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SHARP BOUNDS FOR THE FIRST ZAGREB INDEX AND FIRST ZAGREB COINDEX

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Abstract. Let G be an undirected connected graph with n , $n \geq 2$, vertices and m edges with vertex degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. Lower and upper bounds of a graph invariants $M_1 = \sum_{i=1}^{n} d_i^2$, referred to as the first Zagreb index, and $\bar{M}_1 = \sum_{i \nsim j}(d_i + d_j)$, named the first Zagreb coindex, depending on parameters n, m, Δ and δ are obtained. The obtained results represent improvement of the results reported in the literature.

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1. INTRODUCTION

Let G be an undirected connected graph with n , $n \geq 2$, vertices and m edges, and let $\Delta = d_1 \geq d_2 \geq \ldots \geq d_n = \delta > 0$ be the sequence of its vertex degrees.

In graph theory, a graph invariant is a property of graphs that does not depend on graph representations, such as particular labeling of its vertices or drawings of the graph. A number of different invariants have been introduced so far. One of the oldest was introduced by Gutman and Trinajstić in 1972, known under the name *first Zagreb index*, defined as the sum of squares of vertex degrees of graph, i.e. as

$$M_1 = \sum_{i=1}^{n} d_i^2$$

In [8] Došlić proposed a new graph invariant named *first Zagreb coindex*, defined as

$$\bar{M}_1 = \sum_{i \nsim j}(d_i + d_j).$$

These graph invariants play an important role in many scientific areas, notably in chemistry and network theory (see for example [12] and [1, 18]). In earlier works [2, 3, 5–7, 9–17, 19], several bounds for M_1 and $\bar{M}_1$ were reported. These depend on usual structural parameters (number of vertices, number of edges, vertex degrees, and similar).

In this paper we consider the problem of finding lower and upper bounds of a graph invariants M_1 and $\bar{M}_1$. The obtained results represent improvement of the results reported in the literature.

2. Preliminaries

Here we recall some results from spectral graph theory, and state a few analytical inequalities needed for our work.

Lemma 1 ([9, 16]). *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Then*

$$M_1 \geq \frac{4m^2}{n} \tag{2.1}$$

Equality holds if and only if G is isomorph with a regular graph.

Lemma 2 ([10]). *Let G be simple graph with n, vertices and m edges. Then*

$$M_1 \leq \frac{4m^2}{n} + \frac{n}{4}(\Delta - \delta)^2 \tag{2.2}$$

Lemma 3 ([10, 11, 15, 17]). *Let G be simple graph with n vertices and m edges. Then*

$$M_1 \leq \frac{m^2}{n}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 \tag{2.3}$$

with equality if and only if G is regular graph, or G is bidegreed graph such that $\Delta + \delta$ divides δn and there are exactly $p = \frac{\delta n}{\Delta+\delta}$ vertices of degree Δ, and $q = \frac{\Delta n}{\Delta+\delta}$ vertices of degree δ.

Note that complete conditions when equality in (2.3) occurs were given only in [15].

Lemma 4 ([2]). *Suppose G is a connected graph with exactly n vertices and m edges. Then we have*

$$\bar{M}_1 = 2m(n-1) - M_1. \tag{2.4}$$

Lemma 5 ([14]). *Let G be a simple graph with n vertices and m edges. Then*

$$\bar{M}_1 \leq -\frac{4m^2}{n} + 2m(n-1), \tag{2.5}$$

and

$$\bar{M}_1 \geq 2m(n-1) - \frac{(\Delta+\delta)^2}{n\Delta\delta}m^2. \tag{2.6}$$

The equality holds if and only if G is regular.

Lemma 6 ([4])**.** *Let $p_1, p_2, \dots, p_n$ be non-negative real numbers and $a_1, a_2, \dots, a_n$ and $b_1, b_2, \dots, b_n$, real numbers with the properties*

$$0 < r_1 \le a_i \le R_1 < +\infty \quad \text{and} \quad 0 < r_2 \le b_i \le R_2 < +\infty$$

for each $i = 1, 2, \dots, n$. Further, let S be a subset of $I_n = \{1, 2, \dots, n\}$ which minimizes the expression

$$\left| \sum_{i \in S} p_i - \frac{1}{2} \sum_{i=1}^{n} p_i \right|. \tag{2.7}$$

Then

$$\left| \sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i a_i b_i - \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \right| \le (R_1 - r_1)(R_2 - r_2) \sum_{i \in S} p_i \left(\sum_{i=1}^{n} p_i - \sum_{i \in S} p_i \right). \tag{2.8}$$

3. Main results

3.1. *The first Zagreb index*

The following theorem establishes bound for M_1 depending on parameters n, m, Δ and δ.

Theorem 1. *Let G be an undirected connected graph with n, $n \ge 2$, vertices and m edges. Then*

$$M_1 \ge \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2. \tag{3.1}$$

Equality holds if and only if G is isomorph with k-regular graph, $1 \le k \le n-1$.

Proof. From equality

$$nM_1 - 4m^2 = n \sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} d_i \right)^2 = \sum_{1 \le i \le j \le n} (d_i - d_j)^2$$

and inequality

$$\begin{aligned} \sum_{1 \le i < j \le n} (d_i - d_j)^2 &\ge \sum_{i=2}^{n-1} ((d_1 - d_i)^2 + (d_i - d_n)^2) + (d_1 - d_n)^2 \\ &\ge \sum_{i=2}^{n-1} \frac{1}{2} (d_1 - d_n)^2 + (d_1 - d_n)^2 \\ &= \frac{n-2}{2}(\Delta - \delta)^2 + (\Delta - \delta)^2 = \frac{n}{2}(\Delta - \delta)^2 \end{aligned} \tag{3.2}$$

the inequality (3.1) is obtained.

Since equality in (3.2) holds if and only if $d_1 = d_2 = \dots = d_n$, equality in (3.1) holds if and only if G is isomorph with k-regular graph, $1 \le k \le n-1$. □

Remark 1. Since $(\Delta-\delta)^2 \geq 0$, the inequality (3.1) is stronger than inequality (2.1).

Theorem 2. *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Then*

$$M_1 \leq \frac{4m^2}{n} + n(\Delta-\delta)^2\alpha(n) \tag{3.3}$$

where

$$\alpha(n) = \frac{1}{4}\left(1 - \frac{1+(-1)^{n+1}}{2n^2}\right).$$

Equality in (3.3) holds if and only if G is isomorph with k-regular graph, $1 \leq k \leq n-1$.

Proof. Suppose that S is a subset of the form $S = \{1,2,\dots,k\} \subset I_n = \{1,2,\dots,n\}$ and that $p_i = 1$, $i = 1,2,\dots,n$. Then the expression (2.7) reaches the minimum if $k = \lfloor \frac{n}{2} \rfloor$, i.e. if $S = \{1,2,\dots,\lfloor \frac{n}{2} \rfloor\}$. Now, for $p_i = 1$, $a_i = d_i$, $b_i = d_i$, $i = 1,2,\dots,n$, $r_1 = r_2 = \delta$, $R_1 = R_2 = \Delta$ and $S = \{1,2,\dots,\lfloor \frac{n}{2} \rfloor\}$, the equality (2.8) transforms into

$$n\sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} d_i\right)^2 \leq (\Delta-\delta)^2 \lfloor \frac{n}{2} \rfloor \left(n - \lfloor \frac{n}{2} \rfloor\right), \tag{3.4}$$

i.e.

$$nM_1 - 4m^2 \leq n^2(\Delta-\delta)^2 \frac{1}{n}\lfloor \frac{n}{2} \rfloor \left(1 - \frac{1}{n}\lfloor \frac{n}{2} \rfloor\right).$$

Since

$$\alpha(n) = \frac{1}{n}\lfloor \frac{n}{2} \rfloor \left(1 - \frac{1}{n}\lfloor \frac{n}{2} \rfloor\right) = \frac{1}{4}\left(1 - \frac{1+(-1)^{n+1}}{2n^2}\right)$$

from the above inequality we obtain (3.3).

Since equality in (3.4) holds if and only if $d_1 = d_2 = \cdots = d_n$, equality in (3.3) holds if and only if G is isomorph with k-regular graph, $1 \leq k \leq n-1$. □

Remark 2. If n is even number, $n \geq 2$, then $\alpha(n) = \frac{1}{4}$, and if n is odd, $n \geq 3$, then $\alpha(n) = \frac{(n-1)(n+1)}{4n^2} < \frac{1}{4}$. This means that inequality (3.3) is stronger than inequality (2.2) for each odd n, $n \geq 3$.

Theorem 3. *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Further, let S be a subset of $I_n = \{1,2,\dots,n\}$ that minimizes the expression*

$$\left|\sum_{i\in S} d_i - m\right|. \tag{3.5}$$

Then

$$M_1 \leq \frac{4m^2\left(1 + \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}}\right)^2 \beta(S)\right)}{n} \tag{3.6}$$

where

$$\beta(S)=\frac{1}{2m}\sum_{i\in S}d_i\left(1-\frac{1}{2m}\sum_{i\in S}d_i\right).$$

Equality in (3.6) holds if and only if G is isomorph with k-regular graph, $1\le k\le n-1$, or bidegreed graph such that $\Delta+\delta$ divides $n\delta$ and there are exactly $p=\frac{n\delta}{\Delta+\delta}$ vertices of degree Δ and $q=\frac{n\Delta}{\Delta+\delta}$ vertices of degree δ.

Proof. For $p_i=d_i$, $i=1,2,\dots,n$, the expression (2.7) transforms into (3.5). Suppose that S is subset of $I_n=\{1,2,\dots,n\}$ for which the expression (3.5) reaches a minimum. Now for $p_i=d_i$, $a_i=d_i$, $b_i=\frac{1}{d_i}$, $i=1,2,\dots,n$, $r_1=\delta$, $R_1=\Delta$, $r_2=\frac{1}{\Delta}$ and $R_2=\frac{1}{\delta}$ the inequality (2.8) becomes

$$n\sum_{i=1}^{n}d_i^2-\left(\sum_{i=1}^{n}d_i\right)^2\le(\Delta-\delta)\left(\frac{1}{\delta}-\frac{1}{\Delta}\right)\sum_{i\in S}d_i\left(2m-\sum_{i\in S}d_i\right) \tag{3.7}$$

i.e.

$$nM_1-4m^2\le4m^2\left(\sqrt{\frac{\Delta}{\delta}}-\sqrt{\frac{\delta}{\Delta}}\right)^2\beta(S)$$

wherefrom the inequality (3.6) is obtained.

Equality in (3.7) holds if and only if $d_1=d_2=\cdots=d_n$, therefore the equality in (3.6) holds if and only if G is isomorph with k-regular graph, $1\le k\le n-1$.

Suppose $\Delta+\delta$ divides $n\delta$ and that graph G_1 has exactly $p=\frac{n\delta}{n+\delta}$ vertices of degree Δ and $q=\frac{n\Delta}{\Delta+\delta}$ vertices of degree δ, where $p+q=n$. In that case $m=\frac{n\delta\Delta}{\Delta+\delta}$ and expression (3.5) reaches the minimum if $S=\{1,2,\dots,p\}$ and $\beta(s)=\frac{1}{4}$. This means that equality in (3.5) holds if and only if G is isomorph with bidegreed graph G_1. □

Remark 3. Since for each set $S\subset I_n=\{1,2,\dots,n\}$ holds $\beta(S)\le\frac{1}{4}$, we have that

$$\frac{4m^2\left(1+\left(\sqrt{\frac{\Delta}{\delta}}-\sqrt{\frac{\delta}{\Delta}}\right)^2\beta(S)\right)}{n}\le\frac{m^2\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)^2}{n}.$$

This means that inequality (3.6) is stronger than (2.3).

Corollary 1. *Let G be an undirected connected graph with n , $n\ge2$, vertices and m edges. If $\delta=1$ then*

$$M_1\le\frac{4m^2\left(1+\frac{(n-2)^2}{n-1}\beta(S)\right)}{n}. \tag{3.8}$$

Equality holds if and only if G is isomorph with $K_{1,n-1}$. If $\delta \geq 2$, then

$$M_1 \leq \frac{4m^2\left(1+\frac{(n-3)^2}{2(n-1)}\beta(S)\right)}{n}. \tag{3.9}$$

Equality holds if and only if G is isomorph with graph K_3.

Remark 4. Since $\beta(S) \leq \frac{1}{4}$, it follows that inequalities (3.8) and (3.9) are stronger of the corresponding proved in [15] (their Corollary 2.1) and [17] (their Corollary 2.3).

3.2. *First Zagreb coindex*

Now we give a theorems which provides a lower and upper bounds for $\bar{M}_1$ in terms of parameters n, m, Δ and δ.

Theorem 4. *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Then*

$$\bar{M}_1 \leq \frac{2m}{n}(n(n-1)-2m) - \frac{1}{2}(\Delta-\delta)^2. \tag{3.10}$$

Equality holds if and only if G is isomorph with k-regular graph, $1 \leq k \leq n-1$.

Proof. The proof immediately follows by Lemma 4 and Theorem 1. □

Remark 5. The inequality (3.10) is stronger than (2.5).

Theorem 5. *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Then*

$$\bar{M}_1 \geq \frac{2m}{n}(n(n-1)-2m) - n(\Delta-\delta)^2\alpha(n).$$

Equality holds if and only if G is isomorph with k-regular graph, $1 \leq k \leq n-1$.

Proof. The proof immediately follows by Lemma 4 and Theorem 2. □

Theorem 6. *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Further, let S be a subset of $I_n = \{1, 2, \ldots, n\}$ that minimizes the expression*

$$\left|\sum_{i\in S} d_i - m\right|.$$

Then

$$\bar{M}_1 \geq 2m(n-1) - \frac{4m^2\left(1+\left(\sqrt{\frac{\Delta}{\delta}}-\sqrt{\frac{\delta}{\Delta}}\right)^2\beta(S)\right)}{n} \tag{3.11}$$

where $\beta(s) = \frac{1}{2m}\sum_{i\in S} d_i\left(1-\frac{1}{2m}\sum_{i\in S} d_i\right)$.

Equality in (3.11) holds if and only if G *is isomorph with* k*-regular graph,* $1 \leq k \leq n-1$*, or bidegreed graph such that* $\Delta + \delta$ *divides* $n\delta$ *and there are exactly* $p = \frac{n\delta}{\delta+\delta}$ *vertices of degree* Δ *and* $q = \frac{n\Delta}{\Delta+\delta}$ *vertices of degree* δ*.*

Proof. The proof immediately follows by Lemma 4 and Theorem 3. □

Remark 6. Inequality (3.11) is stronger than (2.6).

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