

Bounds on First Reformulated Zagreb Index of Graph

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ABSTRACT. The first reformulated Zagreb index $EM_1(G)$ of a simple graph G is defined as the sum of the terms $(d_u + d_v - 2)^2$ over all edges uv of G . In this paper, the various upper and lower bounds for the first reformulated Zagreb index of a connected graph in terms of other topological indices are obtained.

Keywords: Zagreb index, reformulated Zagreb index.

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1. INTRODUCTION

A *chemical graph* is a graph whose vertices denote atoms and edges denote bonds between those atoms of any underlying chemical structure. A *topological index* for a (chemical) graph G is a numerical quantity invariant under automorphisms of G and it does not depend on the labeling or pictorial representation of the graph. In the current chemical literature, a large number of graph-based structure descriptors (topological indices) have been put forward, that all depend only on the degrees of the vertices of the molecular graph. More details on vertex-degree-based topological indices and on their comparative study can be found in [5, 6, 9, 11]. The topological indices are graph invariants which have been used for examining quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships

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(QSAR) extensively in which the biological activity or other properties of molecules are correlated with their chemical structures, in [3].

For a (molecular) graph G , The *first Zagreb index* $M_1(G)$ is equal to the sum of the squares of the degrees of the vertices, and the *second Zagreb index* $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices, that is, $M_1(G) = \sum_{u \in V(G)} d_G^2(u) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$,

$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$, where $d_G(u)$ is the degree of a vertex u in G .

Milicević et al. [14] in 2004 reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees $EM_1(G) = \sum_{e \in E(G)} d(e)^2$, where $d(e)$

denotes the degree of the edge e in G , which is defined by $d(e) = d(u) + d(v) - 2$ with $e = uv$. The use of these descriptors in QSPR study was also discussed in their report [14]. Reformulated Zagreb index, particularly its upper and lower bounds has attracted recently threat tension of many mathematicians and computer scientists, in [2, 10, 12, 13, 14, 19, 21]. In this sequence, we obtain here, the various upper and lower bounds for the first reformulated Zagreb index of a connected graph in terms of other topological indices.

2. PRELIMINARIES

In this section, we recall some definitions and notations which will be used throughout the paper.

Let G be a connected graph. We denote by δ and Δ the minimum and maximum 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 . Let $D(G)$ be the diameter of G . For an edge $uv = e \in E(G)$, the number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v in G is denoted by $n_u(e)$; analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v in G is smaller than the distance to the vertex u . The *vertex PI index* of G , denoted by $PI(G)$, is defined as $PI(G) = \sum_{e=uv \in E(G)} (n_u(e) + n_v(e))$.

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

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 $H(G) = \sum_{uv \in E(G)} \frac{1}{d(u)+d(v)}$. Motivated by definition of the Randić

connectivity index, Vukicević 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 $\xi^c(G) = \sum_{uv \in E(G)} d(u)\epsilon(u)$. The eccentric connectivity index can also be expressed as a sum over edges of G , $\xi^c(G) = \sum_{uv \in E(G)} (\epsilon(u) + \epsilon(v))$.

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 $HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2$.

3. BOUNDS FOR EM_1

In this section, we obtain the different kinds of upper and lower bounds for first reformulated Zagreb index of a given connected graph.

Theorem 3.1. *Let G be a triangle free graph. Then $EM_1(G) \leq HM(G) - 4PI(G) + 4m$ with equality if and only if diameter of G is 2.*

Proof. Since $n_u(e) + n_v(e) \geq d(u) + d(v)$ for each edge $e = uv \in E(G)$. Thus

$$\begin{aligned} EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v))^2 - 4 \sum_{uv \in E(G)} (d(u) + d(v)) + 4m \\ &\leq HM(G) - 4 \sum_{uv \in E(G)} (n_u(e) + n_v(e)) + 4m \\ &= HM(G) - 4PI(G) + 4m. \end{aligned}$$

Assume that $D(G) = 2$ and there exists an edge $e = uv$ such that $n_u(e) + n_v(e) > d_G(u) + d_G(v)$. Then there exists a vertex r such that $d_G(u, r) \neq 1$ and $d_G(v, r) \neq 1$. Suppose x is closer to u than v . Hence $d_G(x, v) > d_G(x, u) \geq 2$, which contradicts by our assumption that $D(G) = 2$. Therefore, for each edge $e = uv$, $n_u(e) + n_v(e) = d_G(u) + d_G(v)$ and so $EM_1(G) = HM(G) - 4PI(G) + 4m$. \square

Theorem 3.2. *Let G be a graph with m edges. Then $4m(\delta - 1)^2 \leq EM_1(G) \leq 4m(\Delta - 1)^2$ with equality if and only if G is regular.*

Proof. One can observe that $2\delta - 2 \leq d(u) + d(v) - 2 \leq 2\Delta - 2$ for every edge uv in G . Thus

$$4m(\delta - 1)^2 = \sum_{uv \in E(G)} (2\delta - 2)^2 \leq \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 = EM_1(G) \leq \sum_{uv \in E(G)} (2\Delta - 2)^2 = 4m(\Delta - 1)^2.$$

The equalities hold if and only if $2\delta - 2 = d(u) + d(v) - 2 = 2\Delta - 2$, for each edge $uv \in E(G)$. This implies that G is regular. \square

For positive integer $r \neq s$, a graph G is said to be (r, s) -semiregular if its vertex degrees assume only the value r and s , and if there is atleast one vertex of degree r and atleast one of degree s

Theorem 3.3. *Let G be a graph with m edges and p pendent vertices. If δ_1 is the minimal nonpendent vertex of G , then $4\delta_1^2(m - p) + (1 + \delta_1)^2p + 4m - 4M_2(G) \leq EM_1(G) \leq 4\Delta^2(m - p) + (1 + \Delta)^2p + 4m - 4M_2(G)$ with equality if and only if G is regular (or) $(1, \Delta)$ -semiregular.*

Proof. From the definition of EM_1 ,

$$\begin{aligned} EM_1(G) &= \sum_{uv \in E(G), d(u), d(v) \neq 1} (d(u) + d(v))^2 + \sum_{uv \in E(G), d(u)=1} (1 + d(v))^2 + 4m - 4M_2(G) \\ &\leq \sum_{uv \in E(G), d(u), d(v) \neq 1} (2\Delta)^2 + \sum_{uv \in E(G), d(u)=1} (1 + \Delta)^2 + 4m - 4M_2(G) \\ &= 4\Delta^2(m - p) + (1 + \Delta)^2p + 4m - 4M_2(G). \end{aligned}$$

Similarly, We can prove $EM_1(G) \geq 4\delta_1^2(m - p) + (1 + \delta_1)^2p + 4m - 4M_2(G)$. The equalities hold if and only if $d(u) = d(v) = \delta_1 = \Delta$, for each $uv \in E(G)$, with $d(u), d(v) \neq 1$ and $d(u) = \delta_1 = \Delta$, for each $uv \in E(G)$ with $d(u) = 1$. Thus G is regular if $p = 0$ and G is $(1, \Delta)$ -semiregular if $p > 0$. \square

Theorem 3.4. *Let G be a tree on n vertices. Then $EM_1(G) \leq (n - 1)(n - 2)^2$ with equality if and only if G is a star.*

Proof. Since G is a tree, $d(u) + d(v) - 2 \leq n - 2$ for all $uv \in E(G)$. Thus

$$EM_1(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 \leq m(n - 2)^2 = (n - 1)(n - 2)^2.$$

Equality holds for $d(u) + d(v) - 2 = n - 2$ for all $uv \in E(G)$. Thus G is a star. \square

Lemma 3.5. *(Cauchy-Schwarz inequality) Let $X = (x_1, x_2, \dots, x_n)$ and $Y = (y_1, y_2, \dots, y_n)$ 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 $x_i = cy_i$, for each $1 \leq i \leq n$.*

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

Corollary 3.6. Let x_1, x_2, \dots, 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 $x_1 = x_2 = \dots = x_n$.

Theorem 3.7. Let G be a graph on m edges. Then $EM_1(G) \geq \frac{(M_1(G)-2m)^2}{m}$ with equality if and only if G is regular.

Proof. From the definition of EM_1 , $EM_1(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2$.

By Corollary 3.6, we have

$$EM_1(G) \geq \frac{\left(\sum_{uv \in E(G)} (d(u) + d(v) - 2)\right)^2}{m} = \frac{(M_1(G) - 2m)^2}{m}.$$

The equality is hold if and only if G is regular. □

Lemma 3.8. (Polya-Szego 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 $\sum_{i=1}^n x_i^2 \sum_{i=1}^n y_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}} \right)^2 \left(\sum_{i=1}^n x_i y_i \right)^2$.

Theorem 3.9. Let G be a graph on m edges. Then $EM_1(G) \leq \frac{1}{4m} \frac{(\Delta + \delta - 2)^2}{(\delta - 1)(\Delta - 1)} (M_1(G) - 2m)^2$.

Proof. One can see that $2\delta - 2 \leq d(u) + d(v) - 2 \leq 2\Delta - 2$ for all $uv \in E(G)$. Setting $m_1 = 2\delta - 2$, $x_i = d(u) + d(v) - 2$, $1 \leq i \leq m$, $M_1 = 2\Delta - 2$, $m_2 = y_i = M_2 = 1$, $1 \leq i \leq m$, in Polya-Szego inequality, we have

$$\begin{aligned} \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 \sum_{uv \in E(G)} (1)^2 &\leq \frac{1}{4} \left(\sqrt{\frac{2\Delta - 2}{2\delta - 2}} + \sqrt{\frac{2\delta - 2}{2\Delta - 2}} \right)^2 \left(\sum_{uv \in E(G)} (d(u) + d(v) - 2) \right)^2 \\ &= \frac{1}{4} \left(\sqrt{\frac{\Delta - 1}{\delta - 1}} + \sqrt{\frac{\delta - 1}{\Delta - 1}} \right)^2 (M_1(G) - 2m)^2. \end{aligned}$$

Hence $EM_1(G) \leq \frac{1}{4m} \frac{(\Delta + \delta - 2)^2}{(\delta - 1)(\Delta - 1)} (M_1(G) - 2m)^2$.

Lemma 3.10. (Diaz-Metcalf inequality [4]) Let $x_1, x_2, \dots, x_n, y_1, y_2, \dots, y_n$ be real numbers such that $px_i \leq y_i \leq Px_i$, 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 $y_i = Px_i$ or $y_i = px_i$, for $1 \leq i \leq n$.

Theorem 3.11. Let G be a graph on m edges. Then $EM_1(G) \leq 2(\delta + \Delta - 2)(M_1(G) - 2m) - 4(\delta - 1)(\Delta - 1)m$ with equality if and only if G is regular.

Proof. Setting $p = 2\delta - 2$, $P = 2\Delta - 2$, $x_i = 1$ and $y_i = d(u) + d(v) - 2$, $1 \leq i \leq m$, in Diaz-Metcalf inequality, we have

$$\begin{aligned} \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 + (2\delta - 2)(2\Delta - 2) \sum_{uv \in E(G)} (1)^2 &\leq (2\delta - 2 + 2\Delta - 2) \sum_{uv \in E(G)} (d(u) + d(v) - 2) \\ &= (2\delta + 2\Delta - 4)(M_1(G) - 2m). \end{aligned}$$

This implies that $EM_1(G) \leq 2(\delta + \Delta - 2)(M_1(G) - 2m) - 4(\delta - 1)(\Delta - 1)m$.

Equality holds if and only if $d(u) + d(v) - 2 = 2\delta - 2$ or $d(u) + d(v) - 2 = 2\Delta - 2$ for all $uv \in E(G)$.

$\Rightarrow G$ is regular. \square

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

The *geometric mean* of x_1, x_2, \dots, x_n is equal to $GM(x_1, x_2, \dots, x_n) = \sqrt[n]{x_1 x_2 \dots x_n}$.

The *harmonic mean* of x_1, x_2, \dots, x_n is equal to $HM(x_1, x_2, \dots, x_n) = \frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + \dots + \frac{1}{x_n}}$.

Lemma 3.12. (*AM-GM-HM inequality*). *Let x_1, x_2, \dots, x_n be positive real numbers. Then $AM(x_1, x_2, \dots, x_n) \geq GM(x_1, x_2, \dots, x_n) \geq HM(x_1, x_2, \dots, x_n)$, with equality if and only if $x_1 = x_2 = \dots = x_n$.*

Theorem 3.13. *Let G be a graph on m edges. Then $EM_1(G) \geq 4M_2(G) - 4M_1(G) + 4m$ with equality if and only if G is regular.*

Proof. By using AM-GM inequality, we have

$$\begin{aligned} EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 \\ &= \sum_{uv \in E(G)} [(d(u) + d(v))^2 + 4 - 4(d(u) + d(v))] \\ &\geq \sum_{uv \in E(G)} (2\sqrt{d(u)d(v)})^2 + 4m - 4M_1(G) \\ &= 4M_2(G) - 4M_1(G) + 4m \end{aligned}$$

with equality if and only if $d(u) = d(v)$ for each $uv \in E(G)$. Thus G is regular. \square

Theorem 3.14. *Let G be a graph on m edges. Then $(\delta - 4)M_1(G) + 2M_2(G) + 4m \leq EM_1(G)(\Delta - 4)M_1(G) + 2M_2(G) + 4m$ with equality if and only if G is regular.*

Proof. Since $\delta \leq d(u) \leq \Delta$, for each $u \in V(G)$. Thus

$$\begin{aligned}
 EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 \\
 &= \sum_{uv \in E(G)} [d^2(u) + d^2(v) + 4 + 2d(u)d(v) - 4d(u) - 4d(v)] \\
 &= \sum_{u \in V(G)} d(u)d^2(u) + 4m + 2M_2(G) - 4M_1(G) \\
 &\leq \Delta M_1(G) + 4m + 2M_2(G) - 4M_1(G) \\
 &= (\Delta - 4)M_1(G) + 2M_2(G) + 4m.
 \end{aligned}$$

Similarly we obtain $EM_1(G) \geq (\delta - 4)M_1(G) + 2M_2(G) + 4m$.

Equality hold if and only if $\delta = d(u) = \Delta$, for each $u \in V(G)$. Thus G is regular. \square

Theorem 3.15. *Let G be a graph on m edges. Then $EM_1 \geq m(\sqrt{\pi_1^*(G)^2}) + 4m - 4M_1(G)$ with equality if and only if G is regular.*

Proof. Using AM-GM inequality, we have

$$\begin{aligned}
 EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v))^2 + 4m - 4M_1(G) \\
 &\geq m \left(\sqrt{\prod_{uv \in E(G)} (d(u) + d(v))^2} \right) + 4m - 4M_1(G) \\
 &= m \left(\sqrt{\pi_1^*(G)^2} \right) + 4m - 4M_1(G).
 \end{aligned}$$

Proof.

Theorem 3.16. *For any graph G , $4(\delta - 1)^2 \delta R(G) \leq EM_1(G) \leq 4(\Delta - 1)^2 \delta R(G)$ with equality if and only if G is regular.*

Proof. Clearly $d(u) + d(v) \leq 2\Delta$ for each edge $uv \in E(G)$.

$$4(\delta - 1)^2 \delta = (2\delta - 2)^2 \sqrt{\delta^2} \leq (d(u) + d(v) - 2)^2 \sqrt{d(u)d(v)} \leq (2\Delta - 2)^2 \sqrt{\Delta^2} = 4(\Delta - 1)^2 \delta.$$

By the definition of Randić index, we have

$$4(\delta - 1)^2 \delta R(G) \leq EM_1(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2 \frac{\sqrt{d(u)d(v)}}{\sqrt{d(u)d(v)}} = 4(\Delta - 1)^2 \Delta R(G).$$

Equality hold if and only if $d(u) = d(v) = \Delta = \delta$. This implies G is regular. \square

Theorem 3.17. *Let G be a graph on m edges. Then G , $EM_1(G) \geq \frac{4m^3}{R(G)} - 4M_1(G) + 4m$.*

Proof.

$$\begin{aligned}
\frac{EM_1(G)}{4m} &= \frac{1}{4m} \left[\sum_{uv \in E(G)} (d(u) + d(v))^2 + 4m - 4M_1(G) \right] \\
&= \frac{m}{m^2} \sum_{uv \in E(G)} \left(\frac{(d(u) + d(v))^2}{2} \right) - \frac{M_1(G)}{m} + 1 \\
&\geq \frac{1}{m^2} \left(\sum_{uv \in E(G)} \frac{d(u) + d(v)}{2} \right)^2 - \frac{M_1(G)}{m} + 1 \\
&\geq \left(\frac{\sum_{uv \in E(G)} \sqrt{d(u)d(v)}}{m} \right)^2 - \frac{M_1(G)}{m} + 1 \\
&\geq \left(\frac{m}{\sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}} \right)^2 - \frac{M_1(G)}{m} + 1 \\
&= \left(\frac{m}{R(G)} \right)^2 - \frac{M_1(G)}{m} + 1 \\
EM_1(G) &\geq \frac{4m^3}{R(G)} - 4M_1(G) + 4m,
\end{aligned}$$

where $R(G)$ is the Randic index of G .

Theorem 3.18. *Let G be a graph with m edges. Then*
 $4\delta^3 H(G) + 4m - 4M_1(G) \leq EM_1(G) \leq 4\Delta^3 H(G) + 4m - 4M_1(G)$.

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

$$4\delta^3 = \frac{(2\delta)^3}{2} \leq \frac{(d(u) + d(v))^3}{2} \leq \frac{(2\Delta)^3}{2} = 4\Delta^3.$$

By the definition of first reformulated Zagreb index,

$$\begin{aligned}
EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v))^2 + 4m - 4M_1(G) \\
&= \sum_{uv \in E(G)} \left(\frac{2}{d(u) + d(v)} \right) \left(\frac{(d(u) + d(v))^3}{2} \right) + 4m - 4M_1(G).
\end{aligned}$$

$$EM_1(G) \leq 4\Delta^3 H(G) + 4m - 4M_1(G),$$

where $H(G)$ is the harmonic index of G . □

Similarly, we obtain $4\delta^3 H(G) + 4m - 4M_1(G) \leq EM_1(G)$.

Theorem 3.19. *For any graph G , $EM_1(G) \geq \frac{4\delta^2}{m} (GA(G))^2 + 4m - 4M_1(G)$.*

Proof.

$$\begin{aligned}
 EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v))^2 + 4m - 4M_1(G) \\
 &= 4 \sum_{uv \in E(G)} \left(\frac{d(u) + d(v)}{2} \right)^2 + 4m - 4M_1(G) \\
 &\geq 4 \sum_{uv \in E(G)} \left(\frac{2}{\frac{1}{d(u)} + \frac{1}{d(v)}} \right)^2 + 4m - 4M_1(G) \\
 &= 4 \sum_{uv \in E(G)} \left(\frac{2d(u)d(v)}{d(u) + d(v)} \right)^2 + 4m - 4M_1(G) \\
 &\geq \frac{4}{m} \left(\sum_{uv \in E(G)} \frac{2d(u)d(v)}{d(u) + d(v)} \right)^2 + 4m - 4M_1(G) \\
 &= \frac{4}{m} \left(\sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}\sqrt{d(u)d(v)}}{d(u) + d(v)} \right)^2 + 4m - 4M_1(G) \\
 &\geq \frac{4\delta^2}{m} \left(\sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)} \right)^2 + 4m - 4M_1(G) \\
 &= \frac{4\delta^2}{m} (GA(G))^2 + 4m - 4M_1(G),
 \end{aligned}$$

where $GA(G)$ is the geometric arithmetic index of G . \square

Lemma 3.20. *Let G be a nontrivial connected graph of order n . For each $u \in V(G)$, $\xi_u \leq n - d(u)$, with equality if and only if $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$, where $K_n - iK_2$ denotes the graph obtained from the complete graph K_n by removing i independent edges.*

Theorem 3.21. *For any graph G , $EM_1(G) \leq 4n^2m + \xi_3(G) + 2\xi_2(G) - 4n\xi^c(G) + 4m - 4M_1(G)$, where $\xi_3(G) = \sum_{u \in V(G)} (\xi_u^2 + \xi_v^2)$ and the equality holds if and only if $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$.*

Proof. By the definition of EM_1

$$\begin{aligned}
 EM_1(G) &= \sum_{uv \in E(G)} (d(u) + d(v))^2 + 4m - 4M_1(G) \\
 &\leq \sum_{uv \in E(G)} (n - \xi_u + n - \xi_v)^2 + 4m - 4M_1(G) \\
 &= \sum_{uv \in E(G)} [4n^2 + (\xi_u^2 + \xi_v^2) + 2\xi_u\xi_v - 4n(\xi_u + \xi_v)] + 4m - 4M_1(G), \text{ by Lemma 3.20} \\
 &= 4n^2m + \xi_3(G) + 2\xi_2(G) - 4n\xi^c(G) + 4m - 4M_1(G),
 \end{aligned}$$

where $\xi_3(G) = \sum_{u \in V(G)} (\xi_u^2 + \xi_v^2)$. By Lemma 3.20, the equality holds if and only if $d(u) = n - \xi_u$ for each $u \in V(G)$, which by Lemma 3.20 implies that $G \cong P_4$ or $G \cong K_n - iK_2, 0 \leq i \leq \lfloor \frac{n}{2} \rfloor$. \square

Lemma 3.22. (Zhou and Wu 2005) *Let G be a graph of order $n \geq 4$ such that both G and \bar{G} are connected. Then $\frac{n(n-1)^2}{2} \leq M_1(G) + M_1(\bar{G}) \leq n(n-1)^2$, the right equality holds if and only if G or \bar{G} is the complete graph K_n , the left equality holds if and only if G or \bar{G} is $2k$ -regular graph on $n = 4k + 1$ vertices.*

Theorem 3.23. *Let G be a simple graph with $n \geq 4$ vertices and \bar{G} its complement. If both G and \bar{G} are connected, then $EM_1(G) + EM_1(\bar{G}) \leq HM(G) + HM(\bar{G}) - 2n(n-1)(2n-3)$ and $EM_1(G) + EM_1(\bar{G}) \geq HM(G) + HM(\bar{G}) - 2n(n-1)(n-2)$.*

Proof.

$$\begin{aligned} EM_1(G) + EM_1(\bar{G}) &= \sum_{uv \in E(G)} (d_G(u) + d_G(v) - 2)^2 + \sum_{uv \in E(\bar{G})} (d_{\bar{G}}(u) + d_{\bar{G}}(v) - 2)^2 \\ &= HM(G) - 4M_1(G) + 4m + HM(\bar{G}) - 4M_1(\bar{G}) + 4|E(\bar{G})| \\ &= HM(G) + HM(\bar{G}) - 4(M_1(G) + M_1(\bar{G})) + 2n(2n-1). \end{aligned}$$

By Lemma 3.22, we get the desired result. \square

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