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INEQUALITIES AMONG TOPOLOGICAL DESCRIPTORS

ZEHUI SHAO[1], HUIQIN JIANG[2], AND ZAHID RAZA[3]

Abstract. A topological index is a type of molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are used for example in the development of QSAR QSPR in which the biological activity or other properties of molecules are correlated with their chemical structure. In this paper, we establish several inequalities among the molecular descriptors such as the generalized version of the first Zagreb index, the Randić index, the ABC index, AZI index, and the redefined first, second and third Zagreb indices.

1. Introduction

Graph theory is an important tool to study properties of chemical molecules. In chemical graph theory, the vertices of the graph correspond to the atoms of molecules and the edges correspond to chemical bonds, and such a molecular graph is established to define topological indices which are used to study, or predict its structural features [13]. These topological indices are very important in the the quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies [10]. They can reflect many phisico-chemical properties such as the stability of linear and branched alkanes, strain energy of cycloalkanes [4], heat of formation for heptanes and octanes [7], and the bioactivity of chemical compounds [11].

In this paper, we only consider undirected simple graphs. Let G be a graph, we denote $V(G)$ and $E(G)$ the vertex set and edge set of G, respectively. The complete graph, path, cycle and star on n vertices are denoted by K_n, P_n, C_n and S_n (or $S_{1,n-1}$), respectively. A graph is an (n,m)-graph if it has order n and size m. We denote

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TABLE 1. The most common molecular descriptors defined in last two decays

Atomic Bond Connectivity Index	$ABC(G)$	$\sum_{uv\in E(G)}\left(\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}\right)$
Augmented Zagreb Index	$AZI(G)$	$\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$
Randic Connectivity Index	$R(G)$	$\sum_{uv\in E(G)}\left(\frac{1}{\sqrt{d(u)d(v)}}\right)$
Sum-Connectivity Index	$X(G)$	$\sum_{uv\in E(G)}\left(\frac{1}{\sqrt{d(u)+d(v)}}\right)$
First Zagreb Index	$Zg_1(G)$	$\sum_{uv\in E(G)}(d(u)+d(v))$
Second Zagreb Index	$Zg_2(G)$	$\sum_{uv\in E(G)}(d(u)d(v))$
Generalized Zagreb Index	$M_\alpha(G)$	$\sum_{uv\in E(G)}(d(u)^{\alpha-1}+d(v)^{\alpha-1})$
Modified Zagreb Index	$M_2^*(G)$	$\sum_{uv\in E(G)}\left(\frac{1}{d(u)d(v)}\right)$
Redefined First Zagreb Index	$ReZg_1(G)$	$\sum_{uv\in E(G)}\left(\frac{d(u)+d(v)}{d(u)d(v)}\right)$
Redefined Second Zagreb Index	$ReZg_2(G)$	$\sum_{uv\in E(G)}\left(\frac{d(u)d(v)}{d(u)+d(v)}\right)$
Redefined Third Zagreb Index	$ReZg_3(G)$	$\sum_{uv\in E(G)}(d(u)+d(v))\,d(u)d(v)$
Forgotten Index	$F(G)$	$\sum_{v\in V(G)}(d(v))^3$
Harmonic Index	$H(G)$	$\sum_{v\in V(G)}\left(\frac{2}{d(u)+d(v)}\right)$
Geometric-Arithmetic Index	$GA(G)$	$\sum_{uv\in E(G)}\left(\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}\right)$

by $d(v)$ the degree of a vertex v of a graph G. We denote by $\Delta(G)$ and $\delta(G)$ (or simply Δ and δ) the maximum and minimum degree of G, respectively. A graph is *regular* if $\Delta=\delta$. A bipartite graph is *biregular* if each vertex in the same part has the same degree, e.g., $K_{2,3}$ is a biregular graph. For positive integers s,t, we denote by $E_{s,t}$ the set of edges with two end vertices with degree s and t, respectively. That is $E_{s,t}=\{uv : d(u)=s, d(v)=t\}$. The most common molecular descriptors defined in last two decays are defined in Table 1.

When a new topological index is proposed in chemical graph theory, one of the important problems is to find lower and upper bounds for this index on a class of graphs such as trees or general graphs or graph operations [3,6]. Motivated with the importance of bounds and inequalities, this paper continue to study the inequalities among topological indices.

2. Related Work on Inequalities Among Topological Indices

In recent years, there has been an increasing amount of literature on inequality of topological indices [1, 19–22]. Various relations of different topological indices have been extensively researched, and we summarize main known results as follows.

Theorem 2.1. *Let G be a connected graph having $n \geq 3$ vertices. Then*

$$\left(\frac{1536}{343}\right) X(G) \leq AZI(G) \leq \left(\frac{\sqrt{(n-1)^{13}}}{\sqrt{32}(n-2)^3}\right) X(G),$$

with left equality if and only if $G \cong S_{1,8}$ and right equality if and only if $G \cong K_n$.

Theorem 2.2 ([1])**.** *Let G be a connected graph having $n \geq 3$ vertices. Then*

$$\begin{aligned}
\left(\frac{343\sqrt{7}}{216}\right) R(G) \leq & AZI(G) \leq \left(\frac{\sqrt{(n-1)^7}}{8(n-2)^3}\right) R(G),\\
\left(\frac{375}{64}\right) H(G) \leq & AZI(G) \leq \left(\frac{\sqrt{(n-1)^7}}{8(n-2)^3}\right) H(G),\\
\left(\frac{n-1}{n-2}\right)^{\frac{7}{2}} ABC(G) \leq & AZI(G) \leq \left(\frac{(n-1)^2}{2(n-2)}\right)^{\frac{7}{2}} ABC(G),\\
8GA(G) \leq & AZI(G) \leq \left(\frac{\sqrt{(n-1)^6}}{8(n-2)^3}\right) GA(G), \quad \delta \geq 2,\\
4M_2^*(G) \leq & AZI(G) \leq \left(\frac{\sqrt{(n-1)^4}}{2(n-2)}\right) M_2^*(G).
\end{aligned}$$

The left equality in the above inequalities holds if and only if $G \cong S_{1,7}$, $G \cong S_{1,5}$, $G \cong S_{1,n-1}$, $G \cong C_n$, $G \cong P_3$, respectively and right equality in all the aforementioned inequalities holds if and only if $G \cong K_n$.

Theorem 2.3 ([20])**.** *Let G be a simple connected graph on $n \geq 3$ vertices with minimum degree $\delta \geq s$ and maximum degree $\Delta \leq t$, where $1 \leq s \leq t \leq n-1$ and $t \geq 2$. Then*

(i) $\left(\frac{\sqrt{2t-2}}{t}\right) GA(G) \leq ABC(G)$, *with equality if and only if G is a t-regular graph;*

(ii) $ABC(G) \leq \left(\frac{\sqrt{2s-2}}{s}\right) GA(G)$, *with equality if and only if G is a s-regular graph and $ABC(G) \leq \left(\frac{(s+t)\sqrt{s+t-2}}{st}\right) GA(G)$ if $t \geq 2s-3+\sqrt{5s^2-14s+9}$, with equality if and only if one vertex has degree s and the other vertex has degree t for every edge of G.*

Theorem 2.4 ([1]). *Let G be a connected graph having $n \geq 2$ vertices. Then*
$$\begin{aligned} M_2^*(G) \leq & R(G) \leq (n-1)M_2^*(G), \\ \frac{M_2^*(G)}{\sqrt{2}} \leq & X(G) \leq \left(\frac{(n-1)^{\frac{3}{2}}}{\sqrt{2}}\right) M_2^*(G), \\ M_2^*(G) \leq & H(G) \leq (n-1)M_2^*(G), \\ M_2^*(G) \leq & GA(G) \leq (n-1)^2 M_2^*(G), \\ \sqrt{2}M_2^*(G) \leq & ABC(G) \leq (n-1)\sqrt{2(n-2)}M_2^*(G). \end{aligned}$$
The left equality in the first four inequalities and in the fifth inequality is attained if and only if $G \cong P_2$ and $G \cong P_3$, respectively. The right equality in all inequalities is attained if and only if $G \cong K_n$.

Theorem 2.5 ([19]). *Let G be a connected graph having $n \geq 3$ vertices. Then*
(i) $\left(\sqrt{\frac{3}{2}}\right) X(G) \leq ABC(G)$, *with equality if and only if $G \cong P_3$;*
(ii) $ABC(G) \leq \sqrt{2}X(G)$, *if $n = 3$, the equality holds if and only if $G \cong K_3$, $ABC(G) \leq \left(\sqrt{\frac{8}{3}}\right) X(G)$, if $n = 4$, the equality holds if and only if $G \cong K_4$ or $G \cong S_4$, $ABC(G) \leq \left(\sqrt{\frac{n(n-2)}{n-1}}\right) X(G)$, if $n \geq 5$, the equality holds if and only if $G \cong S_n$.*

Theorem 2.6 ([19]). *Let G be a connected graph having $n \geq 3$ vertices. Then*
(i) $\left(\frac{3\sqrt{2}}{4}\right) H(G) \leq ABC(G)$, *with equality if and only if $G \cong P_3$;*
(ii) $ABC(G) \leq \sqrt{2n-4}H(G)$, *if $3 \leq n \leq 6$, with equality if and only if $G \cong K_n$, $ABC(G) \leq \left(\frac{n}{2}\sqrt{\frac{n-2}{n-1}}\right) H(G)$, if $n \geq 7$, with equality if and only if $G \cong S_n$.*

2.1. Other inequalities and some inequality chains.

Proposition 2.1 ([22]). *Let G be a graph. Then $X(G) \geq \left(\frac{1}{\sqrt{2}}\right) R(G)$ with equality if and only if all non-isolated vertices have degree one. Moreover, if G has no components on two vertices, then $X(G) \geq \left(\sqrt{\frac{2}{3}}\right) R(G)$ with equality if and only if all non-trivial components of G are paths on three vertices, and if no pendant vertices, then $X(G) \geq R(G)$ with equality if and only if all non-isolated vertices have degree two.*

Proposition 2.2 ([22]). *Let G be a graph with m edges. Then $X(G) \leq \sqrt{\frac{mR(G)}{2}}$ with equality if and only if G is regular.*

Theorem 2.7 ([19]). *Let G be a graph with n vertices. Then $\left(\frac{2\sqrt{n-1}}{n}\right) R(G) \leq H(G) \leq R(G)$. The lower bound is attained if and only if $G \cong S_n$, and the upper bound is attained if and only if all connected components of G are regular.*

Theorem 2.8 ([20]). *Let G be a connected graph with $\delta \geq 2$. Then*
$$H(G) \leq R(G) \leq X(G) < ABC(G),$$
where the first inequality holds as equality if and only if G is a regular graph, and the second inequality holds as equality if and only if G is a cycle.

3. Results and Discussion

For a graph G, we say G has Property A if for each edge uv we have $d(u)+d(v)=k$ for some k, and G has Property B if for each edge uv we have $d(u)d(v)=k$ for some k, and G has Property C if for each edge uv we have $\frac{d(u)d(v)}{d(u)+d(v)}=k$ for some k.

Definition 3.1. We define the four classes of graphs as follows.

- Let $\mathcal{G}_1$ be the set of graphs without isolated vertices with property A.
- Let $\mathcal{G}_2$ be the set of graphs without isolated vertices with property B.
- Let $\mathcal{G}_3$ be the set of graphs without isolated vertices with properties A and B.
- Let $\mathcal{G}_4$ be the set of graphs without isolated vertices with property C.

Lemma 3.1. *If G is a graph without isolated vertices we have $d(u_1)d(v_1)=d(u_2)d(v_2)$ and $d(u_1)+d(v_1)=d(u_2)+d(v_2)$ for any pair of edges u_1v_1 and u_2v_2, then G has properties A and B. Equivalently, G is either regular or a biregular.*

Proof. Since $d(u_1)d(v_1)=d(u_2)d(v_2)$ and $d(u_1)+d(v_1)=d(u_2)+d(v_2)$ for any pair of edges u_1v_1 and u_2v_2, we have $d(u)d(v)=k_1$ and $d(u)+d(v)=k_2$ for some k_1 and k_2. Then we have $uv\in E_{s,t}$ where s and t are the roots of the equation $x^2-k_1x+k_2=0$. If $s=t$, then we have G is regular. If $s\neq t$, then the degree of each neighbor of each vertex with degree s is t and thus G is biregular. □

The following lemma is the well known power mean inequality [2].

Lemma 3.2. *Let $x_1,x_2,\ldots,x_n>0$ and $p>q>0$. Then*

$$\sqrt[p]{\frac{x_1^p+x_2^p+\cdots+x_n^p}{n}}\geq\sqrt[q]{\frac{x_1^q+x_2^q+\cdots+x_n^q}{n}},$$

with equality if and only if $x_i=x_j$ for each $i\neq j$.

The Cauchy-Schwarz inequality is arguably one of the most widely used inequalities in mathematics (see [18]).

Lemma 3.3. *Let $(a_1,a_2,\ldots,a_n)$ and $(b_1,b_2,\ldots,b_n)$ be two real sequences. Then $\left(\sum\limits_{i=1}^{n}a_i^2\right)\left(\sum\limits_{i=1}^{n}b_i^2\right)\geq\left(\sum\limits_{i=1}^{n}a_ib_i\right)^2$, with equality if and only if there exists a constant c such that $a_i=cb_i$ for all $i=1,2,\ldots,n$.*

The following is the well known Jensen's inequality (see [14]).

Lemma 3.4. *Let $(x_1,x_2,\ldots,x_n)$ be a real sequence and $f(x)$ be a continuous real function.*

i) *If $f''(x)>0$, then*

$$\frac{\sum\limits_{i=1}^{n}f(x_i)}{n}\geq f\left(\frac{\sum\limits_{i=1}^{n}x_i}{n}\right),$$

with equality if and only if $x_i=x_j$ for each $i\neq j$.

ii) *If $f''(x) < 0$, then*

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

with equality if and only if $x_i = x_j$ for each $i \neq j$.

By Lemma 3.2, the following result is immediate.

Theorem 3.1. *Let G be an (n,m)-graph without isolated vertices, $k = k_1 + k_2$ with $k_1 > 0$ and $k_2 > 0$. Then*

$$\frac{M_k(G)}{n} \geq \left(\frac{M_{k_1}(G)}{n}\right)\left(\frac{M_{k_2}(G)}{n}\right).$$

Proof. Let $x_i = d(v_i)$ for $i = 1, 2, \ldots, n$. Since G has no isolated vertex, so, we have $x_i \geq 1$. Note that $k > k_1$, by Lemma 3.2, we have

$$\left(\frac{x_1^k + x_2^k + \cdots + x_n^k}{n}\right)^{\frac{1}{k}} \geq \left(\frac{x_1^{k_1} + x_2^{k_1} + \cdots + x_n^{k_1}}{n}\right)^{\frac{1}{k_1}}.$$

That is

$$\left(\frac{x_1^k + x_2^k + \cdots + x_n^k}{n}\right)^{\frac{k_1}{k}} \geq \frac{x_1^{k_1} + x_2^{k_1} + \cdots + x_n^{k_1}}{n}. \tag{3.1}$$

Similarly, we have

$$\left(\frac{x_1^k + x_2^k + \cdots + x_n^k}{n}\right)^{\frac{k_2}{k}} \geq \frac{x_1^{k_2} + x_2^{k_2} + \cdots + x_n^{k_2}}{n}. \tag{3.2}$$

By (3.1) $\times$ (3.2), we get

$$\frac{x_1^k + x_2^k + \cdots + x_n^k}{n} \geq \left(\frac{x_1^{k_1} + x_2^{k_1} + \cdots + x_n^{k_1}}{n}\right)\left(\frac{x_1^{k_2} + x_2^{k_2} + \cdots + x_n^{k_2}}{n}\right).$$

That is

$$\frac{M_k(G)}{n} \geq \left(\frac{M_{k_1}(G)}{n}\right)\left(\frac{M_{k_2}(G)}{n}\right).$$ □

Corollary 3.1. *Let G be an (n,m)-graph without isolated vertices and $k \geq 2$. Then*

$$M_k(G) \geq n\left(\frac{M_{k-1}(G)}{n}\right)^{\frac{k}{k-1}}.$$

Proof. By Theorem 3.1 with $k_1 = 1$ and $k_2 = k - 1$, the result holds. □

Remark 3.1. By Corollary 3.1, we have $F(G) \geq n\left(\frac{M_1(G)}{n}\right)^{\frac{3}{2}} \geq \frac{8m^3}{n^2}$.

Theorem 3.2 ([12]). *Suppose a_i and b_i, $1 \leq i \leq n$, are positive real numbers. Then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A-a)(B-b),$$

where a, b, A and B are real constants, that for each i, $1 \leq i \leq n$, $a \leq a_i \leq A$, $b \leq b_i \leq B$. Further, $\alpha(n) = n\lceil \frac{n}{2} \rceil (1 - \frac{1}{n}\lceil \frac{n}{2} \rceil)$.

By Theorem 3.2, we have the following.

Theorem 3.3. *Let G be an (n,m)-graph without isolated vertices, $k = k_1 + k_2$ with $k_1 > 0$ and $k_2 > 0$. Then*

$$M_k(G) \leq \left(\frac{M_{k_1}(G) M_{k_2}(G) + \alpha(n)(\Delta^{k_1} - \delta^{k_1})(\Delta^{k_2} - \delta^{k_2})}{n} \right).$$

Proof. Let $a_i = d(v_i)^{k_1}$, $b_i = d(v_i)^{k_2}$, $A = \Delta^{k_1}$, $B = \Delta^{k_2}$, $a = \delta^{k_1}$ and $b = \delta^{k_2}$, then by Theorem 3.2, we have

$$nM_k(G) - M_{k_1}(G) M_{k_2}(G) \leq \alpha(n)(\Delta^{k_1} - \delta^{k_1})(\Delta^{k_2} - \delta^{k_2}). \tag{3.3}$$

So, we have

$$M_k(G) \leq \left(\frac{M_{k_1}(G) M_{k_2}(G) + \alpha(n)(\Delta^{k_1} - \delta^{k_1})(\Delta^{k_2} - \delta^{k_2})}{n} \right). \qquad \square$$

Theorem 3.4. *Let G be an (n,m)-graph without isolated vertices. Then $R(G)^2 Zg_2(G) \geq m^3$, with equality if and only if $G \in \mathcal{G}_2$.*

Proof. Let $f(x) = \frac{1}{\sqrt{x}}$, then we have $f''(x) = \frac{3}{4x^{\frac{5}{2}}} > 0$ if $x > 0$. By Lemma 3.4, we have

$$\frac{\sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}}{m} \geq \frac{1}{\sqrt{\frac{\sum\limits_{uv \in E(G)} d(u)d(v)}{m}}}.$$

That is

$$\frac{R(G)}{m} \geq \frac{1}{\sqrt{\frac{Zg_2(G)}{m}}}.$$

Consequently, we have $R(G)^2 Zg_2(G) \geq m^3$. The equality holds if and only if

$$\frac{1}{\sqrt{d(u_1)d(v_1)}} = \frac{1}{\sqrt{d(u_2)d(v_2)}},$$

for any two distinct edges $u_1v_1, u_2v_2 \in E(G)$. Since

$$\frac{1}{\sqrt{d(u_1)d(v_1)}} = \frac{1}{\sqrt{d(u_2)d(v_2)}} \Leftrightarrow d(u_1)d(v_1) = d(u_2)d(v_2),$$

we have the equality holds if and only if $G \in \mathcal{G}_2$. $\square$

Theorem 3.5. *Let G be an (n,m)-graph without isolated vertices. Then $X(G)^2 Zg_1(G) \geq m^3$ with equality if and only if $G \in \mathcal{G}_1$.*

Proof. Let $f(x) = \frac{1}{\sqrt{x}}$. Then $f''(x) = \frac{3}{4x^{\frac{5}{2}}} > 0$ for $x > 0$. By Lemma 3.4, we have

$$\frac{\sum\limits_{uv\in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}}{m} \geq \frac{1}{\sqrt{\frac{\sum\limits_{uv\in E(G)} (d(u)+d(v))}{m}}}.$$

That is

$$\frac{X(G)}{m} \geq \frac{1}{\sqrt{\frac{Zg_1(G)}{m}}}.$$

Consequently, we have $X(G)^2 Zg_1(G) \geq m^3$. The equality holds if and only if

$$\frac{1}{\sqrt{d(u_1)+d(v_1)}} = \frac{1}{\sqrt{d(u_2)+d(v_2)}},$$

for any two distinct edges $u_1v_1, u_2v_2 \in E(G)$. Since

$$\frac{1}{\sqrt{d(u_1)+d(v_1)}} = \frac{1}{\sqrt{d(u_2)+d(v_2)}} \Leftrightarrow d(u_1)+d(v_1) = d(u_2)+d(v_2),$$

we have the equality holds if and only if $G \in \mathcal{G}_1$. $\square$

Theorem 3.6. *Let G be an (n,m)-graph without isolated vertices. Then $ABC(G)^2 + 2R(G)^2 \leq mn$ with equality holds if and only if G is regular or biregular.*

Proof. Let $f(x) = \sqrt{x}$, we have $f''(x) < 0$ if $x > 0$. By Lemma 3.4,

$$\begin{aligned}
\frac{ABC(G)}{m} &= \frac{\sum\limits_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}}{m} \\
&\leq \sqrt{\frac{\sum\limits_{uv\in E(G)} \frac{d(u)+d(v)-2}{d(u)d(v)}}{m}} \\
&= \sqrt{\frac{\sum\limits_{uv\in E(G)} (\frac{1}{d(u)} + \frac{1}{d(u)}) - 2\sum\limits_{uv\in E(G)} \frac{1}{d(u)d(v)}}{m}} \\
&= \sqrt{\frac{n - 2\sum\limits_{uv\in E(G)} \frac{1}{d(u)d(v)}}{m}}. \qquad (3.4)
\end{aligned}$$

The equality holds if and only if

$$\frac{d(u_1)+d(v_1)-2}{d(u_1)d(v_1)} = \frac{d(u_2)+d(v_2)-2}{d(u_2)d(v_2)},$$

for any two distinct edges $u_1v_1, u_2v_2 \in E(G)$.

On the other hand, by Lemma 3.3 we have

$$R(G)^2 = \left(\sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}} \right)^2 \leq m \left(\sum_{uv\in E(G)} \frac{1}{d(u)d(v)} \right). \tag{3.5}$$

The equality holds if and only if

$$\frac{1}{\sqrt{d(u_1)d(v_1)}} = \frac{1}{\sqrt{d(u_2)d(v_2)}},$$

for any two distinct edges $u_1v_1, u_2v_2 \in E(G)$.

From (3.4) and (3.5) above, we have

$$\frac{ABC(G)}{m} \leq \sqrt{\frac{n - 2 \sum\limits_{uv\in E(G)} \frac{1}{d(u)d(v)}}{m}} \leq \sqrt{\frac{n - 2\frac{R(G)^2}{m}}{m}}.$$

Then, we get $ABC(G)^2 + 2R(G)^2 \leq mn$. So, we have the equality holds if and only if $G \in \mathcal{G}_3$. Then by Lemma 3.1, we have G is regular or biregular. $\square$

Theorem 3.7. *Let G be an (n, m)-graph without isolated vertices. Then*

$$AZI(G)(mn - 2R(G)^2)^3 \geq m^7$$

and the equality holds if and only if G is regular or biregular.

Proof. Let $f(x) = \frac{1}{x^3}$, we have $f''(x) = 12x^{-5} > 0$ if $x > 0$. By Lemma 3.4, we have

$$\begin{aligned}
\frac{AZI(G)}{m} &= \frac{\left(\sum\limits_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)-2} \right)^3}{m} \\
&\geq \frac{1}{\left(\frac{\sum\limits_{uv\in E} \frac{d(u)+d(v)-2}{d(u)d(v)}}{m} \right)^3} \\
&= \frac{1}{\left(\frac{\sum\limits_{uv\in E(G)} (\frac{1}{d(u)} + \frac{1}{d(u)}) - 2 \sum\limits_{uv\in E(G)} \frac{1}{d(u)d(v)}}{m} \right)^3} \\
&= \frac{1}{\left(\frac{n-2 \sum\limits_{uv\in E(G)} \frac{1}{d(u)d(v)}}{m} \right)^3}. \qquad (3.6)
\end{aligned}$$

The equality holds if and only if

$$\frac{d(u_1) + d(v_1) - 2}{d(u_1)d(v_1)} = \frac{d(u_2) + d(v_2) - 2}{d(u_2)d(v_2)},$$

for any two distinct edges $u_1v_1, u_2v_2 \in E(G)$.

On the other hand, by Lemma 3.3 we have

$$R(G)^2 = \left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}} \right)^2 \leq m \left(\sum_{uv \in E(G)} \frac{1}{d(u)d(v)} \right). \tag{3.7}$$

The equality holds if and only if

$$\frac{1}{\sqrt{d(u_1)d(v_1)}} = \frac{1}{\sqrt{d(u_2)d(v_2)}},$$

for any two distinct edges $u_1v_1, u_2v_2 \in E(G)$.

From (3.6) and (3.7) above, we have

$$\frac{AZI(G)}{m} \geq \frac{1}{\left(\frac{n-2 \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}}{m} \right)^3} \geq \frac{1}{\left(\frac{n-2 \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}}{m} \right)^3}.$$

Then we get $AZI(G)(mn - 2R(G)^2)^3 \geq m^7$. Thus, the equality holds if and only if we have $G \in \mathcal{G}_3$. Then by Lemma 3.1, we have G is regular or biregular. □

Theorem 3.8. *Let G be an (n, m)-graph without isolated vertices. Then*
i) *$ReZg_2(G) \geq \frac{m^2}{n}$ and the equality holds if and only if $G \in \mathcal{G}_4$;*
ii) *$ReZg_2(G)ReZg_3(G) \geq Zg_2(G)^2$ and the equality holds if and only if $G \in \mathcal{G}_1$;*
iii) *$ReZg_1(G)ReZg_3(G) \geq Zg_1(G)^2$ and the equality holds if and only if $G \in \mathcal{G}_2$.*

Proof. i) By Lemma 3.3, we have

$$ReZg_1(G)ReZg_2(G) = \left(\sum_{uv \in E(G)} \frac{d(u) + d(v)}{d(u)d(v)} \right) \left(\sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)} \right) \geq m^2.$$

Since

$$ReZG_1(G)ReZG_2(G) = \sum_{uv \in E(G)} \frac{d(u) + d(v)}{d(u)d(v)} = \sum_{uv \in E(G)} (\frac{1}{d(u)} + \frac{1}{d(u)}) = n,$$

we have $ReZG_2(G) \geq \frac{m^2}{n}$. By Lemma 3.3, we have the equality holds if and only if $G \in \mathcal{G}_4$.

ii) By Lemma 3.3, we have

$$\begin{aligned} ReZg_2(G)ReZg_3(G) &= \left(\sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)} \right) \left(\sum_{uv \in E(G)} d(u)d(v)(d(u) + d(v)) \right) \\ &\geq \left(\sum_{uv \in E(G)} d(u)d(v) \right)^2 \\ &= Zg_2(G)^2. \end{aligned}$$

By Lemma 3.3, we have the equality holds if and only if $G \in \mathcal{G}_1$.

iii) By Lemma 3.3, we have

$$\begin{aligned} ReZg_1(G)ReZg_3(G) &= \left(\sum_{uv\in E(G)} \frac{d(u)+d(v)}{d(u)d(v)}\right)\left(\sum_{uv\in E(G)} d(u)d(v)(d(u)+d(v))\right) \\ &\geq \left(\sum_{uv\in E(G)} (d(u)+d(v))\right)^2 \\ &= Zg_1(G)^2. \end{aligned}$$

By Lemma 3.3, we have the equality holds if and only if $G \in \mathcal{G}_2$. □

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[1]School of Computer Science and Educational Software, Guangzhou University, Guangzhou 510006, China
Email address: zshao@cdu.edu.cn

[2]School of Information Science and Engineering, Chengdu University, Chengdu 610106, China
Email address: jianghuiqin@mail.cdu.edu.cn

[3]Department of mathematics, College of sciences, University of Sharjah, UAE
Email address: zraza@sharjah.ac.ae