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# BOUNDS ON THE HYPER-ZAGREB INDEX

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Abstract. The hyper-Zagreb index $HM(G)$ of a simple graph $G$ is defined as the sum of the terms $(d_u+d_v)^2$ over all edges $uv$ of $G$, where $d_u$ denotes the degree of the vertex $u$ of $G$. In this paper, we present several upper and lower bounds on the hyper-Zagreb index in terms of some molecular structural parameters and relate this index to various well-known molecular descriptors.

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## 1. Introduction

Let $G$ be a finite simple connected graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $d_u$ the degree of the vertex $u$ of $G$. A vertex $u$ is said to be pendent if $d_u = 1$. We denote by $\delta$ and $\Delta$ the minimal and maximal vertex degrees of $G$, respectively. The distance $d_G(u, v)$ between the vertices $u$ and $v$ of $G$ is defined as the length of any shortest path in $G$ connecting $u$ and $v$. The eccentricity $\varepsilon_u$ of a vertex $u$ is the largest distance between $u$ and any other vertex of $G$. For positive integers $s \neq t$, a graph $G$ is said to be $(s, t)$-*semiregular* if its vertex degrees assume only the values $s$ and $t$, and if there is at least one vertex of degree $s$ and at least one of degree $t$. A bipartite graph is said to be $(s, t)$-*semiregular bipartite* or $(s, t)$-*biregular* if any vertex in one side of the given bipartition has degree $s$ and any vertex in the other side of the bipartition has degree $t$.

A *molecular descriptor* (also known as *topological index* or *graph invariant*) is any function on a graph that does not depend on a labeling of its vertices.

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In organic chemistry, topological indices have been found to be useful in chemical documentation, isomer discrimination, quantitative structure-property relationships (QSPR), quantitative structure-activity relationships (QSAR), and pharmaceutical drug design [5, 12].

The *Zagreb indices* are among the oldest topological indices, and were introduced by Gutman and Trinajstić [13] in 1972. These indices have since been used to study molecular complexity, chirality, ZE–isomerism, and hetero–systems. The first and second Zagreb indices of $G$ are denoted by $M_1(G)$ and $M_2(G)$, respectively, and defined as

$$M_1(G) = \sum_{u \in V(G)} {d_u}^2 \quad and \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

The first Zagreb index can also be expressed as a sum over edges of $G$,

$$M_1(G) = \sum_{\mathrm{uv} \in E(G)} (d_u + d_v).$$

A multiplicative version of the first Zagreb index called *multiplicative sum Zagreb index* was proposed by Eliasi et al. [7] in 2010. The multiplicative sum Zagreb index $\Pi_1^*(G)$ of $G$ is defined as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v).$$

In 1975, Milan Randić [16] proposed a structural descriptor, based on the end-vertex degrees of edges in a graph, called the *branching index* that later became the well-known *Randić connectivity index*. The Randić index $R(G)$ of $G$ is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The Randić index is one of the most successful molecular descriptors in QSPR and QSAR studies, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons.

Another variant of the Randić connectivity index named the *harmonic index* was introduced by Fajtlowicz [8] in 1987. The harmonic index $H(G)$ of $G$ is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

Motivated by definition of the Randić connectivity index, Vukičević and Furtula [20] proposed another vertex-degree-based topological index, named the *geometric-arithmetic index*. The geometric-arithmetic index of a graph $G$ is denoted by $GA(G)$ and defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The *eccentric connectivity index* was introduced by Sharma et al. [17] in 1997. The eccentric connectivity index $\xi^c(G)$ of $G$ is defined as

$$\xi^c(G) = \sum_{uv \in E(G)} d_u \varepsilon_u.$$

The eccentric connectivity index can also be expressed as a sum over edges of $G$,

$$\xi^c(G) = \sum_{uv \in E(G)} (\varepsilon_u + \varepsilon_v).$$

The *Zagreb eccentricity indices* were introduced by Vukičević and Graovac [21] in 2010. These indices are defined in analogy with the Zagreb indices by replacing the vertex degrees with the vertex eccentricities. Thus, the first and second Zagreb eccentricity indices of $G$ are defined as

$$\xi_1(G) = \sum_{uv \in E(G)} {\varepsilon_u}^2 \quad and \quad \xi_2(G) = \sum_{uv \in E(G)} \varepsilon_u \varepsilon_v.$$

Recently, Shirdel et al. [18] introduced a variant of the first Zagreb index called *hyper-Zagreb index.* The hyper-Zagreb index of $G$ is denoted by $HM(G)$ and defined as

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2.$$

In this paper, we present several upper and lower bounds on the hyper-Zagreb index in terms of some graph parameters such as the order, size, number of pendant vertices, minimal and maximal vertex degrees, and minimal non-pendent vertex degree, and relate this index to various well-known graph invariants such as the first and second Zagreb indices, multiplicative sum Zagreb index, Randić index, harmonic index, geometric-arithmetic index, eccentric connectivity index, and second Zagreb connectivity index. We refer the reader to consult [1, 2, 3, 6, 9, 10, 11, 19] for more information on computing bounds on vertex-degree-based topological indices.

## 2. Preliminaries

In this section, we recall some well-known inequalities which will be used throughout the paper.

Let $x_1, x_2, \dots, x_n$ be positive real numbers.
The *arithmetic mean* of $x_1, x_2, \dots, x_n$ is equal to

$$AM\left(x_1, x_2, \dots, x_n\right) = \frac{x_1 + x_2 + \cdots + x_n}{n}.$$

The *geometric mean* of $x_1, x_2, \dots, x_n$ is equal to

$$GM\left(x_1, x_2, \dots, x_n\right) = \sqrt[n]{x_1 x_2 \dots x_n}.$$

The *harmonic mean* of $x_1, x_2, \ldots, x_n$ is equal to

$$HM\left(x_1, x_2, \ldots, x_n\right) = \frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + \cdots + \frac{1}{x_n}}.$$

Related to these three means, we have the following well-known inequalities.

**Lemma 2.1** (AM-GM-HM inequality)**.** *Let $x_1, x_2, \ldots, x_n$ be positive real numbers. Then*

$$AM\left(x_1, x_2, \ldots, x_n\right) \geq GM\left(x_1, x_2, \ldots, x_n\right) \geq HM\left(x_1, x_2, \ldots, x_n\right),$$

*with equality if and only if $x_1 = x_2 = \ldots = x_n$.*

**Lemma 2.2** (Cauchy-Schwarz inequality)**.** *Let $X = (x_1, x_2, \ldots, x_n)$ and $Y = (y_1, y_2, \ldots, y_n)$ be two sequences of real numbers. Then*

$$\left(\sum_{i=1}^{n} x_i y_i\right)^2 \leq \sum_{i=1}^{n} {x_i}^2 \sum_{i=1}^{n} {y_i}^2,$$

*with equality if and only if the sequences $X$ and $Y$ are proportional, i.e., there exists a constant $c$ such that $x_i = c y_i$, for each $1 \leq i \leq n$.*

As a special case of the Cauchy-Schwarz inequality, when $y_1 = y_2 = \cdots = y_n$, we get the following result.

**Corollary 2.3.** *Let $x_1, x_2, \ldots, x_n$ be real numbers. Then*

$$\left(\sum_{i=1}^{n} x_i\right)^2 \leq n \sum_{i=1}^{n} {x_i}^2,$$

*with equality if and only if $x_1 = x_2 = \cdots = x_n$.*

**Lemma 2.4** (Pólya-Szegö inequality [15])**.** *Let $0 < m_1 \leq x_i \leq M_1$ and $0 < m_2 \leq y_i \leq M_2$, for $1 \leq i \leq n$. Then*

$$\sum_{i=1}^{n} {x_i}^2 \sum_{i=1}^{n} {y_i}^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}}\right)^2 \left(\sum_{i=1}^{n} x_i y_i\right)^2.$$

**Lemma 2.5** (Diaz-Metcalf inequality [4])**.** *Let $x_1, x_2, \ldots, x_n,\ y_1, y_2, \ldots, y_n$ be real numbers such that $p x_i \leq y_i \leq P x_i$, for $1 \leq i \leq n$. Then*

$$\sum_{i=1}^{n} {y_i}^2 + pP \sum_{i=1}^{n} {x_i}^2 \leq (p + P) \sum_{i=1}^{n} x_i y_i,$$

*with equality if and only if $y_i = P x_i$ or $y_i = p x_i$, for $1 \leq i \leq n$.*

**Lemma 2.6** ([14])**.** *Let $G$ be a nontrivial connected graph of order $n$. For each vertex $u \in V(G)$,*

$$\varepsilon_u \leq n - d_u,$$

*with equality if and only if $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor$, where $P_4$ denotes the path on 4 vertices and $K_n - iK_2$ denotes the graph obtained from the complete graph $K_n$ by removing $i$ independent edges.*

## 3. Results and discussion

In this section, we present several upper and lower bounds on the hyper-Zagreb index in terms of some graph parameters and various molecular descriptors.

Throughout this section, we assume that $G$ is a nontrivial simple connected graph with order $n$ and size $m$. Note that, the connectivity of $G$ is not an important restriction, since if $G$ has connected components $G_1, G_2, \ldots, G_r$, then $HM(G) = \sum_{i=1}^{r} HM(G_i)$. Furthermore, every molecular graph is connected.

**Theorem 3.1.** *For any graph $G$,*

$$4m\delta^2 \leq HM(G) \leq 4m\Delta^2,$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Since $2\delta \leq d_u + d_v \leq 2\Delta$, for each $uv \in E(G)$, we have

$$4m\delta^2 = \sum_{uv\in E(G)} (2\delta)^2 \leq HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2 \leq \sum_{uv\in E(G)} (2\Delta)^2 = 4m\Delta^2.$$

The equalities hold if and only if $d_u + d_v = 2\Delta = 2\delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. □

**Theorem 3.2.** *For any graph $G$ with $p$ pendant vertices and minimal non-pendent vertex degree $\delta_1$,*

$$4{\delta_1}^2 (m-p) + (1+\delta_1)^2 p \leq HM(G) \leq 4\Delta^2 (m-p) + (1+\Delta)^2 p,$$

*with equality if and only if $G$ is regular or $(1, \Delta)$-semiregular.*

*Proof.* From the definition of the hyper-Zagreb index,

$$\begin{aligned} HM(G) &= \sum_{\substack{uv\in E(G)\\ d_u,d_v\neq 1}} (d_u + d_v)^2 + \sum_{\substack{uv\in E(G)\\ d_u=1}} (1 + d_v)^2 \\ &\leq \sum_{\substack{uv\in E(G)\\ d_u,d_v\neq 1}} (2\Delta)^2 + \sum_{\substack{uv\in E(G)\\ d_u=1}} (1 + \Delta)^2 \\ &= 4\Delta^2 (m-p) + (1+\Delta)^2 p. \end{aligned}$$

Similarly,

$$HM(G) \geq \sum_{\substack{uv\in E(G)\\ d_u,d_v\neq 1}} (2\delta_1)^2 + \sum_{\substack{uv\in E(G)\\ d_u=1}} (1+\delta_1)^2 = 4{\delta_1}^2 (m-p) + (1+\delta_1)^2 p.$$

The above equalities hold if and only if $d_u = d_v = \Delta = \delta_1$, for each $uv \in E(G)$, with $d_u, d_v \neq 1$, and $d_v = \Delta = \delta_1$, for each $uv \in E(G)$, with $d_u = 1$. This implies that, $G$ is $(1, \Delta)$-semiregular if $p > 0$, and $G$ is regular if $p = 0$. □

**Theorem 3.3.** *Let $G$ be a tree. Then*

$$HM(G) \leq n^2(n-1),$$

*with equality if and only if $G$ is a star graph.*

*Proof.* Since $d_u + d_v \leq n$, for each $uv \in E(G)$, we have

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2 \leq \sum_{uv \in E(G)} n^2 = n^2 m = n^2(n-1),$$

with equality if and only if $d_u + d_v = n$, for each $uv \in E(G)$, which implies that $G$ is a star graph. □

**Theorem 3.4.** *For any graph $G$,*

$$HM(G) \geq \frac{M_1(G)^2}{m},$$

*with equality if and only if $G$ is regular or biregular.*

*Proof.* By Corollary 2.3, we obtain

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2 \geq \frac{\left(\sum_{uv \in E(G)} (d_u + d_v)\right)^2}{m} = \frac{M_1(G)^2}{m}.$$

The equality holds if and only if there exists a constant $c$ such that $d_u + d_v = c$, for each $uv \in E(G)$. If $uv, uz \in E(G)$, then $d_u + d_v = d_u + d_z$, which implies that $d_v = d_z$. Consequently, for each $u \in V(G)$, every neighbor of $u$ has the same degree. Since $G$ is connected, this holds if and only if $G$ is regular or biregular. □

**Theorem 3.5.** *For any graph $G$,*

$$HM(G) \leq \frac{(\delta + \Delta)^2}{4m\delta\Delta} M_1(G)^2.$$

*Proof.* Using the fact that, $2\delta \leq d_u + d_v \leq 2\Delta$, for each $uv \in E(G)$, and setting $m_1 = 2\delta$, $x_i = d_u + d_v$, $1 \leq i \leq m$, $M_1 = 2\Delta$, and $m_2 = y_i = M_2 = 1$, $1 \leq i \leq m$, in Pólya-Szegö inequality, we obtain

$$\sum_{uv \in E(G)} (d_u + d_v)^2 \sum_{uv \in E(G)} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{2\Delta}{2\delta}} + \sqrt{\frac{2\delta}{2\Delta}}\right)^2 \Big(\sum_{uv \in E(G)} (d_u + d_v)\Big)^2,$$

which is easily simplified into

$$HM(G) \leq \frac{1}{4m}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 M_1(G)^2 = \frac{(\delta + \Delta)^2}{4m\delta\Delta} M_1(G)^2.$$

□

**Theorem 3.6.** *For any graph $G$,*

$$HM(G) \leq 2\,(\delta+\Delta)\,M_1(G) - 4m\delta\Delta,$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* By setting $p = 2\delta$, $P = 2\Delta$, $x_i = 1$, and $y_i = d_u + d_v$, $1 \leq i \leq m$, in Diaz-Metcalf inequality, we obtain

$$\sum_{uv\in E(G)} (d_u + d_v)^2 + 4\delta\Delta \sum_{uv\in E(G)} 1^2 \leq 2\,(\delta+\Delta) \sum_{uv\in E(G)} (d_u + d_v),$$

which is easily simplified into

$$HM(G) \leq 2\,(\delta+\Delta)\,M_1(G) - 4m\delta\Delta.$$

By Lemma 2.5, the equality holds if and only if $d_u + d_v = 2\delta$ or $d_u + d_v = 2\Delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. □

**Theorem 3.7.** *For any graph $G$,*

$$HM(G) \geq 4M_2(G),$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Using the AM-GM inequality, we get

$$HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2 \geq \sum_{uv\in E(G)} \left(2\sqrt{d_u d_v}\right)^2 = 4M_2(G).$$

By Lemma 2.1, the equality holds if and only if $d_u = d_v$, for each $uv \in E\,(G)$, which implies that $G$ is a regular graph. □

**Theorem 3.8.** *For any graph $G$,*

$$\delta M_1(G) + 2M_2(G) \leq HM(G) \leq \Delta M_1(G) + 2M_2(G),$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Using the definitions of the hyper-Zagreb and Zagreb indices, we have

$$\begin{aligned} HM(G) &= \sum_{uv\in E(G)} (d_u + d_v)^2 = \sum_{uv\in E(G)} \left({d_u}^2 + {d_v}^2\right) + \sum_{uv\in E(G)} 2d_u d_v \\ &= \sum_{u\in V(G)} d_u.{d_u}^2 + 2M_2(G). \end{aligned}$$

Now using the fact that, $\delta \leq d_u \leq \Delta$, for each $u \in V\,(G)$, we obtain

$$\delta M_1(G) + 2M_2(G) \leq HM(G) \leq \Delta M_1(G) + 2M_2(G).$$

The equalities hold if and only if $d_u = \Delta = \delta$, for each $u \in V\,(G)$, which implies that $G$ is a regular graph. □

**Theorem 3.9.** *For any graph $G$,*

$$HM(G) \geq m \sqrt[m]{\Pi_1^*(G)^2},$$

*with equality if and only if $G$ is regular or biregular.*

*Proof.* Using the AM-GM inequality, we get

$$HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2 \geq m \sqrt[m]{\prod_{uv\in E(G)} (d_u + d_v)^2} = m \sqrt[m]{\Pi_1^*(G)^2}.$$

By Lemma 2.1, the equality holds if and only if there exists a constant $c$ such that $(d_u + d_v)^2 = c$, for each $uv \in E(G)$. This implies that, $d_u + d_v = \sqrt{c}$, for each $uv \in E(G)$. As explained in the proof of Theorem 3.4, this holds if and only if $G$ is regular or biregular. □

**Theorem 3.10.** *For any graph $G$,*

$$4\delta^3 R(G) \leq HM(G) \leq 4\Delta^3 R(G),$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* It is easy to see that, for each $uv \in E(G)$,

$$4\delta^3 = (2\delta)^2\sqrt{\delta^2} \leq (d_u + d_v)^2\sqrt{d_u d_v} \leq (2\Delta)^2\sqrt{\Delta^2} = 4\Delta^3.$$

Now, from the definition of the hyper-Zagreb index,

$$4\delta^3 R(G) \leq HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2 \frac{\sqrt{d_u d_v}}{\sqrt{d_u d_v}} \leq 4\Delta^3 R(G).$$

The equalities hold if and only if $d_u = d_v = \delta = \Delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. □

**Theorem 3.11.** *For any graph $G$,*

$$HM(G) \geq \frac{4m^3}{R(G)^2},$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Using the AM-HM inequality, AM-GM inequality, and Corollary 2.3, respectively, we obtain

$$\begin{aligned}\left(\frac{m}{R(G)}\right)^2 &= \left(\frac{m}{\sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}}\right)^2 \leq \left(\frac{\sum_{uv\in E(G)} \sqrt{d_u d_v}}{m}\right)^2 \\ &\leq \frac{1}{m^2}\left(\sum_{uv\in E(G)} \frac{d_u + d_v}{2}\right)^2 \leq \frac{m}{m^2} \sum_{uv\in E(G)} \left(\frac{d_u + d_v}{2}\right)^2 = \frac{1}{4m} HM(G).\end{aligned}$$

By Lemma 2.1, the above first equality holds if and only if there exists a constant $c$ such that $\sqrt{d_u d_v} = c$, for each $uv \in E(G)$. If $uv, uz \in E(G)$, then $\sqrt{d_u d_v} = \sqrt{d_u d_z}$, which implies that $d_v = d_z$. Consequently, for each vertex

$u \in V(G)$, every neighbor of $u$ has the same degree. This holds if and only if $G$ is regular or biregular. By Lemma 2.1, the second equality holds if and only if $d_u = d_v$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. By Corollary 2.3, the third equality holds if and only if there exists a constant $c$ such that $\frac{d_u+d_v}{2} = c$, or equivalently, $d_u + d_v = 2c$, for each $uv \in E(G)$. As explained in the proof of Theorem 3.4, this holds if and only if $G$ is regular or biregular. Consequently, $HM(G) \geq \frac{4m^3}{R(G)^2}$, with equality if and only if $G$ is a regular graph. □

**Theorem 3.12.** *For any graph $G$,*

$$4\delta^3 H(G) \leq HM(G) \leq 4\Delta^3 H(G),$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* It is easy to see that, for each $uv \in E(G)$,

$$4\delta^3 = \frac{(2\delta)^3}{2} \leq \frac{(d_u + d_v)^3}{2} \leq \frac{(2\Delta)^3}{2} = 4\Delta^3.$$

Now, from the definition of the hyper-Zagreb index,

$$4\delta^3 H(G) \leq HM(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \times \frac{(d_u + d_v)^3}{2} \leq 4\Delta^3 H(G).$$

The equalities hold if and only if $d_u = d_v = \delta = \Delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. □

**Theorem 3.13.** *For any graph $G$,*

$$HM(G) \geq \frac{4\delta m^2}{H(G)},$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Using the Cauchy-Schwartz inequality, we get

$$\begin{aligned} HM(G)H(G) =& \sum_{uv \in E(G)} (d_u + d_v)^2 \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \\ \geq& \Big( \sum_{uv \in E(G)} (d_u + d_v) \sqrt{\frac{2}{d_u + d_v}} \Big)^2 \\ =& 2 \Big( \sum_{uv \in E(G)} \sqrt{d_u + d_v} \Big)^2 \geq 2 \Big( \sum_{uv \in E(G)} \sqrt{2\delta} \Big)^2 = 4\delta m^2. \end{aligned}$$

By Lemma 2.2, the above first equality holds if and only if there exists a constant $c$ such that $d_u + d_v = c\sqrt{\frac{2}{d_u+d_v}}$, for each $uv \in E(G)$. This implies that $(d_u + d_v)^3 = 2c^2$, for each $uv \in E(G)$. If $uv, uz \in E(G)$, then $(d_u + d_v)^3 = (d_u + d_z)^3$, which is then easily simplified into $d_v = d_z$. Consequently, for each vertex $u \in V(G)$, every neighbor of $u$ has the same degree. This holds if and only if $G$ is regular or biregular. The second equality holds if and only if $d_u = d_v = \delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. Consequently, $HM(G) \geq \frac{4\delta m^2}{H(G)}$, with equality if and only if $G$ is a regular graph. □

**Theorem 3.14.** *For any graph $G$,*

$$HM(G) \geq \frac{4\delta^2}{m}(GA(G))^2,$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Using the AM-HM inequality and Corollary 2.3, we obtain

$$\begin{aligned}\frac{HM(G)}{4} &= \sum_{uv\in E(G)}\Big(\frac{d_u+d_v}{2}\Big)^2 \geq \sum_{uv\in E(G)}\Big(\frac{2}{\frac{1}{d_u}+\frac{1}{d_v}}\Big)^2 = \sum_{uv\in E(G)}\Big(\frac{2d_ud_v}{d_u+d_v}\Big)^2\\ &\geq \frac{1}{m}\Big(\sum_{uv\in E(G)}\frac{2d_ud_v}{d_u+d_v}\Big)^2 = \frac{1}{m}\Big(\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}\sqrt{d_ud_v}\Big)^2\\ &\geq \frac{1}{m}\Big(\delta\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}\Big)^2 = \frac{\delta^2}{m}(GA(G))^2.\end{aligned}$$

By Lemma 2.1, the above first equality holds if and only if $d_u = d_v$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. By Corollary 2.3, the second equality holds if and only if there exists a constant $c$ such that $\frac{2d_ud_v}{d_u+d_v} = c$, for each $uv \in E(G)$. If $uv, uz \in E(G)$, then $\frac{2d_ud_v}{d_u+d_v} = \frac{2d_ud_z}{d_u+d_z}$. Then $d_v(d_u + d_z) = d_z(d_u + d_v)$, which is easily simplified into $d_v = d_z$. So, every neighbor of $u$ has the same degree, which implies that $G$ is regular or biregular. The third equality holds if and only if $d_u = d_v = \delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. Consequently, $HM(G) \geq \frac{4\delta^2}{m}(GA(G))^2$, with equality if and only if $G$ is a regular graph. □

**Theorem 3.15.** *For any graph $G$,*

$$HM(G) \geq \frac{4m^2\delta^2}{GA(G)},$$

*with equality if and only if $G$ is a regular graph.*

*Proof.* Using the AM-HM inequality, we obtain

$$\begin{aligned}\frac{m}{GA(G)} &= \frac{m}{\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}} \leq \frac{1}{m}\sum_{uv\in E(G)}\frac{d_u+d_v}{2\sqrt{d_ud_v}}\\ &= \frac{1}{2m}\sum_{uv\in E(G)}\frac{d_u+d_v}{\sqrt{d_ud_v}}\times\frac{d_u+d_v}{d_u+d_v}\\ &= \frac{1}{2m}\sum_{uv\in E(G)}(d_u+d_v)^2\times\frac{1}{\sqrt{d_ud_v}(d_u+d_v)} \leq \frac{1}{4m\delta^2}HM(G).\end{aligned}$$

By Lemma 2.1, the above first equality holds if and only if there exists a constant $c$ such that $\frac{d_u+d_v}{2\sqrt{d_u d_v}} = c$, for each $uv \in E(G)$. Using the same argument as in the previous theorems, this holds if and only if $G$ is regular or biregular. The second equality holds if and only if $d_u = d_v = \delta$, for each $uv \in E(G)$, which implies that $G$ is a regular graph. Consequently, $HM(G) \geq \frac{4m^2\delta^2}{GA(G)}$, with equality if and only if $G$ is a regular graph. □

**Theorem 3.16.** *For any graph G,*

$$HM(G) \leq 4n^2m + \xi_3(G) + 2\xi_2(G) - 4n\xi^c(G),$$

*where* $\xi_3(G) = \sum_{u\in V(G)} \left({\varepsilon_u}^2 + {\varepsilon_v}^2\right)$, *and the equality holds if and only if* $G \cong P_4$ *or* $G \cong K_n - iK_2$, $0 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor$.

*Proof.* Using the definition of the hyper-Zagreb index and Lemma 2.6, we get

$$\begin{aligned} HM(G) = &\sum_{uv\in E(G)} (d_u + d_v)^2 \leq \sum_{uv\in E(G)} (n - \varepsilon_u + n - \varepsilon_v)^2 \\ = &\sum_{uv\in E(G)} \left(4n^2 + \left({\varepsilon_u}^2 + {\varepsilon_v}^2\right) + 2\varepsilon_u\varepsilon_v - 4n(\varepsilon_u + \varepsilon_v)\right) \\ = &4n^2m + \xi_3(G) + 2\xi_2(G) - 4n\xi^c(G). \end{aligned}$$

By Lemma 2.6, the equality holds if and only if $d_u = n - \varepsilon_u$, for each $u \in V(G)$, which by Lemma 2.6 implies that, $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \left\lfloor \frac{n}{2} \right\rfloor$. □

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