k-1}\}$. Thus

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

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

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

(1) Applying Lemma 3 with $p=2$, $s=n-k-1$, $a_i=d(v_i)$, and $b_i=1$, where $i=1,2,\cdots,n-k-1$, the ideas in the proof of (1) in Theorem 1, and the conditions in (1) in Theorem 2, we have

$$(k+1)\delta^2+\frac{\delta^2(2e+n-k-1)}{2\delta+1}\le Z_1(G)\le(k+1)\delta^2+\frac{\delta^2(2e+n-k-1)}{2\delta+1}.$$

Thus

$$Z_1(G)=(k+1)\delta^2+\frac{\delta^2(2e+n-k-1)}{2\delta+1}.$$

Therefore G is a regular bipartite graph with partition sets of I and $V-I$ which implies that $|I|=|V-I|=(k+1)$. Lemma 5 implies that G is Hamiltonian, a contradiction.

This completes the proof of (1) in Theorem 2.

(2) Applying Lemma 4 with $s=n-k-1$, $p_i=d(v_i)$ and $q_i=1$, where $i=1,2,\cdots,n-k-1$, the ideas in the proof of (2) in Theorem 1, and the conditions in (2) in Theorem 2, we have

$$(k+1)\delta^2+\frac{e^2(\Delta^2+1)}{(n-k-1)\Delta^2}-(n-k-1)$$
$$\le Z_1(G)\le(k+1)\delta^2+\frac{e^2(\Delta^2+1)}{(n-k-1)\Delta^2}-(n-k-1).$$

Thus G is a bipartite graph with partition sets of I and $V-I$ such that $|I|=(k+1)$, $d(u)=\delta$ for each $u\in I$, and $d(v)=\Delta$ for each $v\in V-I$. $\delta|I|=e=\Delta|V-I|$ and $\delta\le\Delta$, we have that $|V-I|\le|I|=(k+1)$. Notice that $n\ge 2\delta+1\ge 2k+1$ otherwise $\delta\ge k\ge n/2$ and G is Hamiltonian. Thus $|V-I|=|V|-|I|\ge k$. Therefore $|V-I|=k$ or $|V-I|=(k+1)$. If $|V-I|=k$, then G is $K_{k,k+1}$. If $|V-I|=(k+1)$, Lemma 5 implies that G is Hamiltonian, a contradiction.

This completes the proof of (2) in Theorem 2.

The proof of Theorem 3 is similar to the proof of Theorem 2. For the sake of completeness, we still present a full proof of Theorem 3 below.

Proof of Theorem 3. Let G be a k-connected ($k\ge 1$) graph with $n\ge 9$ vertices and e edges satisfying exactly one of two conditions in Theorem 3. Suppose G is not traceable. Then Lemma 2 implies that $\beta\ge k+2$. Let $I_1:=\{u_1,u_2,\cdots,u_\beta\}$ be a maximum independent set in G. Then $I:=\{u_1,u_2,\cdots,u_{k+2}\}$ is an independent set in G. Set $V-I=\{v_1,v_2,\cdots,v_{n-k-2}\}$. Thus

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

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

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

(1) Applying Lemma 3 with $p=2$, $s=n-k-2$, $a_i=d(v_i)$, and $b_i=1$, where $i=1,2,\cdots,n-k-2$, the ideas in the proof of (1) in Theorem 1, and the conditions in (1) in Theorem 3, we have

$$(k+2)\delta^2+\frac{\delta^2(2e+n-k-2)}{2\delta+1}\le Z_1(G)\le(k+2)\delta^2+\frac{\delta^2(2e+n-k-2)}{2\delta+1}.$$

Thus

$$Z_1(G)=(k+2)\delta^2+\frac{\delta^2(2e+n-k-2)}{2\delta+1}.$$

Therefore G is a regular bipartite graph with partition sets of I and $V-I$ which implies that $|I|=|V-I|=(k+2)$. Since $n=2k+4\ge 9$, we have that $k\ge 3$. Thus Lemma 5 implies that G is Hamiltonian and thereby G is traceable, a contradiction.

This completes the proof of (1) in Theorem 3.

(2) Applying Lemma 4 with $s=n-k-2$, $p_i=d(v_i)$ and $q_i=1$, where $i=1,2,\cdots,n-k-2$, the ideas in the proof of (2) in Theorem 1, and the conditions in (2) in Theorem 3, we have

$$(k+2)\delta^2+\frac{e^2(\Delta^2+1)}{(n-k-2)\Delta^2}-(n-k-2)$$
$$\le Z_1(G)\le(k+2)\delta^2+\frac{e^2(\Delta^2+1)}{(n-k-2)\Delta^2}-(n-k-2).$$

Thus G is a bipartite graph with partition sets of I and $V-I$ such that $|I|=(k+2)$, $d(u)=\delta$ for each $u\in I$, and $d(v)=\Delta$ for each $v\in V-I$. Since $\delta|I|=e=\Delta|V-I|$ and $\delta\le\Delta$, we have that $|V-I|\le|I|=(k+2)$. Notice that $n\ge 2\delta+2\ge 2k+2$ otherwise $\delta\ge k\ge(n-1)/2$ and G is traceable. Thus $|V-I|=|V|-|I|\ge k$. Therefore $|V-I|=k$ or $|V-I|=(k+1)$ or $|V-I|=(k+2)$. If $|V-I|=k$, then G is $K_{k,k+2}$. If $|V-I|=(k+1)$, Lemma 6 implies that G has a cycle of length at least $(n-1)$ and thereby G is traceable, a contradiction. If $|V-I|=(k+2)$, since $n=2k+4\ge 9$, we have that $k\ge 3$. Thus Lemma 5 implies that G is Hamiltonian and thereby G is traceable, a contradiction.

This completes the proof of (2) in Theorem 3.

Acknowledgements

The author would like to thank the referees for their suggestions or comments which improve the initial version of the paper.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

References

[1] Bondy, J.A. and Murty, U.S.R. (1976) Graph Theory with Applications. Elsevier.

[2] Gutman, I. and Trinajstić, N. (1972) Graph Theory and Molecular Orbitals. Total φ-Electron Energy of Alternant Hydrocarbons. *Chemical Physics Letters*, **17**, 535-538.

https://doi.org/10.1016/0009-2614(72)85099-1

[3] Gutman, I., Ruščić, B., Trinajstić, N. and Wilcox, C.F. (1975) Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes. *The Journal of Chemical Physics*, **62**, 3399-3405. https://doi.org/10.1063/1.430994

[4] Borovićanin, B., Das, K., Furtula, B. and Gutman, I. (2017) Bounds for Zagreb Indices. *MATCH Communications in Mathematical and in Computer Chemistry*, **78**, 17-100.

[5] Li, R. and Taylor, M.M. (2017) The First Zagreb Index and Some Hamiltonian Properties of the Line Graph of a Graph. *Journal of Discrete Mathematical Sciences and Cryptography*, **20**, 445-451. https://doi.org/10.1080/09720529.2015.1103009

[6] Li, R. (2019) The Hyper-Zagreb Index and Some Hamiltonian Properties of Graphs. *Discrete Mathematics Letters*, **1**, 54-58.

[7] An, M. (2022) The First Zagreb Index, Reciprocal Degree Distance and Hamiltonian-Connectedness of Graphs. *Information Processing Letters*, **176**, Article ID: 106247. https://doi.org/10.1016/j.ipl.2022.106247

[8] Lu, Y. and Zhou, Q. (2022) On Hyper-Zagreb Index Conditions for Hamiltonicity of Graphs. *Czechoslovak Mathematical Journal*, **72**, 653-662. https://doi.org/10.21136/cmj.2022.0089-21

[9] Jahanbani, A. and Sheikholeslam, S. (2023) The Topological Indices and Some Hamiltonian Properties of Graphs. *Applied Mathematics E-Notes*, **23**, 260-264.

[10] Li, R. (2024) The First General Zagreb Index and Some Hamiltonian Properties of Graphs. *Mathematical Aspects of Topological Indices*, **6**, 43-48.

[11] Li, R. (2024) The General First Zagreb Index Conditions for Hamiltonian and Traceable Graphs. *Discrete Mathematics Letters*, **14**, 31-35.

[12] Li, R. (2024) The First Zagreb Index and Some Hamiltonian Properties of Graphs. *Mathematics*, **12**, Article 3902. https://doi.org/10.3390/math12243902

[13] Li, R. (2024) The Harmonic Index and Some Hamiltonian Properties of Graphs. *Discrete Mathematics Letters*, **14**, 103-107.

[14] Li, R. (2025) The First Zagreb Index Conditions for Hamiltonian and Traceable Graphs. *Open Journal of Discrete Applied Mathematics*, **8**, 45-51. https://doi.org/10.30538/psrp-odam2025.0115

[15] Li, R. (2025) On General Zagreb Indices and Some Hamiltonian Properties of Graphs. *Electronic Journal of Mathematics*, **9**, 88-92. https://doi.org/10.47443/ejm.2025.011

[16] Chvátal, V. and Erdös, P. (1972) A Note on Hamiltonian Circuits. *Discrete Mathematics*, **2**, 111-113. https://doi.org/10.1016/0012-365x(72)90079-9

[17] Bosch, P., Rodríguez, J.M., Sigarreta, J.M. and Tourís, E. (2024) Some New Milne-Type Inequalities. *Journal of Inequalities and Applications*, **2024**, Article No. 106. https://doi.org/10.1186/s13660-024-03184-4

[18] Dragomir, S.S. (2003) A Survey on Cauchy-Bunyakovsky-Schwarz Type Discrete Inequalities. *Journal of Inequalities in Pure and Applied Mathematics*, **4**, Article 63. http://jipam.vu.edu.au/

[19] Moon, J. and Moser, L. (1963) On Hamiltonian Bipartite Graphs. *Israel Journal of Mathematics*, **1**, 163-165. https://doi.org/10.1007/bf02759704

[20] Jackson, B. (1985) Long Cycles in Bipartite Graphs. *Journal of Combinatorial Theory, Series B*, **38**, 118-131. https://doi.org/10.1016/0095-8956(85)90077-2