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Some inequalities between degree- and distance-based topological indices

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Abstract

The first Zagreb index M_1 and the second Zagreb index M_2 belong to the class of degree-based topological indices which are defined for a simple connected graph $\mathbf{G}$ with vertex set $V = \{\upsilon_1, \upsilon_2, \cdots, \upsilon_n\}$ as $M_1(\mathbf{G}) = \sum_{i=1}^{n} d_i^2$ and $M_2(\mathbf{G}) = \sum_{\upsilon_i \sim \upsilon_j} d_i d_j$, where d_i is the degree of vertex υ_i and $\upsilon_i \sim \upsilon_j$ represents the adjacency of vertices υ_i and υ_j in $\mathbf{G}$. The eccentric connectivity index (ECI) is a distance based topological index, denoted by ξ^c, is defined as $\xi^c(\mathbf{G}) = \sum_{i=1}^{n} \varepsilon_i d_i$, where ε_i is the eccentricity of υ_i in $\mathbf{G}$. The aim of this paper is to derive the inequalities between ECI and the Zagreb indices. Moreover, we establish the inequalities between some variants of ECI and the Zagreb indices.

Keyword: *Degree (of vertex), eccentricity (of vertex), Zagreb indices, eccentricity-based topological indices.*

Mathematics Subject Classification: *05C07; 05C35; 92E10.*

1. Introduction

All the graphs concerned in this paper are finite, undirected and simple. Let $\mathbf{G}$ be a graph with vertex set $V = \{\upsilon_1, \upsilon_2, \cdots, \upsilon_n\}$ and edge set $E = E(\mathbf{G})$, where $n = |V|$ and $m = |E|$ are known as order and size of $\mathbf{G}$, respectively. The minimum number of edges lying in the paths connecting the vertices υ_i and υ_j is known as distance between them and is represented by $d(i, j)$. If $d(i, j) = 1$, then we write $\upsilon_i \sim \upsilon_j$. The eccentricity ε_i of vertex $\upsilon_i \in V$ is defined as $\varepsilon_i = \max_{\upsilon_j \in V}\{d(i, j)\}$. Then, the radius r and the diameter d of $\mathbf{G}$ is defined as $r = \min_{\upsilon_i \in V}\{\varepsilon_i\}$ and $d = \max_{\upsilon_i \in V}\{\varepsilon_i\}$, respectively. Assume that the sequence of vertex eccentricities $(\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_n)$ satisfies $d = \varepsilon_1 \geq \varepsilon_2 \geq \cdots \geq \varepsilon_n = r > 0$. If this sequence is constant, i.e., $\varepsilon_i = r = d$, for every vertex υ_i in $\mathbf{G}$, then $\mathbf{G}$ is named as a self-centered graph. For a given vertex υ_i, let $N(\upsilon_i) = \{\upsilon_j \in V \mid d(i, j) = 1\}$, then the degree d_i of vertex υ_i, is defined as $d_i = |N(\upsilon_i)|$. Also, the minimum degree δ and maximum degree Δ of $\mathbf{G}$ is defined as $\delta = \min_{\upsilon_i \in V}\{d_i\}$ and $\Delta = \max_{\upsilon_i \in V}\{d_i\}$, respectively. We assume that the sequence $(d_1, d_2, \cdots, d_n)$ satisfies $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. If this sequence is constant, i.e., $d_i = \delta = \Delta$, for every vertex υ_i in $\mathbf{G}$, then $\mathbf{G}$ is termed a regular graph. Further, for a given vertex υ_i, we define $S_i = \sum_{\upsilon_i \sim \upsilon_j} d_j$. It is easy to observe that $\delta^2 = \min_{\upsilon_i \in V}\{S_i\}$ and $\Delta^2 = \max_{\upsilon_i \in V}\{S_i\}$.

Graph theory has contributed to the development of chemistry by providing a variety of valuable mathematical tools, like as topological indices [28]. Molecular structures of molecules and chemical compounds are usually modeled by graphs. A unique number that is calculated from the parameters of a graph, is declared a topological index (TI) if it correlates with some molecular property of the corresponding molecule/chemical compound. TIs are the conclusive results of a mathematical and logical procedure that converts the chemical phenomena hidden inside a molecule's symbolic representation into a useful number, and they have been shown to be useful in modelling a variety of physicochemical properties in various QSAR and QSPR studies. [8, 27].

Topological indices are generally classified into three types: degree-based indices [4, 16, 20], distance-based indices [3, 24] and spectrum-based indices [17, 22, 23]. The Zagreb indices (ZIs) are among the oldest, best known and most studied vertex degrees-based topological indices which were put forward in [14]. Later, they were enhanced in [15] and utilized in the modeling of structure-property relationship [27]. The first and second Zagreb indices $M_i(\mathbf{G})$ $(i = 1, 2)$ of G are respectively defined as:

$$M_1(\mathbf{G}) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2(\mathbf{G}) = \sum_{\upsilon_i \sim \upsilon_j} d_i d_j.$$

Eccentricity-based topological indices (ETIs) relate to the class of distance-based topological indices which can be defined in three ways, as follows:

$$ETI_1(\mathbf{G}) = \sum_{i=1}^{n} F(\varepsilon_i, d_i), \tag{1.1}$$

$$ETI_2(\mathbf{G}) = \sum_{i=1}^{n} H(\varepsilon_i, S_i), \tag{1.2}$$

and

$$ETI_3(\mathbf{G}) = \sum_{i=1}^{n} Z(\varepsilon_i) \tag{1.3}$$

where F, H and Z are suitably selected functions and the sum runs over all vertices of $\mathbf{G}$.

Sharma et al. [26] proposed a classical ETI, named as eccentric connectivity index (ECI), denoted as ξ^c, and is defined by taking the function $F = \varepsilon_i d_i$ in 1.1. From the following fact: For every function $\theta : [1, \infty) \to R$, we have

$$\sum_{\upsilon_i \sim \upsilon_j} (\theta(\upsilon_i) + \theta(\upsilon_j)) = \sum_{i=1}^{n} d_i \theta(\upsilon_i),$$

we can write ECI as follows:

$$\xi^c(\mathbf{G}) = \sum_{i=1}^{n} \varepsilon_i d_i = \sum_{\upsilon_i \sim \upsilon_j} (\varepsilon_i + \varepsilon_j).$$

ECI has been successfully utilized to build a variety of mathematical models for the prediction of biological activities of diverse nature [13, 24, 25]. Another version of ECI was proposed by Gupta et al. [12], named as connective eccentric index (CEI), represented by ξ^{ce}, and is formulated by choosing the function $F = \frac{d_i}{\varepsilon_i}$ in 1.1. A modified version of ECI was proposed in

[1], called the modified eccentric connectivity index (MECI) which is represented by ξ_c and is defined by setting the function $H = \varepsilon_i S_i$ in 1.2. The Ediz eccentric connectivity index (EECI) was put forward in [10]. This index is symbolized by ${}^{E}\zeta^{c}$ and is defined by selecting the function $H = \frac{S_i}{\varepsilon_i}$ in 1.2. Another version of ECI based on vertex eccentricities was presented in [11], called the total eccentricity index (TEI). This index is represented by ζ and is defined by taking the function $Z = \varepsilon_i$ in 1.3. Similar to this index, Dankelmann et al. [5] proposed the average eccentricity index (AEI) which is symbolized by *avec* and is defined by selecting the function $Z = \frac{1}{n}\varepsilon_i$ in 1.3.
Das and Trinajstić [6] studied the comparison between ECI and ZIs. They investigated that for a tree T with $\Delta \leq 4$, $\xi^c(T) \geq M_i(T)$, $i = 1, 2$. Further, they proved that for a graph G with $\Delta \leq 4$ and $d \geq 7$, $\xi^c(\mathbf{G}) > M_1(\mathbf{G})$. Recently, the inequalities between some ETIs and some degree-based topological indices (other than the ZIs), have been put forward in [19]. In this paper, we derive the inequalities between some ETIs such as ECI, CEI, MECI, and EECI and the ZIs.

2. Some known inequalities

We will review some analytic inequalities for real number sequences before moving on to the rest of the paper.
The following result may be found in [2].

Theorem 1. *Let p_i and q_i be sequences of positive real numbers, then for real constants p, q, P, and Q, we have*

$$\left| n\sum_{i=1}^{n} p_i q_i - \sum_{i=1}^{n} p_i \sum_{i=1}^{n} q_i \right| \leq \tau(n)\,(P-p)\,(Q-q) \tag{2.1}$$

where $p \leq p_i \leq P$ and $q \leq q_i \leq Q$, for each i, $1 \leq i \leq n$, and $\tau(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$. Further, equality attains if and only if $p_1 = p_2 = \cdots = p_n$ and $q_1 = q_2 = \cdots = q_n$.

We find the following Diaz−Metcalf inequality in [9].

Lemma 1. *Let a_i and b_i be real numbers for which t and T are real constants such that $ta_i \leq b_i \leq Ta_i$ holds for each i $(1 \leq i \leq n)$. Then*

$$\sum_{i=1}^{n} b_i^2 + tT\sum_{i=1}^{n} a_i^2 \leq (t+T)\sum_{i=1}^{n} a_i b_i, \tag{2.2}$$

where equality is attained if and only if $b_i = ta_i$ *or* $b_i = Ta_i$.

The following generalized Diaz-Metcalf's inequality can be found in [18].

Theorem 2. *Let* p *and* q *be real numbers with the condition* $0 < q \leq p < 1$, $p + q = 1$ *and let* w_k, a_k *and* b_k *be real numbers for which* t *and* T *are real constants such that* $ta_k \leq b_k \leq Ta_k$ *holds for each* k $(1 \leq k \leq m)$. *Then*

$$p \sum_{k=1}^{m} w_k b_k^2 + tT \sum_{k=1}^{n} q w_k a_k^2 \leq (qt + pT) \sum_{k=1}^{m} w_k a_k b_k \tag{2.3}$$

and equality is attained if and only if $b_k = ta_k$ *or* $b_k = Ta_k$.

In [21], we find the following Radon's inequality.

Lemma 2. *If* $a_i \geq 0$ *and* $b_i > 0$ $(1 \leq i \leq n)$ *are real numbers, then for real number* $p > 0$,

$$\sum_{i=1}^{n} \frac{a_i^{p+1}}{b_i^p} \geq \frac{\left(\sum\limits_{i=1}^{n} a_i\right)^{p+1}}{\left(\sum\limits_{i=1}^{n} b_i\right)^{p}} \tag{2.4}$$

with equality is attained if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_n}{b_n}$.

3. Relations between some ETIs and the first Zagreb index

In this section, we derive the relation of each ECI, CEI, MECI, and EECI with the first Zagreb index.

Theorem 3. *Let* $\mathbf{G}$ *be a connected graph having the defined parameters* n, m, δ, Δ, r *and* d. *Then*

$$\xi^c(\mathbf{G}) \leq \frac{1}{n} \left[2m\zeta(\mathbf{G}) + \tau(n)(\Delta - \delta)(d - r)\right] \tag{3.1}$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$ *and equality is attained if and only if* $\mathbf{G}$ *is a self-centered regular graph.*

Proof. We choose $p_i = d_i$, $q_i = \varepsilon_i$, $p = \delta$, $P = \Delta$, $q = r$, and $Q = d$, for which

$$\delta \leq d_i \leq \Delta \text{ and } r \leq \varepsilon_i \leq d$$

for each i $(1 \leq i \leq n)$. Then, inequality (2.1) becomes

$$n \sum_{i=1}^{n} d_i \varepsilon_i - \sum_{i=1}^{n} d_i \sum_{i=1}^{n} \varepsilon_i \leq \tau(n)(\Delta - \delta)(d - r),$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$.
Since $\sum_{i=1}^{n} d_i = 2m$. So, we have

$$n\xi^c(\mathbf{G}) - 2m\zeta(\mathbf{G}) \leq \tau(n)(\Delta - \delta)(d - r)$$

and the required inequality (3.1) follows.
Equality attains in (2.1) if and only if $p_1 = p_2 = \cdots = p_n$ and $q_1 = q_2 = \cdots = q_n$. This means that equality attains in (3.1) if and only if $d_i = \delta = \Delta$ and $\varepsilon_i = r = d$, for every vertex $v_i \in V$. This is equivalent to $\mathbf{G}$ being a self-centered regular graph. □
In [7], we find the following relation between the average eccentricity and the first Zagreb index.

Theorem 4. *Let* $\mathbf{G}$ *be a connected graph with the defined parameters* n *and* m*. Then*

$$avec(\mathbf{G}) \leq \sqrt{\frac{M_1(\mathbf{G}) + n^3 - 4mn}{n}} \tag{3.2}$$

with equality is attained if and only if $\mathbf{G} \cong K_n$ *or* $\mathbf{G}$ *is isomorphic to a unique* $(n-2)$*-regular graph.*

Corollary 1. *Let* $\mathbf{G}$ *be a connected graph having the defined parameters* n, m, δ, Δ, r *and* d*. Then*

$$\xi^c(\mathbf{G}) \leq 2m\sqrt{\frac{n^3 - 4mn + M_1(\mathbf{G})}{n}} + \frac{\tau(n)}{n}(\Delta - \delta)(d - r) \tag{3.3}$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$ *and the equality attains if and only if* $\mathbf{G} \cong K_n$.

Proof. The relation between TEI and AEI, for a connected graph $\mathbf{G}$ with order n, as follows:

$$avec(\mathbf{G}) = \frac{1}{n}\zeta(\mathbf{G}).$$

With this, (3.2) becomes

$$\zeta(\mathbf{G}) \leq n\sqrt{\frac{M_1(\mathbf{G}) + n^3 - 4mn}{n}}. \tag{3.4}$$

From (3.1) and (3.4), we get

$$\xi^c(\mathbf{G}) \leq 2m\sqrt{\frac{n^3 - 4mn + M_1(\mathbf{G})}{n}} + \frac{\tau(n)}{n}(\Delta - \delta)(d - r)$$

where $\tau(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$.
Since every Complete graph K_n is a regular self-centered graph, whereas $(n-2)$-regular graph may not be a self-centered graph. Therefore, from (3.1) and (3.2), equality attains in (3.3) if and only if $\mathbf{G} \cong K_n$. □

Theorem 5. *Let* $\mathbf{G}$ *be a connected graph having the defined parameters* n, δ, Δ, r *and* d. *Then*

$$\xi^{ce}(\mathbf{G}) \geq \frac{1}{\Delta d + \delta r}\left[\frac{n^3 \Delta \delta r d}{(\zeta(\mathbf{G}))^2} + M_1(\mathbf{G})\right] \tag{3.5}$$

and equality attains if and only if $\mathbf{G}$ *is a self-centered regular graph.*

Proof. We take $a_i = d_i$, $b_i = \frac{1}{\varepsilon_i}$, $t = \frac{1}{\Delta d}$, and $T = \frac{1}{\delta r}$, for which

$$\frac{1}{\Delta d} \leq \frac{b_i}{a_i} \leq \frac{1}{\delta r}$$

for each i $(1 \leq i \leq n)$. Then, inequality (2.2) takes the form

$$\sum_{i=1}^{n} \frac{1}{\varepsilon_i^2} + \frac{1}{\Delta d \delta r} \sum_{i=1}^{n} d_i^2 \leq \left(\frac{1}{\Delta d} + \frac{1}{\delta r}\right) \sum_{i=1}^{n} \frac{d_i}{\varepsilon_i}. \tag{3.6}$$

For $a_i = 1$, $b_i = \varepsilon_i$ and $p = 2$, the inequality (2.4) becomes

$$\sum_{i=1}^{n} \frac{1}{\varepsilon_i^2} \geq \frac{\left(\sum\limits_{i=1}^{n} 1\right)^3}{\left(\sum\limits_{i=1}^{n} \varepsilon_i\right)^2}. \tag{3.7}$$

From (3.6) and (3.7), it implies that

$$\frac{\left(\sum\limits_{i=1}^{n} 1\right)^3}{\left(\sum\limits_{i=1}^{n} \varepsilon_i\right)^2} + \frac{1}{\Delta d \delta r} M_1(\mathbf{G}) \leq \left(\frac{\Delta d + \delta r}{\Delta d \delta r}\right) \xi^{ce}(\mathbf{G}),$$

$$\frac{n^3}{(\zeta(\mathbf{G}))^2} + \frac{1}{\Delta d \delta r} M_1(\mathbf{G}) \leq \left(\frac{\Delta d + \delta r}{\Delta d \delta r}\right) \xi^{ce}(\mathbf{G}),$$

and the desired inequality (3.5) is achieved.
Equality holds in (2.2) if and only if $b_i = ta_i$ or $b_i = Ta_i$, for $1 \leq i \leq n$. This implies that equality attains in (3.6) if and only if $d_i\varepsilon_i = \Delta d$ or $d_i\varepsilon_i = \delta r$, for every vertex $\upsilon_i \in V$, i.e., $d_i\varepsilon_i = c =$ constant, for every vertex $\upsilon_i \in V$. Also, equality attains in (2.4) if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_n}{b_n}$. This means that equality attains in (3.7) if and only if $\frac{1}{\varepsilon_i} = c_2 =$ constant, for every vertex $\upsilon_i \in V$. Let $\upsilon_i, \upsilon_j \in V$, then $d_i\varepsilon_i = d_j\varepsilon_j$ and $\frac{1}{\varepsilon_i} = \frac{1}{\varepsilon_j} \Rightarrow \varepsilon_i = \varepsilon_j$. Then, equality attain in (3.6) and (3.7) if and only if $\varepsilon_i = \varepsilon_j = c_3 =$ constant and $d_i c_3 = d_j c_3 \Rightarrow d_i = d_j$. Finally, we conclude that equality attains in (3.5) if and only if $\mathbf{G}$ is a self-centered regular graph. $\square$ The following Corollary of Theorem 5 can be proved by the similar arguments, presented in Corollary 1.

Corollary 2. *Let* $\mathbf{G}$ *be a connected graph with the defined parameters* n, m, δ, Δ, r *and* d. *Then*

$$\xi^{ce}(\mathbf{G}) \geq \frac{1}{\Delta d + \delta r}\left[\frac{n^2 \Delta \delta r d}{n(n^2 - 4m) + M_1(\mathbf{G})} + M_1(\mathbf{G})\right]$$

and equality attains if and only if $\mathbf{G} \cong K_n$.

Theorem 6. *Let* $\mathbf{G}$ *be a connected graph with the defined parameters* n, δ, Δ, r *and* d. *Then*

$$\xi_c(\mathbf{G}) \leq \frac{1}{n}\left[M_1(\mathbf{G})\zeta(\mathbf{G}) + \tau(n)\left(\Delta^2 - \delta^2\right)(d - r)\right], \tag{3.8}$$

where $\tau(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$ *and equality attains if and only if* $\mathbf{G}$ *is a self-centered regular graph.*

Proof. We define $p_i = S_i$, $q_i = \varepsilon_i$, $p = \delta^2$, $P = \Delta^2$, $q = r$, and $Q = d$, for which

$$\delta^2 \le S_i \le \Delta^2 \quad \text{and} \quad r \le \varepsilon_i \le d$$

for each i $(1 \le i \le n)$. Then, from inequality (2.1), we have

$$n \sum_{i=1}^{n} S_i \varepsilon_i - \sum_{i=1}^{n} S_i \sum_{i=1}^{n} \varepsilon_i \le \tau(n) \left(\Delta^2 - \delta^2\right)(d-r) \tag{3.9}$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$.
It is easy to observe that

$$M_1(\mathbf{G}) = \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} S_i. \tag{3.10}$$

From (3.9) and (3.10), we have

$$n\xi_c(\mathbf{G}) - M_1(\mathbf{G})\zeta(\mathbf{G}) \le \tau(n) \left(\Delta^2 - \delta^2\right)(d-r).$$

and we obtain inequality (3.8).
Equality attains in (2.1) if and only if $p_1 = p_2 = \cdots = p_n$ and $q_1 = q_2 = \cdots = q_n$. This implies that equality attains in (3.8) if and only if $\varepsilon_i = r = d$ and $S_i = \delta^2 = \Delta^2$, for every vertex $v_i \in V$. This is equivalent to $\mathbf{G}$ being a self-centered graph and $d_i = \delta = \Delta$, for every vertex $v_i \in V$. Consequently, equality attains in (3.8) if and only if $\mathbf{G}$ is a self-centered regular graph. $\square$

By the similar arguments presented in Corollary 1, the following corollary of Theorem 6 can be proved.

Corollary 3. *Let* $\mathbf{G}$ *be a connected graph* $\mathbf{G}$ *having the defined parameters* n, δ, Δ, r *and* d*. Then*

$$\xi_c(\mathbf{G}) \le M_1(\mathbf{G}) \sqrt{\frac{M_1(\mathbf{G}) + n^3 - 4mn}{n}} + \frac{\tau(n)}{n} \left(\Delta^2 - \delta^2\right)(d-r),$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$ *and equality is attained if and only if* $\mathbf{G} \cong K_n$.

Theorem 7. *Let* $\mathbf{G}$ *be a connected graph having the defined parameters* n, δ, Δ, r *and* d*. Then*

$${}^{E}\zeta^{c}(\mathbf{G}) \ge \frac{1}{\Delta^2 d + \delta^2 r} \left[\frac{n^3}{(\zeta(\mathbf{G}))^2} + \frac{M_1(\mathbf{G})}{n} \right], \tag{3.11}$$

where equality is attained if and only if $\mathbf{G}$ *is a self-centered regular graph.*

Proof. We choose $a_i = S_i$, $b_i = \frac{1}{\varepsilon_i}$, $t = \frac{1}{\Delta^2 d}$, $T = \frac{1}{\delta^2 r}$, for which

$$\frac{1}{\Delta^2 d} \leq \frac{b_i}{a_i} \leq \frac{1}{\delta^2 r}.$$

for each i $(1 \leq i \leq n)$. Then, inequality (2.2) becomes

$$\sum_{i=1}^{n} \frac{1}{\varepsilon_i^2} + \frac{1}{\Delta^2 d \delta^2 r} \sum_{i=1}^{n} S_i^2 \leq \left(\frac{1}{\Delta^2 d} + \frac{1}{\delta^2 r} \right) \sum_{i=1}^{n} \frac{S_i}{\varepsilon_i}. \tag{3.12}$$

For $a_i = S_i$, $b_i = 1$, and $p = 1$, inequality (2.4) becomes

$$\sum_{i=1}^{n} S_i^2 \geq \frac{\left(\sum\limits_{i=1}^{n} S_i\right)^2}{\sum\limits_{i=1}^{n} 1}. \tag{3.13}$$

From (3.7) and (3.13), inequality (3.12) becomes

$$\frac{\left(\sum\limits_{i=1}^{n} 1\right)^3}{\left(\sum\limits_{i=1}^{n} \varepsilon_i\right)^2} + \frac{1}{\Delta^2 d \delta^2 r} \frac{\left(\sum\limits_{i=1}^{n} S_i\right)^2}{\left(\sum\limits_{i=1}^{n} 1\right)} \leq \left(\frac{\Delta^2 d + \delta^2 r}{\Delta^2 d \delta^2 r} \right) {}^{E}\zeta^{c}(\mathbf{G}),$$

$$\frac{n^3}{(\zeta(\mathbf{G}))^2} + \frac{1}{\Delta^2 d \delta^2 r} \frac{(M_1(\mathbf{G}))^2}{n} \leq \left(\frac{\Delta^2 d + \delta^2 r}{\Delta^2 d \delta^2 r} \right) {}^{E}\zeta^{c}(\mathbf{G}),$$

and we achieve the required inequality (3.11).
Equality attains in (2.2) if and only if $b_i = ta_i$ or $b_i = Ta_i$, for $1 \leq k \leq n$. This means that equality holds in (3.12) if and only if $S_i \varepsilon_i = \Delta^2 d$ or $S_i \varepsilon_i = \delta^2 r$, for every vertex $\upsilon_i \in V$, i.e., $S_i \varepsilon_i = c = \textit{constant}$, for every vertex $\upsilon_i \in V$. Let $\upsilon_i, \upsilon_j \in V$, then $S_i \varepsilon_i = S_j \varepsilon_j$. Also, equality attains in (2.4) if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_n}{b_n}$. This implies that equality attains in (3.13) if and only if $S_i = c_1 =$ constant, for every vertex $\upsilon_i \in V$. Thus, equality attains in (3.12) and (3.13) if and only if $S_i = c_1$ and $c_1 \varepsilon_i = c_1 \varepsilon_j \Rightarrow \varepsilon_i = \varepsilon_j$. We have already proved in Theorem 5 that equality attains in (3.7) if and only if $\mathbf{G}$ is a self-centered graph. Finally, we conclude that equality attains in (3.11) if and only if $\mathbf{G}$ is a self-centered regular graph. □ From the similar arguments given in Corollary 1, the following Corollary of Theorem 7 can be proved.

Corollary 4. *Let* $\mathbf{G}$ *be a connected graph* $\mathbf{G}$ *having the defined parameters* n, m, δ, Δ, r *and* d. *Then*

$$^{E}\zeta^{c}(\mathbf{G}) \geq \frac{1}{\Delta^2 d + \delta^2 r}\left[\frac{n^2}{n^3 - 4mn + M_1(\mathbf{G})} + \frac{M_1(\mathbf{G})}{n}\right],$$

where equality attains if and only if $\mathbf{G} \cong K_n$.

4. Relations between some ETIs and the second Zagreb index

In this section, we establish the following relations: between ECI and the second Zagreb index, between CEI, MECI, and the second Zagreb index, and between ECI, EECI, and the second Zagreb index.

Theorem 8. *Let* $\mathbf{G}$ *be a connected graph having the defined parameters* δ, Δ, r *and* d. *Then*

$$\frac{\xi^{c}(\mathbf{G})}{M_2(\mathbf{G})} + \frac{4rd}{\Delta^2\delta^2}\frac{M_2(\mathbf{G})}{\xi^{c}(\mathbf{G})} \leq 2\left(\frac{d}{\delta^2} + \frac{r}{\Delta^2}\right) \tag{4.1}$$

and equality attains if and only if $\mathbf{G}$ *is a self-centered regular graph.*

Proof. Let $\mathbf{G}$ be a connected graph with size m. For each edge e_k, incident to the vertices υ_i and υ_j, we define $a_k = d_i d_j$, $b_k = \varepsilon_i + \varepsilon_j$, $w_k = \frac{1}{d_i d_j}$, $t = \frac{2r}{\Delta^2}$, and $T = \frac{2d}{\delta^2}$, for which

$$\frac{2r}{\Delta^2} \leq \frac{b_k}{a_k} = \frac{\varepsilon_i + \varepsilon_j}{d_i d_j} \leq \frac{2d}{\delta^2}$$

for each k $(1 \leq k \leq m)$, and by taking $p = q = \frac{1}{2}$, inequality (2.3) becomes

$$\sum_{\upsilon_i \sim \upsilon_j} \frac{(\varepsilon_i + \varepsilon_j)^2}{d_i d_j} + \frac{4rd}{\Delta^2\delta^2}\sum_{\upsilon_i \sim \upsilon_j} d_i d_j \leq \left(\frac{2r}{\Delta^2} + \frac{2d}{\delta^2}\right)\sum_{\upsilon_i \sim \upsilon_j}(\varepsilon_i + \varepsilon_j). \tag{4.2}$$

Also, we define $a_k = \varepsilon_i + \varepsilon_j$ and $b_k = d_i d_j$. By taking $p = 1$, inequality (2.4) becomes

$$\sum_{\upsilon_i \sim \upsilon_j} \frac{(\varepsilon_i + \varepsilon_j)^2}{d_i d_j} \geq \frac{\left(\sum\limits_{\upsilon_i \sim \upsilon_j}(\varepsilon_i + \varepsilon_j)\right)^2}{\sum\limits_{\upsilon_i \sim \upsilon_j} d_i d_j}. \tag{4.3}$$

From (4.2) and (4.3), we have

$$\frac{\left(\sum\limits_{v_i\sim v_j}(\varepsilon_i+\varepsilon_j)\right)^2}{\sum\limits_{v_i\sim v_j} d_id_j}+\frac{4rd}{\Delta^2\delta^2}M_2(\mathbf{G})\leq 2\left(\frac{d}{\delta^2}+\frac{r}{\Delta^2}\right)\xi^c(\mathbf{G}),$$

$$\frac{(\xi^c(\mathbf{G}))^2}{M_2(\mathbf{G})}+\frac{4rd}{\Delta^2\delta^2}M_2(\mathbf{G})\leq 2\left(\frac{d}{\delta^2}+\frac{r}{\Delta^2}\right)\xi^c(\mathbf{G})$$

and we obtain the required inequality (4.1).
Equality holds in (2.3) if and only if $b_i = ta_i$ or $b_i = Ta_i$ for $1 \leq i \leq n$. This implies that equality attains in (4.2) if and only if either $2rd_id_j = \Delta^2(\varepsilon_i+\varepsilon_j)$ or $2dd_id_j = \delta^2(\varepsilon_i + \varepsilon_j)$ for every edge of $\mathbf{G}$, i.e., $\frac{d_id_j}{\varepsilon_i+\varepsilon_j} = c =$ constant, for every edge of $\mathbf{G}$. Also, equality attains in (4.3) if and only if $\frac{\varepsilon_i+\varepsilon_j}{d_id_j} = c_1 =$ constant, for every edge of $\mathbf{G}$. Let v_j, v_t be vertices adjacent to vertex v_i, that is $v_i \sim v_j$ and $v_i \sim v_t$, then $\frac{d_id_j}{\varepsilon_i+\varepsilon_j} = \frac{d_id_t}{\varepsilon_i+\varepsilon_t} \Rightarrow \frac{d_j}{\varepsilon_i+\varepsilon_j} = \frac{d_t}{\varepsilon_i+\varepsilon_t}$. This implies that equality attains in (4.2) and (4.3) if and only if $d_j = d_t = c_2 =$ constant and $\frac{c_2}{\varepsilon_i+\varepsilon_j} = \frac{c_2}{\varepsilon_i+\varepsilon_t} \Rightarrow \varepsilon_i + \varepsilon_j = \varepsilon_i + \varepsilon_t \Rightarrow \varepsilon_j = \varepsilon_t$. Hence, equality attains in (4.1) if and only if $\mathbf{G}$ is a self-centered regular graph. □

Observation 1. *Let G be a graph. From the definition of $M_2(G)$, it is easy to observe that*

$$M_2(\mathbf{G}) = \sum_{v_i\sim v_j} d_id_j = \frac{1}{2}\sum_{i=1}^{n} d_i \sum_{v_j\in N(v_i)} d_j = \frac{1}{2}\sum_{i=1}^{n} d_iS_i. \tag{4.4}$$

Theorem 9. *Let $\mathbf{G}$ be a connected graph $\mathbf{G}$ having the defined parameters n, δ, Δ, r and d. Then*

$$M_2(\mathbf{G}) \geq \frac{\Delta\delta}{2n\left(\Delta^3d^2+\delta^3r^2\right)}\left[(\xi_c(\mathbf{G}))^2+\Delta\delta\left(rd\xi^{ce}(\mathbf{G})\right)^2\right] \tag{4.5}$$

and equality is attained if and only if $\mathbf{G}$ is a self-centered regular graph.

Proof. We take $a_i = \frac{d_i}{\varepsilon_i}$, $b_i = \varepsilon_iS_i$, $t = \frac{r^2\delta^2}{\Delta}$, and $T = \frac{d^2\Delta^2}{\delta}$, for which

$$\frac{r^2\delta^2}{\Delta} \leq \frac{b_i}{a_i} = \frac{\varepsilon_i^2S_i}{d_i} \leq \frac{d^2\Delta^2}{\delta}$$

for each i $(1 \leq i \leq n)$. Then, from inequality (2.2), we have

$$\sum_{i=1}^{n} (\varepsilon_i S_i)^2 + \frac{r^2\delta^2 d^2\Delta^2}{\Delta\delta} \sum_{i=1}^{n} \left(\frac{d_i}{\varepsilon_i}\right)^2 \leq \left(\frac{r^2\delta^2}{\Delta} + \frac{d^2\Delta^2}{\delta}\right) \sum_{i=1}^{n} d_i S_i.$$

From (4.4), we have

$$\sum_{i=1}^{n} (\varepsilon_i S_i)^2 + r^2 d^2 \Delta\delta \sum_{i=1}^{n} \left(\frac{d_i}{\varepsilon_i}\right)^2 \leq 2M_2(G) \left(\frac{\Delta^3 d^2 + \delta^3 r^2}{\Delta\delta}\right). \tag{4.6}$$

For $a_i = \varepsilon_i S_i$, $b_i = 1$ and $p = 1$, inequality (2.4) becomes

$$\sum_{i=1}^{n} (\varepsilon_i S_i)^2 \geq \frac{\left(\sum\limits_{i=1}^{n} \varepsilon_i S_i\right)^2}{\sum\limits_{i=1}^{n} 1}. \tag{4.7}$$

Also, for $a_i = \frac{d_i}{\varepsilon_i}$, $b_i = 1$ and $p = 1$, inequality (2.4) becomes

$$\sum_{i=1}^{n} \left(\frac{d_i}{\varepsilon_i}\right)^2 \geq \frac{\left(\sum\limits_{i=1}^{n} \frac{d_i}{\varepsilon_i}\right)^2}{\sum\limits_{i=1}^{n} 1}. \tag{4.8}$$

From inequalities (4.6), (4.7) and (4.8), we have

$$\frac{\left(\sum\limits_{i=1}^{n} \varepsilon_i S_i\right)^2}{\sum\limits_{i=1}^{n} 1} + r^2 d^2 \Delta\delta \frac{\left(\sum\limits_{i=1}^{n} \frac{d_i}{\varepsilon_i}\right)^2}{\sum\limits_{i=1}^{n} 1} \leq 2M_2(\mathbf{G}) \left(\frac{\Delta^3 d^2 + \delta^3 r^2}{\Delta\delta}\right),$$

$$\frac{(\xi_c(\mathbf{G}))^2}{n} + r^2 d^2 \Delta\delta \frac{(\xi^{ce}(\mathbf{G}))^2}{n} \leq 2M_2(\mathbf{G}) \left(\frac{\Delta^3 d^2 + \delta^3 r^2}{\Delta\delta}\right)$$

and here we obtain the desired inequality (4.5).
Equality attains in (2.3) if and only if $b_i = ta_i$ or $b_i = Ta_i$ for $1 \leq k \leq n$. This means that equality holds in (4.6) if and only if $\frac{\varepsilon_i^2 S_i}{d_i} = \frac{r^2\delta^2}{\Delta}$ or $\frac{\varepsilon_i^2 S_i}{d_i} = \frac{d^2\Delta^2}{\delta}$, for every vertex $v_i \in V$, i.e., $\frac{\varepsilon_i^2 S_i}{d_i} = c =$ constant, for every vertex $v_i \in V$. Also, equality attains in (4.7) if and only if $\varepsilon_i S_i = c_1 =$ constant, for every vertex $v_i \in V$. Further, equality attains in (4.8) if and only if $\frac{d_i}{\varepsilon_i} = c_2 =$ constant, for every vertex $v_i \in V$. By combining $\varepsilon_i S_i = c_1$

and $\frac{d_i}{\varepsilon_i} = c_2$, we have $S_i d_i = c_3 =$ constant, for every vertex $\upsilon_i \in V$. We claim that G is a regular graph. For otherwise, $d_i \neq d_j$, for some vertices $\upsilon_i, \upsilon_j \in V$. Also, by the definition of S_i, $S_i \geq d_i$ for every vertex $\upsilon_i \in V$. For $d_i \neq d_j$, we have $S_i \geq d_i$ and $S_j \geq d_j$. This implies that $S_i d_i \neq S_j d_j$, i.e. $S_i d_i \neq$ constant. This contradicts to the given statement that $S_i d_i = c_3 =$ constant, for every vertex $\upsilon_i \in V$. Hence, **G** is a regular graph. So, $d_i = c_4 =$ constant and $S_i = c_4^2$, for every vertex $\upsilon_i \in V$. Then, $\frac{\varepsilon_i^2 S_i}{d_i} = c \Rightarrow \frac{\varepsilon_i^2 c_4^2}{c_4} = c \Rightarrow \varepsilon_i = c_5 =$ constant, for every vertex $\upsilon_i \in V$. Finally, we conclude that equality attains in (4.5) if and only if **G** is a self-centered regular graph. □

Theorem 10. *Let* **G** *be a connected graph having the defined parameters* n, δ, Δ, r *and* d. *Then*

$$M_2(\mathbf{G}) \leq \frac{1}{2n}\left[{}^{E}\zeta^c(\mathbf{G})\xi^c(\mathbf{G}) + \frac{\tau(n)}{rd}(\Delta d - \delta r)\left(\Delta^2 d - \delta^2 r\right)\right] \tag{4.9}$$

where $\tau(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$ *and equality attains if and only if* **G** *is a self-centered regular graph.*

Proof. We define $p_i = \frac{S_i}{\varepsilon_i}$, $q_i = \varepsilon_i d_i$, $p = \frac{\delta^2}{d}$, $P = \frac{\Delta^2}{r}$, $q = r\delta$, and $Q = d\Delta$, for which

$$\frac{\delta^2}{d} \leq p_i \leq \frac{\Delta^2}{r} \quad \text{and} \quad r\delta \leq q_i \leq d\Delta$$

for each i $(1 \leq i \leq n)$. Then, inequality (2.1) takes the form

$$n\sum_{i=1}^{n} d_i S_i - \sum_{i=1}^{n} \frac{S_i}{\varepsilon_i} \sum_{i=1}^{n} \varepsilon_i d_i \leq \tau(n)\left(\frac{\Delta^2}{r} - \frac{\delta^2}{d}\right)(\Delta d - \delta r)$$

where $\tau(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$.
From (4.4), it follows that

$$2nM_2(\mathbf{G}) - {}^{E}\zeta^c(\mathbf{G})\xi^c(\mathbf{G}) \leq \frac{\tau(n)}{rd}\left(\Delta^2 d - \delta^2 r\right)(\Delta d - \delta r)$$

and the desired inequality (4.9) follows.
Equality attains in (2.1) if and only if $p_1 = p_2 = \cdots = p_n$ and $q_1 = q_2 = \cdots = q_n$. This implies that equality attains in (4.9) if and only

if $\frac{S_i}{\varepsilon_i} = \frac{\delta^2}{d} = \frac{\Delta^2}{r}$ and $\varepsilon_i d_i = r\delta = d\Delta$, for every vertex $\upsilon_i \in V$, i.e., $\frac{S_i}{\varepsilon_i} = c =$ constant and $\varepsilon_i d_i = c_1 =$ constant, for every vertex $\upsilon_i \in V$. By combining, we have $S_i d_i = c_2 =$ constant, for every vertex $\upsilon_i \in V$. This implies that $\mathbf{G}$ is a regular graph, i.e., $d_i = c_3 =$ constant. Also, $\varepsilon_i d_i = c_1 \Rightarrow \varepsilon_i c_3 = c_1 \Rightarrow \varepsilon_i = c_4 =$ constant, for every vertex $\upsilon_i \in V$. Hence, we conclude that equality attains in (4.9) if and only if $\mathbf{G}$ is a self-centered regular graph. □

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