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SOME INEQUALITIES ON THE INVERSE SUM INDEG COINDEX

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Abstract. Topological indices and coindices play an important role in mathematical chemistry. In this paper we establish some lower and upper bounds for the inverse sum indeg coindex in terms of different graph parameters associated with the structure of the graph. We also obtain relations between the inverse sum indeg coindex and some other indices and coindices.

1. Introduction

In this paper we are concerned with simple graphs, that is graphs without directed, weighted or multiple edges, and without self loops. Let $G=(V,E)$ be such a graph, where $V=\{v_1,v_2,\dots,v_n\}$ is its vertex set and E is its edge set. The order of G is the number $n=|V|$, and size of G is the number $m=|E|$. The degree of vertex v_i, denoted by $d(v_i)$ (or d_i if it is clear from the context) is the number of first neighbors of v_i. Denote by $(d_1,d_2,\dots,d_n)$ the sequence of vertex degrees satisfying $\Delta=d_1\geqslant d_2\geqslant\cdots\geqslant d_n=\delta>0$. The complement of G, denoted as $\bar{G}$, has the same vertex set $V(G)$, and two vertices are adjacent in $\bar{G}$ if and only if they are not adjacent in G, that is $\bar{G}=(V,\bar{E})$, where $\bar{m}=|\bar{E}|=\frac{n(n-1)}{2}-m$. If vertices v_i and v_j of G are adjacent, we write $i\sim j$. On the other hand, if v_i and v_j are adjacent in $\bar{G}$, we write $i\nsim j$. In addition, we will use the following notation: $\bar{\Delta}_e=\max\limits_{i\nsim j}\{d_i+d_j\}$, $\bar{\delta}_e=\min\limits_{i\nsim j}\{d_i+d_j\}$, $\bar{\Delta}=\max\{d_i\,|\,v_i\in V, d_i\neq n-1\}$, and $\bar{\delta}=\min\{d_i\,|\,v_i\in V, d_i\neq n-1\}$. Note that the following relations are valid for these quantities: $2=\bar{\delta}_e\leqslant\bar{\Delta}_e\leqslant 2(n-2)$ and $1\leqslant\bar{\delta}\leqslant\bar{\Delta}\leqslant n-2$.

In graph theory, an invariant is a numerical quantity of graphs that depends only on their abstract structure, not on labeling of vertices or edges, or on the drawings of the graphs. In chemical graph theory such quantities are also referred to as topological indices. Hundreds of various topological indices have been introduced in mathematical chemistry literature in order to describe physical and chemical properties of molecules, especially for studying quantitative structure–activity relationships (QSAR) and quantitative structure–property relationships (QSPR) for predicting different properties of

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chemical compounds (see for example [33, 34]). Many of them are defined as simple functions of the degrees of the vertices of (molecular) graph and can commonly be represented as [17, 19]

$$TI(G) = \sum_{i\sim j} F(d_i, d_j), \tag{1}$$

where $F(x,y)$ a is a real non-negative function with the property $F(x,y) = F(y,x)$.

In [7] a concept of topological coindices was introduced. In this case the sum runs over the edges of the complement of G. In a view of (1) the corresponding coindex of G can be defined as

$$\overline{TI}(G) = \sum_{i\nsim j} F(d_i, d_j).$$

Note that if G is a complete graph, $G \cong K_n$, then its complement $\bar{G} = \bar{K}_n$ has no edges, and hence $TI(\bar{K}_n) = \overline{TI}(K_n) = 0$.

The first and second Zagreb indices are vertex-degree-based graph invariants defined as

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

The quantity M_1 was first time considered in 1972 [15], whereas M_2 in 1975 [16]. These terms were recognized to be a measure of the extent of branching of the carbon–atom skeleton of the underlying molecule. The first Zagreb index became one of the most popular and most extensively studied graph-based molecular structure descriptors. In [29] it was shown that M_1 can also be represented as

$$M_1(G) = \sum_{i\sim j} (d_i + d_j).$$

The corresponding coindices were conceived in [7] as

$$\overline{M}_1(G) = \sum_{i\nsim j} (d_i + d_j) \qquad \text{and} \qquad \overline{M}_2(G) = \sum_{i\nsim j} d_i d_j.$$

Multiplicative versions of the first and second Zagreb coindices were introduced in [38], and defined as

$$\overline{\Pi}_1(G) = \prod_{i\nsim j} (d_i + d_j) \qquad \text{and} \qquad \overline{\Pi}_2(G) = \prod_{i\nsim j} d_i d_j.$$

In [15], another quantity, the sum of cubes of vertex degrees

$$F(G) = \sum_{i=1}^{n} d_i^3 = \sum_{i\sim j} (d_i^2 + d_j^2),$$

was encountered, as well. This quantity is also a measure of branching and it was found that its predictive ability is quite similar to that of $M_1(G)$. However, for the unknown reasons, it did not attracted any attention until 2015 when it was reinvented in

[12] and named the *forgotten topological index*. The forgotten topological coindex, or F-coindex, is defined as [13] (see also [6])

$$\overline{F}(G) = \sum_{i \nsim j} (d_i^2 + d_j^2).$$

In [9] the inverse degree index was introduced. It is conceived to be

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i \sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right).$$

Accordingly, the corresponding coindex is

$$\begin{aligned} \overline{ID}(G) &= \sum_{i \nsim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) \\ &= \sum_{i=1}^{n} (n-1-d_i) \frac{1}{d_i^2}. \end{aligned}$$

In [1] Albertson introduced the quantity called the *imbalance* of an edge e as $imb(e) = |d_i - d_j|$, and used it to define the irregularity measure of a graph as

$$Alb(G) = \sum_{i \sim j} |d_i - d_j|,$$

which is sometimes referred to as *Albertson index* [22, 23] or the *third Zagreb index* [11]. The Albertson coindex, $\overline{Alb}(G)$ was defined in [35].

A family of 148 discrete Adriatic indices was introduced and analyzed in [37] (see also [36]). An especially interesting subclass of these indices consists of 20 indices which are useful for predicting certain physicochemical properties of chemical compounds. The so called inverse sum indeg index, $ISI(G)$, is one of them. It is defined as

$$ISI(G) = \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j}.$$

The $ISI(G)$ is a significant predictor of total surface area for octane isomers [37]. More on its applications and mathematical properties can be found in [2, 10, 18, 21, 26, 32]. The corresponding coindex could be defined as

$$\overline{ISI}(G) = \sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j}.$$

In this paper we determine lower and upper bounds on $\overline{ISI}(G)$ as well as relationships between $\overline{ISI}(G)$ and the above mentioned indices and coindices.

2. Preliminaries

In this section we recall a few discrete inequalities for real number sequences which will be often used in proofs of theorems.

Let $p=(p_i)$ and $a=(a_i)$, $i=1,2,\dots,n$, be two positive real number sequences such that $p_1+p_2+\cdots+p_n=1$ and $0<r\leqslant a_i\leqslant R<+\infty$, where r and R are positive real numbers. In [31] (see also [28]) the following inequality was proved

$$\sum_{i=1}^{n} p_i a_i + rR\sum_{i=1}^{n}\frac{p_i}{a_i} \leqslant r+R. \tag{2}$$

Equality holds if and only if $a_i\in\{r,R\}$, for $i=1,2,\dots,n$.

Let $p=(p_i)$, $i=1,2,\dots,n$, be a sequence of nonnegative real numbers, and $a=(a_i)$, $i=1,2,\dots,n$ a sequence of positive real numbers. Then, for any real r, $r\leqslant 0$ or $r\geqslant 1$, holds [28]

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1}\sum_{i=1}^{n} p_i a_i^r \geqslant \left(\sum_{i=1}^{n} p_i a_i\right)^{r}. \tag{3}$$

When $0\leqslant r\leqslant 1$, the opposite inequality is valid. Equality is attained if and only if either $r=0$, or $r=1$, or $a_1=a_2=\cdots=a_n$, or $p_1=\cdots=p_t$ and $a_{t+1}=\cdots=a_n$, for some t, $1\leqslant t\leqslant n-1$.

Let $x=(x_i)$, $i=1,2,\dots,n$ be a sequence of nonnegative real numbers and $a=(a_i)$, $i=1,2,\dots,n$ a sequence of positive real numbers. In [30] it was proved that for any real $r\geqslant 0$ holds

$$\sum_{i=1}^{n}\frac{x_i^{r+1}}{a_i^r} \geqslant \frac{\left(\sum_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^{r}}. \tag{4}$$

Equality holds if and only if $r=0$ or $\frac{x_1}{a_1}=\frac{x_2}{a_2}=\cdots=\frac{x_n}{a_n}$.

3. Main results

In the next theorem we determine a lower bound for $\overline{ISI}(G)$ that depends on n, m and $ID(G)$ and an upper bound in terms of n, m and $M_1(G)$.

THEOREM 1. *Let G, $G\ncong K_n$, be a simple connected graph with $n\geqslant 3$ vertices and m edges. Then, we have*

$$\frac{(n(n-1)-2m)^2}{4((n-1)ID(G)-n)} \leqslant \overline{ISI}(G) \leqslant \frac{1}{4}(2m(n-1)-M_1(G)). \tag{5}$$

Equality in the left-hand part of (5) holds if and only if $\frac{1}{d_i}+\frac{1}{d_j}$ is a constant for every non-adjacent pair of vertices v_i and v_j in G. Equality in the right-hand side of (5) holds if $d_i=d_j$ for every non-adjacent pair of vertices v_i and v_j in G.

Proof. Having in mind the inequality between arithmetic and harmonic means for real numbers, that is AM-HM inequality (see e.g. [28]), we have that

$$\sum_{i \nsim j} \frac{d_i + d_j}{d_i d_j} \sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j} \geqslant \overline{m}^2 ,$$

that is

$$\overline{ISI}(G) \sum_{i \nsim j} \frac{d_i + d_j}{d_i d_j} \geqslant \frac{1}{4}(n(n-1) - 2m)^2 . \tag{6}$$

On the other hand, we have that

$$\sum_{i \nsim j} \frac{d_i + d_j}{d_i d_j} = \sum_{i \nsim j} \left(\frac{1}{d_i} + \frac{1}{d_j} \right) = \sum_{i=1}^{n} (n-1-d_i) \frac{1}{d_i} = (n-1) ID(G) - n . \tag{7}$$

Combining (6) and (7) we obtain

$$((n-1)ID(G) - n)\overline{ISI}(G) \geqslant \frac{1}{4}(n(n-1) - 2m)^2 .$$

Since $G \ncong K_n$, we have that $(n-1)ID(G) - n \neq 0$, from which left-hand side of (5) is obtained.

Equality in (6), and consequently in the left-hand side of (5), holds if and only if $\frac{1}{d_i} + \frac{1}{d_j}$ is a constant for every pair of non-adjacent vertices v_i and v_j in G, $G \ncong K_n$.

From the inequality between the arithmetic and geometric means for real numbers, the AM-GM inequality (see [28]), we have that

$$d_i d_j \leqslant \frac{1}{4} (d_i + d_j)^2 ,$$

that is

$$\frac{d_i d_j}{d_i + d_j} \leqslant \frac{d_i + d_j}{4} .$$

After summation of the above inequality over all edges of $\overline{G}$ we get

$$\overline{ISI}(G) = \sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j} \leqslant \frac{1}{4} \sum_{i \nsim j} (d_i + d_j) = \frac{\overline{M}_1(G)}{4} . \tag{8}$$

From the above and identity

$$\overline{M}_1(G) = 2m(n-1) - M_1(G) , \tag{9}$$

which was proved in [4] (see also [7, 13, 25]), we obtain the right-hand side of the inequality (5).

Equality in (8), and thus in the right-hand side of (5), holds if and only if $d_i = d_j$ for every pair of non-adjacent vertices v_i and v_j in G. $\square$

REMARK 1. As far as the right-hand side of (5) is concerned, the condition $G \ncong K_n$ is surplus. However, since $\overline{TI}(K_n) = 0$, for any vertex–degree-based topological index, the condition $G \ncong K_n$ does not deteriorate the generality.

COROLLARY 1. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$\overline{ISI}(G) \leqslant \frac{m}{2n}(n(n-1)-2m). \tag{10}$$

Equality holds if and only if G is regular.

Proof. In [8] (see also [24, 39]) it was proved that

$$M_1(G) \geqslant \frac{4m^2}{n},$$

with equality if and only if G is regular. According to the above and right-hand side of (5) we obtain (10). □

COROLLARY 2. *Let U be a simple connected unicyclic graph with $n \geqslant 3$ vertices. Then*

$$\overline{ISI}(U) \leqslant \frac{n(n-3)}{2},$$

with equality if and only if $U \cong C_n$.

COROLLARY 3. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edgse. Then*

$$ISI(G) + \overline{ISI}(G) \leqslant \frac{m(n-1)}{2}.$$

Equality holds if and only if G is regular.

Proof. The required result is obtained from the right-hand side of (5) and the inequality

$$ISI(G) \leqslant \frac{M_1(G)}{4},$$

which was proved in [10]. □

COROLLARY 4. *Let U be a simple connected unicyclic graph with $n \geqslant 3$ vertices. Then*

$$ISI(U) + \overline{ISI}(U) \leqslant \frac{n(n-1)}{2},$$

with equality if and only if $U \cong C_n$.

In the next theorem we establish an upper bound for $\overline{ISI}(G)$ in terms of n, m, $M_1(G)$, $M_2(G)$ and $F(G)$.

THEOREM 2. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then, we have*

$$\overline{ISI}(G) \leqslant \frac{1}{4}\sqrt{\frac{(n(n-1)-2m)(4m^2+(n-2)M_1(G)-F(G)-2M_2(G))}{2}}. \tag{11}$$

Equality holds if and only if $d_i = d_j$ for every pair of non-adjacent vertices v_i and v_j in G.

Proof. Since [3, 13, 20]

$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G) \tag{12}$$

and

$$\overline{F}(G) = (n-1)M_1(G) - F(G) \tag{13}$$

we have that

$$4m^2 + (n-2)M_1(G) - F(G) - 2M_2(G) = \overline{F}(G) + 2\overline{M}_2(G) = 4\sum_{i \nsim j}\left(\frac{d_i+d_j}{2}\right)^2. \tag{14}$$

According to AM-HM inequality we have that

$$\sum_{i \nsim j}\left(\frac{d_i+d_j}{2}\right)^2 \geqslant \sum_{i \nsim j}\left(\frac{2}{\frac{1}{d_i}+\frac{1}{d_j}}\right)^2 = 4\sum_{i \nsim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2. \tag{15}$$

On the other hand , for $r := 2$, $p_i := 1$, $a_i := \frac{d_id_j}{d_i+d_j}$, where summation is performed over all edges of $\overline{G}$, the inequality (3) transforms into

$$\sum_{i \nsim j} 1 \sum_{i \nsim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2 \geqslant \left(\sum_{i \nsim j}\frac{d_id_j}{d_i+d_j}\right)^2,$$

that is, under assumption that $G \ncong K_n$,

$$\sum_{i \nsim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2 \geqslant \frac{\overline{ISI}(G)^2}{\overline{m}} = \frac{2\overline{ISI}(G)^2}{n(n-1)-2m}. \tag{16}$$

Now, the inequality (11) is obtained from (14), (15) and (16).

Equality in (15) holds if and only if $\frac{d_i+d_j}{2} = \frac{2d_id_j}{d_i+d_j}$, that is if and only if $d_i = d_j$ for every non-adjacent pair of vertices v_i and v_j in G. The equality in (16), and consequently in (11), holds under the same condition. □

The following theorem relates $\overline{ISI}(G)$ with $M_1(G)$ and $\overline{Alb}(G)$.

THEOREM 3. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geqslant 3$ vertices and m edges. Then*

$$\overline{ISI}(G) \leqslant \frac{1}{4}\left(2m(n-1) - M_1(G) - \frac{\overline{Alb}(G)^2}{2m(n-1) - M_1(G)}\right). \tag{17}$$

Equality holds if and only if $\frac{|d_i - d_j|}{d_i + d_j}$ is constant for any pair of non-adjacent vertices v_i and v_j in G.

Proof. We have that

$$\overline{M}_1(G) - 4\overline{ISI}(G) = \sum_{i \nsim j}\left((d_i + d_j) - \frac{4d_i d_j}{d_i + d_j}\right) = \sum_{i \nsim j} \frac{(d_i - d_j)^2}{d_i + d_j}. \tag{18}$$

On the other hand, for $r := 1$, $x_i := |d_i - d_j|$, $a_i := d_i + d_j$, where summation is performed over all edges of $\overline{G}$, the inequality (4) becomes

$$\sum_{i \nsim j} \frac{|d_i - d_j|^2}{d_i + d_j} \geqslant \frac{\left(\sum_{i \nsim j} |d_i - d_j|\right)^2}{\sum_{i \nsim j} (d_i + d_j)} = \frac{\overline{Alb}(G)^2}{\overline{M}_1(G)} = \frac{\overline{Alb}(G)^2}{2m(n-1) - M_1(G)}. \tag{19}$$

From the above and equality (18) we obtain

$$2m(n-1) - M_1(G) - 4\overline{ISI}(G) \geqslant \frac{\overline{Alb}(G)^2}{2m(n-1) - M_1(G)},$$

from which we arrive at (17).

Equality in (19), and hence in (17), holds if and only if $\frac{|d_i - d_j|}{d_i + d_j}$ is constant for any pair of non-adjacent vertices v_i and v_j in G, $G \ncong K_n$. □

REMARK 2. Since

$$\overline{ISI}(G) \leqslant \frac{1}{4}\left(2m(n-1) - M_1(G) - \frac{\overline{Alb}(G)^2}{2m(n-1) - M_1(G)}\right) \leqslant \frac{2m(n-1) - M_1(G)}{4},$$

the inequality (17) is stronger than the right-hand side of (5).

THEOREM 4. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geqslant 3$ vertices and m edges. Then*

$$\overline{ISI}(G) \leqslant \frac{\bar{\Delta}_e + \bar{\delta}_e}{2\bar{\Delta}_e \bar{\delta}_e}\left(4m^2 - M_1(G) - 2M_2(G)\right) - \frac{(2m(n-1) - M_1(G))^2}{\bar{\Delta}_e \bar{\delta}_e((n-1)ID(G) - n)}. \tag{20}$$

Equality holds if and only if $d_i = d_j$ for any pair of non-adjacent vertices v_i and v_j in G.

Proof. For $p_i := \frac{d_i d_j}{\overline{M}_2(G)}$, $a_i := d_i + d_j$, $r := \bar{\delta}_e$, $R := \bar{\Delta}_e$, where summation is performed over all edges of $\overline{G}$, $G \ncong K_n$, the inequality (2) becomes

$$\frac{\sum_{i \nsim j} d_i d_j (d_i + d_j)}{\overline{M}_2(G)} + \bar{\Delta}_e \bar{\delta}_e \frac{\sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j}}{\overline{M}_2(G)} \leqslant \bar{\Delta}_e + \bar{\delta}_e \,,$$

that is

$$\sum_{i \nsim j} d_i d_j (d_i + d_j) + \bar{\Delta}_e \bar{\delta}_e \overline{ISI}(G) \leqslant (\bar{\Delta}_e + \bar{\delta}_e) \overline{M}_2(G) \,. \tag{21}$$

On the other hand, for $r := 1$, $x_i := d_i + d_j$, $a_i := \frac{1}{d_i} + \frac{1}{d_j}$, where summation is performed over all edges of $\overline{G}$, $G \ncong K_n$, the inequality (4) transforms into

$$\sum_{i \nsim j} d_i d_j (d_i + d_j) = \sum_{i \nsim j} \frac{(d_i + d_j)^2}{\frac{1}{d_i} + \frac{1}{d_j}} \geqslant \frac{\left(\sum_{i \nsim j} (d_i + d_j)\right)^2}{\sum_{i \nsim j} \left(\frac{1}{d_i} + \frac{1}{d_j}\right)} \,,$$

that is

$$\sum_{i \nsim j} d_i d_j (d_i + d_j) \geqslant \frac{\overline{M}_1(G)^2}{\sum_{i \nsim j} \left(\frac{1}{d_i} + \frac{1}{d_j}\right)} \,. \tag{22}$$

The inequality (20) is obtained from inequalities (21) and (22), and identities (7), (9) and (12).

Equality in (21) holds if and only if $d_i + d_j \in \{\bar{\Delta}_e, \bar{\delta}_e\}$ for any pair of non-adjacent vertices v_i and v_j in G. Equality in (22) holds if and only if $d_i d_j$ is constant for any pair of non-adjacent vertices v_i and v_j in G. This implies that equality in (20) holds if and only if $d_i = d_j$ for any pair of non-adjacent vertices v_i and v_j in G. □

THEOREM 5. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geqslant 3$ vertices and m edges. Then*

$$\overline{ISI}(G) \geqslant \frac{\bar{\Delta}\bar{\delta}(2m(n-1) - M_1(G))}{(\bar{\Delta} + \bar{\delta})^2} \,. \tag{23}$$

Equality holds if and only if $d_i = d_j$ for any pair of non-adjacent vertices v_i and v_j in G.

Proof. We have that

$$\overline{ISI}(G) = \sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j} = \sum_{i \nsim j} \frac{d_i + d_j}{\left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}\right)^2} \,. \tag{24}$$

On the other hand, for any pair of non-adjacent vertices v_i and v_j in G holds

$$\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}} \leqslant \sqrt{\frac{\bar{\Delta}}{\bar{\delta}}} + \sqrt{\frac{\bar{\delta}}{\bar{\Delta}}} \,. \tag{25}$$

From the above and equality (24) we obtain (23).

Equality in (25), and consequently in (23), holds if and only if $d_i = d_j$ for any pair of non-adjacent vertices v_i and v_j in G. $\square$

COROLLARY 5. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geqslant 3$ vertices and m edges. Then*

$$\overline{ISI}(G) \geqslant \frac{m\bar{\Delta}\bar{\delta}(n(n-1)-2m)}{(n-1)(\bar{\Delta}+\bar{\delta})^2}.$$

Equality holds if and only if $G \cong K_{1,n-1}$.

Proof. In [8] it was proved that

$$M_1(G) \leqslant m\left(\frac{2m}{n-1}+n-2\right),$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$ [5]. From the above and inequality (23) we obtain the required result. $\square$

In the next theorem we determine a lower bound for $\overline{ISI}(G)$ that depends on n, m and multiplicative coindices $\overline{\Pi}_1(G)$ and $\overline{\Pi}_2(G)$.

THEOREM 6. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geqslant 3$ vertices and m edges. Then*

$$\overline{ISI}(G) \geqslant \frac{n(n-1)-2m}{2}\left(\frac{\overline{\Pi}_2(G)}{\overline{\overline{\Pi}}_1(G)}\right)^{\frac{2}{n(n-1)-2m}}. \tag{26}$$

Equality holds if and only if $\frac{1}{d_i}+\frac{1}{d_j}$ is constant for any pair of vertices v_i and v_j in G.

Proof. Based on the AM–GM inequality we have that

$$\overline{ISI}(G) = \sum_{i \nsim j} \frac{d_i d_j}{d_i+d_j} \geqslant \overline{m}\left(\prod_{i \nsim j}\frac{d_i d_j}{d_i+d_j}\right)^{1/\overline{m}} = \overline{m}\left(\frac{\prod_{i \nsim j} d_i d_j}{\prod_{i \nsim j}(d_i+d_j)}\right)^{1/\overline{m}}, \tag{27}$$

wherefrom (26) is obtained.

Equality in (27), and hence in (26), holds if and only if $\frac{d_i d_j}{d_i+d_j}$, that is $\frac{1}{d_i}+\frac{1}{d_j}$, is constant for any pair of non-adjacent vertices v_i and v_j in G, $G \ncong K_n$. $\square$

REMARK 3. Since

$$(n-1)ID(G)-n = \sum_{i=1}^{n}(n-1-d_i)\frac{1}{d_i} = \sum_{i \nsim j}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) = \sum_{i \nsim j}\frac{d_i+d_j}{d_i d_j} \geqslant \overline{m}\left(\frac{\overline{\Pi}_1(G)}{\overline{\overline{\Pi}}_2(G)}\right)^{1/\overline{m}},$$

we have that

$$\left(\frac{\overline{\Pi}_2(G)}{\overline{\Pi}_1(G)}\right)^{\frac{2}{n(n-1)-2m}} \geqslant \frac{n(n-1)-2m}{2((n-1)ID(G)-n)}.$$

From the above inequality we have that

$$\overline{ISI}(G) \geqslant \frac{n(n-1)-2m}{2}\left(\frac{\overline{\Pi}_2(G)}{\overline{\Pi}_1(G)}\right)^{\frac{2}{n(n-1)-2m}} \geqslant \frac{(n(n-1)-2m)^2}{4((n-1)ID(G)-n)},$$

which means that inequality (26) is stronger than (5).

THEOREM 7. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$\frac{(n-1)M_1(G)-F(G)}{2\overline{\Delta}_e} \leqslant \frac{2m(n-1)-M_1(G)}{2} - \overline{ISI}(G) \leqslant \frac{(n-1)M_1(G)-F(G)}{2\overline{\delta}_e}. \tag{28}$$

Equality holds if and only if $d_i + d_j$ is constant for any pair of non-adjacent vertices v_i and v_j in G.

Proof. We have that

$$\frac{1}{2}\overline{M}_1(G) - \overline{ISI}(G) = \sum_{i\nsim j}\left(\frac{d_i+d_j}{2} - \frac{d_id_j}{d_i+d_j}\right) = \sum_{i\nsim j}\frac{d_i^2+d_j^2}{2(d_i+d_j)}. \tag{29}$$

On the other hand, we have that

$$\frac{1}{2\overline{\Delta}_e}\sum_{i\nsim j}(d_i^2+d_j^2) \leqslant \sum_{i\nsim j}\frac{d_i^2+d_j^2}{2(d_i+d_j)} \leqslant \frac{1}{2\overline{\delta}_e}\sum_{i\nsim j}(d_i^2+d_j^2),$$

that is

$$\frac{\overline{F}(G)}{2\overline{\Delta}_e} \leqslant \sum_{i\nsim j}\frac{d_i^2+d_j^2}{2(d_i+d_j)} \leqslant \frac{\overline{F}(G)}{2\overline{\delta}_e}. \tag{30}$$

Combining (29) and (30) we get

$$\frac{\overline{F}(G)}{2\overline{\Delta}_e} \leqslant \frac{1}{2}\overline{M}_1(G) - \overline{ISI}(G) \leqslant \frac{\overline{F}(G)}{2\overline{\delta}_e}.$$

From the above inequalities and identities (9) and (13) we arrive at (28).

Equalities in (30), and hence in (28), hold if and only if $d_i + d_j$ is constant for any pair of non-adjacent vertices v_i and v_j in G. □

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