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The First Zagreb Index Conditions For 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 $\sum_{u \in V} d^2(u)$, where $d(u)$ is the degree of vertex u in G. In this paper, we present the first Zagreb index conditions for some Hamiltonian properties of a graph and an upper bound for the first Zagreb index of a graph.

1 Introduction

We consider only finite undirected graphs without loops or multiple edges. Notation and terminology not defined here follow those in [2]. Let $G = (V(G), E(G))$ be a graph with n vertices and e edges, the degree of a vertex v is denoted by $d_G(v)$. We use δ and Δ to denote the minimum degree and maximum degree of G, respectively. A set of vertices in a graph G is independent if the vertices in the set are pairwise nonadjacent. A maximum independent set in a graph G is an independent set of largest possible size. The independence number, denoted by $\beta(G)$, of a graph G is the cardinality of a maximum independent set in G. For disjoint vertex subsets X and Y of $V(G)$, we use $E(X, Y)$ to denote the set of all the edges in $E(G)$ such that one end vertex of each edge is in X and another end vertex of the edge is in Y. Namely, $E(X, Y) := \{\, e : e = xy \in E, x \in X, y \in Y\,\}$. A bipartite graph G with vertex partition sets X and Y is called balanced if $|X| = |Y|$. A cycle C in a graph G is called a Hamiltonian cycle of G if C contains all the vertices of G. A graph G is called Hamiltonian if G has a Hamiltonian cycle. A path P in a graph G is called a Hamiltonian path of G if P contains all the vertices of G. A graph G is called traceable if G has a Hamiltonian path.

The first Zagreb index of a graph was introduced by Gutman and Trinajstić in [5]. For a graph G, its first Zagreb index, denoted $Z_1(G)$, is defined as $\sum_{u \in V(G)} d_G^2(u)$. In recent years, the sufficient conditions based on the first Zagreb index or its variants for the Hamiltonian and traceable graphs have been obtained. Some of them can be found in [1, 7, 8, 9, 10, 11, 12, 13, 16]. In this paper, we, using the Pólya-Szegő inequality, present the first Zagreb index conditions for the Hamiltonian and traceable graphs and an upper bound for the first Zagreb index of a graph. The main results are as follows.

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

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

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. If*

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

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

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

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

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 $P = \{\, x : x \in I, d(x) = n-\beta \,\}$, $Q = \{\, y : y \in I, d(y) = \delta \,\}$, and $|P| = \frac{\delta\beta}{\delta+n-\beta}$ and $|Q| = \frac{(n-\beta)\beta}{\delta+n-\beta}$ are integers.

2 Lemmas

We will use the following results as our lemmas. The first two are from [3].

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

Lemma 2 (C. Chvátal and P. Erdös, [3]) *Let G be a k-connected graph of order n. If $\beta \leq k+1$, then G is traceable.*

Lemma 3 is the Pólya-Szegő inequality in [15]. The following one is Corollary 3 on Page 66 in [4].

Lemma 3 (J. Diaz and F. Metcalf, [4]) *Let the real numbers a_k and b_k $(k = 1, 2, \cdots, s)$ satisfy $0 < m_1 \leq a_k \leq M_1$ and $0 < m_2 \leq b_k \leq M_2$. Then*

$$\sum_{k=1}^{s} a_k^2 \sum_{k=1}^{s} b_k^2 \leq \frac{(M_1M_2 + m_1m_2)^2}{4m_1m_2M_1M_2} \left(\sum_{k=1}^{s} a_k b_k \right)^2 .$$

If $M_1M_2 > m_1m_2$, then the equality sign holds in above inequality if and only if

$$\nu = \frac{M_1 m_2}{M_1 m_2 + m_1 M_2} s$$

is an integer; while, at the same time, for ν values of k one has $(a_k, b_k) = (m_1, M_2)$ and for the remaining $s - \nu$ values of k one has $(a_k, b_k) = (M_1, m_2)$. If $M_1M_2 = m_1m_2$, the equality always holds.

Lemma 4 below is from [14].

Lemma 4 (J. Moon and L. Moser, [14]) *Let G be a balanced bipartite graph of order $2n$ with 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 5 below is from [6].

Lemma 5 (B. Jackson, [6]) *Let G be a 2-connected bipartite graph with bipartition $(A,\, B)$, where $|A| \geq |B|$. 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 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 $I_1 := \{\, u_1, u_2, ..., u_\beta \,\}$ be a maximum independent set in G. Then $I := \{u_1, u_2, ..., u_{k+1}\}$ 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 $u \in I$. Applying Lemma 3 with $s = k+1$, $a_i = 1$ and $b_i = d(u_i)$ with $i = 1, 2, ..., (k+1)$, $m_1 = 1 > 0$, $M_1 = 1$, $m_2 = \delta > 0$ and $M_2 = n-k-1$, we have

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

Thus

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

Therefore,

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

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

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

and $\sum_{i=1}^{k+1} d(u_i) = e$ which implies $\sum_{v\in V-I} d(v) = e$ and G is a bipartite graph with partition sets of I and $V - I$. 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 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 4 implies 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, 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

$$|P| = \frac{\delta(k+1)}{\delta+n-k-1}, \quad |Q| = (k+1) - |P| = \frac{(n-k-1)(k+1)}{\delta+n-k-1}$$

and $I = P \cup Q$. Choose one vertex x in P and one vertex z in $V-I$. Then $n-k-1 = d(x) \leq \Delta = d(z) \leq k+1$. 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 4 implies that G is Hamiltonian, a contradiction. If $n = 2k+1$, then G is $K_{k,\,k+1}$ which implies $n-k-1 = \delta$, a contradiction.

This completes the proof of Theorem 1. ■

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 $I_1 := \{ u_1, u_2, ..., u_\beta \}$ be a maximum independent set in G. Then $I := \{ u_1, u_2, ..., u_{k+2} \}$ 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 $u \in I$. Applying Lemma 3 with $s = k+2$, $a_i = 1$ and $b_i = d(u_i)$ with $i = 1, 2, ..., (k+2)$, $m_1 = 1 > 0$, $M_1 = 1$, $m_2 = \delta > 0$ and $M_2 = n-k-2$, we have

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

Thus

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

Therefore,

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

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

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

and $\sum_{i=1}^{k+2} d(u_i) = e$ which implies $\sum_{v \in V-I} d(v) = e$ and G is a bipartite graph with partition sets of I and $V-I$. 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 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 $k \geq 3$ since $n \geq 9$. Thus Lemma 4 implies that G is Hamiltonian and thereby G is traceable, a contradiction. If $n = 2k+3$, then $k \geq 3$ since $n \geq 9$. Thus Lemma 5 implies 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, 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

$$|P| = \frac{\delta(k+2)}{\delta+n-k-2}, \quad |Q| = (k+2) - |P| = \frac{(n-k-2)(k+2)}{\delta+n-k-2} \quad \text{and } I = P \cup Q.$$

Choose one vertex x in P and one vertex z in $V-I$. Then

$$n-k-2=d(x)\leq\Delta=d(z)\leq k+2.$$

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 $n\geq 9$. Thus Lemma 4 implies that G is Hamiltonian and thereby G is traceable, a contradiction. If $n=2k+3$, then $k\geq 3$ since $n\geq 9$. Thus Lemma 5 implies 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 $K_{k,\,k+2}$ which implies $n-k-2=\delta$, a contradiction.

This completes the proof of Theorem 2. ■

Proof of Theorem 3. Let G be a graph with n vertices, e edges, and $\delta\geq 1$. Clearly, $\beta<n$. Let $I:=\{u_1,u_2,...,u_\beta\}$ 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 $u\in I$. Applying Lemma 3 with $s=\beta$, $a_i=1$ and $b_i=d(u_i)$ with $i=1,2,...,\beta$, $m_1=1>0$, $M_1=1$, $m_2=\delta>0$ and $M_2=n-\beta$, we have

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

Thus

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

Therefore,

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

If

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

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

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

and $\sum_{i=1}^{\beta}d(u_i)=e$ which implies $\sum_{v\in V-I}d(v)=e$ and G is a bipartite graph with partition sets of I and $V-I$. 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 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 $I = P \cup Q$, $|P| = \frac{\delta\beta}{\delta+n-\beta}$ which is an integer, and $|Q| = \beta - |P| = \frac{(n-\beta)\beta}{\delta+n-\beta}$ which is an integer.. Suppose G is $K_{\beta,\, n-\beta}$. Since $V - I$ is independent in G, $n - \beta \leq \beta$ and thereby $\delta = n - \beta$. A simple computation can verify that

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

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 $P = \{\, x : x \in I,\, d(x) = n - \beta\}$, $Q = \{\, y : y \in I,\, d(y) = \delta\}$, and $|P| = \frac{\delta\beta}{\delta+n-\beta}$ and $|Q| = \frac{(n-\beta)\beta}{\delta+n-\beta}$ are integer. Then

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

Thus

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

This completes the proof of Theorem 3. ■

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References

[1] M. An, The first Zagreb index, reciprocal degree distance and Hamiltonian-connectedness of graphs, Information Processing Letters, 176(2022), 106247.

[2] J. A. Bondy and U. S. R. Murty, Graph Theory with Applications, Macmillan, London and Elsevier, New York, 1976.

[3] C. Chvátal and P. Erdös, A note on Hamiltonian circuits, Discrete Mathematics, 2(1973), 111–113.

[4] J. Diaz and F. Metcalf, Complementary inequalities I: inequalities complementary to Cauchy's inequalities for sums of real numbers, J. Math. Anal. Appl., 9(1964), 59–74.

[5] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals, total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17(1972), 535–538.

[6] B. Jackson, Long cycles in bipartite graphs, . Comb. Theory Ser. B, 38(1985), 118–131.

[7] A. Jahanbani and S. Sheikholeslam, The topological indices and some Hamiltonian properties of graphs, Applied Mathematics E-Notes, 23(2023), 260–264.

[8] Y. Jin, S. Zhou, T. Tian and K. C. Das, Sufficient conditions for Hamiltonian properties of graphs based on the difference of Zagreb indices, Comp. Appl. Math. 43(2024), Article 385.

[9] R. Li, The general first Zagreb index conditions for Hamiltonian and traceable graphs, Discrete Math. Lett., 14(2024), 31–35.

[10] R. Li, The first general Zagreb index and some Hamiltonian properties of graphs, Math. Asp. Topol. Indices, 6(2024), 43–48.

[11] R. Li, The hyper-Zagreb index and some Hamiltonian properties of graphs, Discrete Math. Lett., 1(2019), 54–58.

[12] R. Li and M. Taylor, The first Zagreb index and some Hamiltonian properties of the line graph of a graph, Journal of Discrete Mathematical Sciences and Cryptography, 20(2017), 445–451.

[13] Y. Lu and Q. Zhou, On hyper-Zagreb index conditions for Hamiltonicity of graphs, Czechoslovak Mathematical Journal, 72(2022), 653–662.

[14] J. Moon and L. Moser, On Hamiltonian bipartite graphs, Israel J. Math., 1(1963), 163–165.

[15] G. Pólya and G. Szegő, Aufgaben und Lehrsätze aus der Analysis, Springer, Vol. I, Berlin, 1925.

[16] G. Su and Z. Li, Sufficient conditions for a graph to be k-edge-hamiltonian, k-path-coverable, traceable and Hamilton-connected, Australas. J. Combin., 77(2020), 269–284.