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# SHARP INEQUALITIES FOR THE ATOM–BOND (SUM) CONNECTIVITY INDEX

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*Abstract.* For a graph $G$, its atom-bond connectivity (ABC) index (respectively, atom-bond sum connectivity (ABS) index) is defined as the addition of the numbers $\sqrt{d_i+d_j-2}(d_id_j)^{-1/2}$ (respectively, $\sqrt{d_i+d_j-2}(d_i+d_j)^{-1/2}$) over all unordered pairs of adjacent vertices $\{v_i,v_j\}$ of $G$, where $d_i$ and $d_j$ denote the degrees of $v_i$ and $v_j$, respectively. In this paper, sharp upper bounds on the ABC and ABS indices are derived. All the graphs that attain the obtained bounds are also completely characterized.

## 1. Introduction

Let $G=(V,E)$, $V=\{v_1,v_2,\dots,v_n\}$, $E=\{e_1,e_2,\dots,e_m\}$, be a simple graph of order $n\geqslant 2$ and size $m$ without isolated vertices. Denote by $\Delta=d_1\geqslant d_2\geqslant\cdots\geqslant d_n=\delta>0$, $d_i=d(v_i)$, a sequence of vertex degrees given in a non-increasing order. Let $e=\{v_i,v_j\}$ denote an edge incident to vertices $v_i$ and $v_j$. Degree of an edge $e$ is defined to be $d(e)=d_i+d_j-2$. Let $\Delta_e=d(e_1)+2\geqslant d(e_2)+2\geqslant\cdots\geqslant d(e_n)+2=\delta_e$. Denote by $i\sim j$ the edge connecting the vertices $v_i,v_j\in V(G)$.

A topological index for a graph is a numerical quantity which is invariant under isomorphism of the graph. The study of the mathematical aspects of the degree-based topological indices is considered to be one of the very active research areas within the field of chemical graph theory.

The general sum connectivity index, $H_\alpha(G)$, is defined as [50]

$$H_\alpha(G)=\sum_{i\sim j}(d_i+d_j)^\alpha=\sum_{i=1}^{m}(d(e_i)+2)^\alpha,\quad H_0(G)=m,$$

where $\alpha$ is an arbitrary real number. Some special cases include:

— the first Zagreb index, $M_1(G)=H_1(G)$ [19],
— the sum connectivity index $SC(G)=H_{-1/2}(G)$ [51],
— the harmonic index $H(G)=2H_{-1}(G)$ [17].

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The general Randić index $R_\alpha$ of a graph $G$ is a graph invariant defined as [7]

$$R_\alpha(G) = \sum_{i\sim j}(d_i d_j)^\alpha\,, \quad R_0(G) = m\,,$$

where $\alpha$ is an arbitrary real number. When $\alpha = 1$, then the second Zagreb index $M_2(G) = R_1(G)$ is obtained [20]; for $\alpha = -1/2$ the Randić index $R(G) = R_{-1/2}(G)$ is obtained [42]. For $\alpha = -1$ the modified second Zagreb index, $M_2^*(G)$, defined in [38] is obtained (see also [8]).

The arithmetic–geometric index was introduced in [45]. It is a modification of the well–known geometric–arithmetic index. It is defined as

$$AG(G) = \sum_{i\sim j}\frac{d_i + d_j}{2\sqrt{d_i d_j}}\,.$$

The atom-bond connectivity index, ABC index for short, is defined [3, 16] (see for example also [25]) as

$$ABC(G) = \sum_{i\sim j}\sqrt{\frac{d_i + d_j - 2}{d_i d_j}}\,.$$

It was shown that ABC index can be used for modeling thermodynamic properties of organic chemical compounds. Various papers on the mathematical properties of the *ABC* index have been published as well (see the recent review [3]).

For a graph $G$, its atom-bond sum-connectivity (ABS) index (see [5, 4]) is defined as

$$ABS(G) = \sum_{i\sim j}\sqrt{1 - \frac{2}{d_i + d_j}}.$$

Some chemical applications of the ABS index can be found in [5, 37]; these two papers together with [39] also provide some mathematical aspects of the ABS index. In the present paper, we investigate the relationship between *ABC* and *ABS* indices and some other degree-based invariants. More precisely, we derive sharp upper bounds on the ABC and ABS indices by using an inequality of real numbers.

## 2. Preliminaries

In order to obtain the main results, we need to establish some preliminary results. To that end, in this section we recall some results for the atom-bond connectivity index published in the literature that are of interest for this paper.

LEMMA 2.1. [23] *Let $G$ be a graph with $n$ vertices and $m$ edges. Then*

$$ABC(G) \leqslant \sqrt{m\left(n - \frac{2m^2}{M_2(G)}\right)}, \tag{2.1}$$

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

Let us note that in the proof of Lemma 2.1 the inequality

$$ABC(G) \leqslant \sqrt{m(n-2R_{-1}(G))}, \tag{2.2}$$

with equality if and only if $G$ is a regular or semiregular bipartite graph, was proven. Interestingly, the inequality (2.2) is stronger than (2.1).

The inequality (2.2) was also proved in [49]. It was proved that equality is attained if and only if $G$ is a regular or semiregular bipartite graph, or every edge is incident with a vertex of degree two.

LEMMA 2.2. [6] *If $G$ is a connected graph of order $n \geqslant 2$ and size $m$, then*

$$ABC(G) \leqslant \sqrt{(n-1)(m-R_{-1}(G))}, \tag{2.3}$$

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

Note that the bounds on the $ABC(G)$ given in (2.2) and (2.3), involve the same parameters. However, these bounds are not comparable in general.

LEMMA 2.3. [49] *Let $G$ be a graph of size $m$. Then*

$$ABC(G) \leqslant \sqrt{(M_1(G)-2m)R_{-1}(G)}, \tag{2.4}$$

*with equality if and only if either $m=0$, or every component of $G$ is either a regular graph of degree $r$ for all such components (if exist), or semiregular bipartite graph with the degree set $\{s,t\}$ provided that $\frac{st}{s+t-2}$ is constant in all such components (if exist), and $\frac{st}{s+t-2} = r^2(2r-2)$ if there exist both types of the components.*

Let us note that (2.4) was obtained as a corollary of more general results proved in [11, 13]. In [12] the inequality (2.4) was proven for the graphs with tree structure.

## 3. Main results

Our starting point is the inequality reported in [41] for the real number sequences.

LEMMA 3.1. [41] *Let $x=(x_i)$, $i=1,2,\ldots,n$, be a sequence of non-negative real numbers, and $a=(a_i)$, $i=1,2,\ldots,n$, a sequence of positive real numbers. Then, for any $r \geqslant 0$, holds*

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \geqslant \frac{\left(\sum_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^{r}}. \tag{3.1}$$

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

REMARK 3.1. The result in Lemma 3.1 is given in its original form. However, let us note that the inequality (3.1) is valid both if $r \leqslant -1$ or $r \geqslant 0$. When $-1 \leqslant r \leqslant 0$, the opposite inequality is valid. Equality in (3.1) is also valid when $r=-1$.

In the next theorem we establish a relationship $ABC(G)$ and harmonic index, $H(G)$.

THEOREM 3.1. *Let $G$ be a graph of order $n$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{n(m - H(G))}. \tag{3.2}$$

*Equality holds if and only if $G$ is a regular or semiregular bipartite graph.*

*Proof.* The following identities are valid

$$\begin{aligned} m &= \sum_{i\sim j} 1 = \sum_{i\sim j} \frac{d_i+d_j}{d_i+d_j} = \sum_{i\sim j} \frac{2}{d_i+d_j} + \sum_{i\sim j} \frac{d_i+d_j-2}{d_i+d_j} \\ &= H(G) + \sum_{i\sim j} \frac{d_i+d_j-2}{d_i+d_j}. \end{aligned} \tag{3.3}$$

On the other hand, after replacing $r := 1$, $x_i := \sqrt{\frac{d_i+d_j-2}{d_i d_j}}$, $a_i := \frac{d_i+d_j}{d_i d_j}$ and summation over all pairs of adjacent vertices $v_i, v_j$ in $G$, the inequality (3.1) transforms into

$$\sum_{i\sim j} \frac{\left(\sqrt{\frac{d_i+d_j-2}{d_i d_j}}\right)^2}{\frac{d_i+d_j}{d_i d_j}} \geqslant \frac{\left(\sum_{i\sim j} \sqrt{\frac{d_i+d_j-2}{d_i d_j}}\right)^2}{\sum_{i\sim j} \frac{d_i+d_j}{d_i d_j}},$$

that is

$$\sum_{i\sim j} \frac{d_i+d_j-2}{d_i+d_j} \geqslant \frac{ABC(G)^2}{n}, \tag{3.4}$$

because $\sum_{i\sim j} \frac{d_i+d_j}{d_i d_j} = n$ (see Lemma 1 in [15]). The inequality (3.2) is obtained from (3.3) and (3.4).

By Lemma 3.1, the equality in (3.4) holds if and only if $\frac{\sqrt{(d_i+d_j-2)d_i d_j}}{d_i+d_j}$ is constant for every pair of adjacent vertices in $G$. Suppose that vertices $v_j$ and $v_k$ are both adjacent to $v_i$. Then, the equation

$$\frac{\sqrt{(d_i+d_j-2)d_i d_j}}{d_i+d_j} = \frac{\sqrt{(d_i+d_k-2)d_i d_k}}{d_i+d_k},$$

holds if and only if $d_j = d_k$, which implies that the equality in (3.4) holds if and only if $G$ is either regular or semiregular bipartite graph. □

REMARK 3.2. The harmonic index, $H(G)$, is well elaborated in the literature (see for example [1,9,33,43]). From the known lower bounds on $H(G)$ and inequality (3.2) it is possible to derive a number of upper bounds for the $ABC$ index. In the following corollaries of Theorem 3.1 we illustrate this fact.

In [26] it was proven that

$$H(G) \geqslant \frac{2m^2}{M_1(G)}, \tag{3.5}$$

where the equality holds if and only if $G$ is either regular or semiregular bipartite graph. From (3.2) and (3.5) we obtain the following result.

COROLLARY 3.1. *Let $G$ be a graph of order $n$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{nm\left(1 - \frac{2m}{M_1(G)}\right)}, \tag{3.6}$$

*with equality if and only if $G$ is regular or semiregular bipartite graph.*

In [33] it was proven that

$$H(G) \geqslant \frac{2m^2}{M_1(G)} + \frac{(\sqrt{\Delta_e} - \sqrt{\delta_e})^2}{\Delta_e \delta_e},$$

where the equality holds if and only if $G$ is either regular or semiregular bipartite graph. The above inequality is stronger than (3.5). Now we have the following corollary of Theorem 3.1.

COROLLARY 3.2. *Let $G$ be a graph of order $n \geqslant 3$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{n\left(m - \frac{2m^2}{M_1(G)} - \frac{\left(\sqrt{\Delta_e} - \sqrt{\delta_e}\right)^2}{\Delta_e \delta_e}\right)}.$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

In [47] the following lower bound for the harmonic index was obtained

$$H(G) \geqslant \frac{2m^2}{2m(\Delta + \delta) - n\delta\Delta},$$

where the equality holds if and only if one end-vertex is of degree $\Delta$ and the other one is of degree $\delta$ for every edge of $G$. From the above inequality and (3.2) we obtain the next result.

COROLLARY 3.3. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{nm\left(1 - \frac{2m}{2m(\Delta + \delta) - n\delta\Delta}\right)}. \tag{3.7}$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

REMARK 3.3. In [10] (see also [24, 30, 31]) the following inequality was proven

$$M_1(G) \leqslant 2m(\Delta+\delta) - n\delta\Delta. \tag{3.8}$$

The inequality (3.7) can be also obtained from (3.6) and (3.8).

Based on the arithmetic–geometric mean inequality (see for example [36]) we have that

$$2\sqrt{n\delta\Delta M_1(G)} \leqslant M_1(G) + n\delta\Delta \leqslant 2m(\Delta+\delta),$$

that is

$$M_1(G) \leqslant \frac{m^2(\Delta+\delta)^2}{n\delta\Delta},$$

which was proven in [27]. Now we obtain the following result:

COROLLARY 3.4. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{n\left(m - \frac{2n\delta\Delta}{(\Delta+\delta)^2}\right)}.$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

In [44] it was proven that

$$H(G) \geqslant \frac{2n\Delta}{(\Delta+1)^2}.$$

So we have the following result:

COROLLARY 3.5. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{n\left(m - \frac{2n\Delta}{(\Delta+1)^2}\right)}.$$

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

In [48] it was proven that

$$H(G) \geqslant \frac{2(n-1)}{n}.$$

From the above and inequality (3.2) we obtain the next two results.

COROLLARY 3.6. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{nm - 2(n-1)}.$$

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

COROLLARY 3.7. *Let $T$ be a tree with $n \geqslant 2$ vertices. Then*

$$ABC(T) \leqslant \sqrt{n(n-1-H(T))} \leqslant \sqrt{(n-2)(n-1)}. \tag{3.9}$$

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

REMARK 3.4. The second inequality in (3.9) was proven in [18].

In [33] it was proven that

$$H(G) \geqslant \frac{2SC(G)^2}{m}.$$

From the above and (3.2) we obtain the following result.

COROLLARY 3.8. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{n\left(m - \frac{2SC(G)^2}{m}\right)}.$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

In [46] it was proven that

$$H(G) \geqslant \frac{m}{n-r(G)},$$

where $r(G)$ is rank of $G$. Now we have the following corollary of Theorem 3.1.

COROLLARY 3.9. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{mn\left(1 - \frac{1}{n-r(G)}\right)}.$$

*Equality holds if and only if $G \cong K_n$.*

In [14] it was proven that

$$H(G) \geqslant \chi(G) - \frac{n}{2},$$

where $\chi(G)$ is the chromatic number of $G$. Now we have that the following result is valid.

COROLLARY 3.10. *Let $G$ be a connected graph with $n \geqslant 2$ vertices and $m$ edges with chromatic number $\chi(G)$. Then*

$$ABC(G) \leqslant \sqrt{n\left(m - \chi(G) + \frac{n}{2}\right)}.$$

*Equality holds if and only if $G \cong K_n$.*

In the next theorem we determine a relationship between $ABC(G)$, $AG(G)$ and $R(G)$.

THEOREM 3.2. *Let $G$ be a graph without isolated vertices. Then*

$$ABC(G) \leqslant \sqrt{2R(G)(AG(G)-R(G))}. \tag{3.10}$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

*Proof.* The following identities are valid

$$\begin{aligned} AG(G) &= \sum_{i\sim j} \frac{d_i+d_j}{2\sqrt{d_id_j}} = \frac{1}{2}\sum_{i\sim j}\frac{d_i+d_j-2}{\sqrt{d_id_j}} + \sum_{i\sim j}\frac{1}{\sqrt{d_id_j}} \\ &= R(G) + \frac{1}{2}\sum_{i\sim j}\frac{d_i+d_j-2}{\sqrt{d_id_j}}. \end{aligned} \tag{3.11}$$

On the other hand, for $r:=1$, $x_i := \sqrt{\frac{d_i+d_j-2}{d_id_j}}$, $a_i := \frac{1}{\sqrt{d_id_j}}$ and summation performed over all pairs of adjacent vertices $v_i$ and $v_j$ in $G$, the inequality (3.1) transforms into

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

that is

$$\sum_{i\sim j}\frac{d_i+d_j-2}{\sqrt{d_id_j}} \geqslant \frac{ABC(G)^2}{R(G)}. \tag{3.12}$$

The inequality (3.10) immediately follows from (3.11) and (3.12).

By Lemma 3.1, the equality in (3.12) holds if and only if $d_i+d_j$ is constant for every pair of adjacent vertices $v_i$ and $v_j$ in $G$, which implies that equality in (3.10) holds if and only if $G$ is a regular or semiregular bipartite graph. □

The following upper bound for the arithmetic–geometric index was proven in [34]

$$AG(G) \leqslant \frac{nm}{2R(G)} + \frac{1}{8}\left(\sqrt{\Delta_e}-\sqrt{\delta_e}\right)^2,$$

with equality if and only if $G$ is regular or semiregular bipartite graph. From the above and inequality (3.10) we have the following corollary of Theorem 3.2.

COROLLARY 3.11. *Let $G$ be a connected graph of order $n \geqslant 2$ and size $m$. Then we have*

$$ABC(G) \leqslant \sqrt{mn + \left(\frac{1}{4}\left(\sqrt{\Delta_e}-\sqrt{\delta_e}\right)^2 - 2R(G)\right)R(G)}.$$

*Equality holds if and only if $G$ is a regular or a semiregular bipartite graph.*

Since

$$AG(G) = \sum_{i\sim j} \frac{d_i + d_j}{2\sqrt{d_i d_j}} \leqslant \frac{\Delta_e R(G)}{2},$$

with equality if and only if $G$ is a regular or a semiregular bipartite graph, we have another corollary of Theorem 3.2.

COROLLARY 3.12. *Let $G$ be a connected graph. Then*

$$ABC(G) \leqslant R(G)\sqrt{\Delta_e - 2}.$$

*Equality holds if and only if $G$ is a regular or a semiregular bipartite graph.*

Since $\Delta_e \leqslant 2\Delta$ and $R(G) \leqslant \frac{m}{\delta}$, the following results are valid.

COROLLARY 3.13. *Let $G$ be a connected graph. Then*

$$ABC(G) \leqslant \sqrt{2(\Delta-1)}R(G). \tag{3.13}$$

*Equality holds if and only if $G$ is a regular graph.*

COROLLARY 3.14. *Let $G$ be a connected graph of order $m$. Then*

$$ABC(G) \leqslant \frac{m\sqrt{2(\Delta-1)}}{\delta}. \tag{3.14}$$

*Equality holds if and only if $G$ is a regular graph.*

Let us note that inequalities (3.13) and (3.14) were proven in [12, 22].

The reciprocal sum–connectivity index, denoted by $RSC(G)$, is defined as [2]

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

Later, in [28], this index is defined under the name Nirmala index (see also [21, 29]).

The proof of the next result is fully analogous to that of Theorem 3.2 and thence it is omitted.

THEOREM 3.3. *Let $G$ be a graph without isolated vertices. Then*

$$ABS(G) \leqslant \sqrt{SC(G)(RSC(G) - 2\cdot SC(G))}. \tag{3.15}$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

THEOREM 3.4. *Let $G$ be a graph of size $m$ without isolated vertices. Then*

$$ABS(G) \leqslant \sqrt{\frac{(M_1(G) - 2m)H(G)}{2}}. \tag{3.16}$$

*Equality holds if and only if $G$ is a regular or semiregular bipartite graph.*

*Proof.* The following identity is valid

$$M_1(G)-2m=\sum_{i\sim j}(d_i+d_j-2)=\sum_{i\sim j}\frac{d_i+d_j-2}{d_i+d_j}(d_i+d_j)=\sum_{i\sim j}\frac{\frac{d_i+d_j-2}{d_i+d_j}}{\frac{1}{d_i+d_j}}. \tag{3.17}$$

On the other hand, for $r=1$, $x_i:=\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}$, $a_i:=\frac{1}{d_i+d_j}$, with summation performed over all adjacent vertices, the inequality (3.1) becomes

$$\sum_{i\sim j}\frac{\frac{d_i+d_j-2}{d_i+d_j}}{\frac{1}{d_i+d_j}}\geqslant\frac{\left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\right)^2}{\sum_{i\sim j}\frac{1}{d_i+d_j}}, \tag{3.18}$$

that is

$$\sum_{i\sim j}\frac{\frac{d_i+d_j-2}{d_i+d_j}}{\frac{1}{d_i+d_j}}\geqslant\frac{ABS(G)^2}{\frac{1}{2}H(G)}.$$

From the above and equality (3.17) we arrive at (3.16).

Equality in (3.18) holds if and only if $\sqrt{(d_i+d_j-2)(d_i+d_j)}$ is constant for every pair of adjacent vertices in $G$. Suppose that vertices $v_j$ and $v_k$ are both adjacent to $v_i$. Then the equation

$$\sqrt{(d_i+d_j-2)(d_i+d_j)}=\sqrt{(d_i+d_k-2)(d_i+d_k)},$$

that is

$$(d_j-d_k)(2d_i+d_j+d_k-2)=0,$$

holds if and only if $d_j=d_k$, which implies that equality in (3.16) holds if and only if $G$ is either regular or semiregular bipartite graph. □

REMARK 3.5. The Platt index, proposed in [40] for predicting paraffin properties, belongs to the oldest degree based topological indices. It is defined as

$$Pl(G)=\sum_{i\sim j}(d_i+d_j-2).$$

Since

$$Pl(G)=M_1(G)-2m,$$

the inequality (3.16) can be written as

$$ABS(G)\leqslant\sqrt{\frac{Pl(G)H(G)}{2}}.$$

The inverse degree index, $ID(G)$, is a vertex–degree-based index defined in [17] as

$$ID(G)=\sum_{i=1}^{n}\frac{1}{d_i}.$$

The following relation between the first Zagreb index and inverse degree index was established in [32]

$$M_1(G) \leqslant 2m(\Delta+2\delta)+\Delta\delta^2 ID(G)-n\delta(2\Delta+\delta). \tag{3.19}$$

Based on (3.19) and (3.16), we get the following corollary of Theorem 3.4.

COROLLARY 3.15. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then we have*

$$ABS(G) \leqslant \sqrt{\frac{(2m(\Delta+2\delta-1)+\Delta\delta^2 ID(G)-n\delta(2\Delta+\delta))H(G)}{2}}. \tag{3.20}$$

*Equality holds if and only if $\Delta = d_1 = \cdots = d_t \geqslant d_{t+1} = \cdots = d_n = \delta$, for some $t$, $1 \leqslant t \leqslant n-1$.*

From (3.8) and (3.16) we get the following corollary of Theorem 3.4.

COROLLARY 3.16. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABS(G) \leqslant \sqrt{\frac{(2m(\Delta+\delta-1)-n\Delta\delta)H(G)}{2}}. \tag{3.21}$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

REMARK 3.6. Since (see [32])

$$2m+\Delta\delta ID(G) \leqslant n(\Delta+\delta),$$

the following inequality is valid

$$M_1(G) \leqslant 2m((\Delta+2\delta)+\Delta\delta^2 ID(G)-n\delta(2\Delta+\delta) \leqslant 2m(\Delta+\delta)-n\delta\Delta,$$

which means that inequality (3.20) is stronger than (3.21).

When $G$ has a tree structure, $G = T$, the following inequality is valid [32]

$$M_1(T) \leqslant 2(n-1)+(n-2)\Delta.$$

From the above and inequality (3.16), we get the following result.

COROLLARY 3.17. *Let $T$ be a tree with $n \geqslant 3$ vertices. Then*

$$ABS(T) \leqslant \sqrt{\frac{(n-2)\Delta H(T)}{2}}.$$

*Equality holds if and only if $\Delta = d_1 = \cdots = d_t \geqslant d_{t+1} = \cdots = d_n = \delta = 1$, for some $t$, $1 \leqslant t \leqslant n-1$.*

In [35] it was proven that

$$M_1(G)+\frac{\Delta_e\delta_e}{2}H(G)\leqslant m(\Delta_e+\delta_e)\,.$$

From the above inequality and (3.16) we obtain the following result.

COROLLARY 3.18. *Let $G$ be a graph of size $m\geqslant 1$ without isolated vertices. Then*

$$ABS(G)\leqslant\sqrt{\frac{(2m(\Delta_e+\delta_e-2)-\Delta_e\delta_e H(G))H(G)}{4}}\,.$$

*Equality holds if and only if $\Delta=d_1=\cdots=d_t\geqslant d_{t+1}=\cdots=d_n=\delta$, for some $t$, $1\leqslant t\leqslant n-1$.*

Denote with $\omega(G)+1$ the number of vertices of the complete graph which cannot be an induced subgraph of $G$. In [52] it was proven that

$$M_1(G)\leqslant\frac{\omega(G)-1}{\omega(G)}2mn\,.$$

From the above inequality and (3.16) we get the following result.

COROLLARY 3.19. *Let $G$ be a graph of order $n\geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABS(G)\leqslant\sqrt{\frac{m((n-1)\omega(G)-n)H(G)}{\omega(G)}}\,.$$

In the next theorem we establish an upper bound for $M_1(G)$ in terms of $m$, $\Delta$, $\delta$ and the second Zagreb index, $M_2(G)$.

LEMMA 3.2. *Let $G$ be a graph with $m\geqslant 1$ vertices. Then*

$$M_1(G)\leqslant\min\left\{\frac{1}{\Delta}(M_2(G)+m\Delta^2),\frac{1}{\delta}(M_2(G)+m\delta^2)\right\}\,. \tag{3.22}$$

*Equality holds if and only if $G$ is such a graph that either each vertex is adjacent to the vertex with degree $\Delta$, or each vertex is adjacent to the vertex with degree $\delta$.*

*Proof.* For any pair of vertices $v_i$ and $v_j$ in $G$, holds that

$$(\Delta-d_i)(\Delta-d_j)\geqslant 0 \qquad\text{and}\qquad (d_i-\delta)(d_j-\delta)\geqslant 0\,.$$

From the above we obtain that

$$\Delta(d_i+d_j)\leqslant d_id_j+\Delta^2 \qquad\text{and}\qquad \delta(d_i+d_j)\leqslant d_id_j+\delta^2\,.$$

After summation of the above inequalities over all adjacent vertices $v_i$ and $v_j$ in $G$, we obtain

$$\Delta\sum_{i\sim j}(d_i+d_j)\leqslant\sum_{i\sim j}d_id_j+\sum_{i\sim j}\Delta^2 \tag{3.23}$$

and

$$\delta \sum_{i\sim j}(d_i+d_j) \leqslant \sum_{i\sim j} d_i d_j + \sum_{i\sim j} \delta^2 , \tag{3.24}$$

that is

$$M_1(G) \leqslant \frac{1}{\Delta}(M_2(G)+m\Delta^2),$$

and

$$M_1(G) \leqslant \frac{1}{\delta}(M_2(G)+m\delta^2).$$

The inequality (3.22) directly follows from the above inequalities.

Equality in (3.23) holds if and only if each vertex of $G$ is adjacent to the vertex with degree $\Delta$. Equality in (3.24) holds if and only if each vertex of $G$ is adjacent to the vertex with degree $\delta$. This implies that equality in (3.22) holds if and only if either each vertex of $G$ is adjacent to the vertex with degree $\Delta$, or each vertex of $G$ is adjacent to the vertex with degree $\delta$. □

From the inequalities (3.16) and (3.22) we have the following result.

COROLLARY 3.20. *Let $G$ be a graph of order $n \geqslant 2$ and size $m$ without isolated vertices. Then*

$$ABS(G) \leqslant \sqrt{\frac{\left(\min\left\{\frac{1}{\Delta}(M_2(G)+m\Delta^2), \frac{1}{\delta}(M_2(G)+m\delta^2)\right\} - 2m\right) H(G)}{2}}.$$

The modified Platt index, ${}^{m}Pl(G)$, is defined as

$${}^{m}Pl(G) = \sum_{i\sim j} \frac{1}{d_i+d_j-2}.$$

Let $L(G)$ be a line graph of graph $G$. Since

$${}^{m}Pl(G) = \sum_{i\sim j} \frac{1}{d_i+d_j-2} = \sum_{i=1}^{m} \frac{1}{d(e_i)} = ID(L(G)),$$

in essence, ${}^{m}Pl(G)$ is not a new topological index.

In the next theorem we establish a relationship between $ABS(G)$ and ${}^{m}Pl(G)$.

THEOREM 3.5. *Let $G$ be a connected graph of size $m$. Then we have*

$$ABS(G) \geqslant \frac{m^{3/2}}{\sqrt{m+2\,{}^{m}Pl(G)}}. \tag{3.25}$$

*Equality holds if and only if $G$ is regular or semiregular bipartite graph.*

*Proof.* By the arithmetic–geometric mean (AM-HM) inequality (see e.g. [36]), we have that

$$\sum_{i\sim j}\sqrt{\frac{d_i+d_j}{d_i+d_j-2}}\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\geqslant m^2\,,$$

that is

$$ABS(G)\sum_{i\sim j}\sqrt{\frac{d_i+d_j}{d_i+d_j-2}}\geqslant m^2\,. \tag{3.26}$$

Also, the following identity is valid

$$\sum_{i\sim j}\frac{d_i+d_j}{d_i+d_j-2}=\sum_{i\sim j}\left(1+\frac{2}{d_i+d_j-2}\right)=m+2^mPl(G)\,. \tag{3.27}$$

On the other hand, for $r=1$, $x_i:=\frac{d_i+d_j}{d_i+d_j-2}$, $a_i:=1$, with summation performed over all adjacent vertices $v_i$ and $v_j$ in $G$, the inequality (3.1) becomes

$$\sum_{i\sim j}\frac{d_i+d_j}{d_i+d_j-2}\geqslant\frac{\left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j}{d_i+d_j-2}}\right)^2}{\sum_{i\sim j}1}=\frac{\left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j}{d_i+d_j-2}}\right)^2}{m}\,. \tag{3.28}$$

From the above inequality and identity (3.27) we obtain

$$\sum_{i\sim j}\sqrt{\frac{d_i+d_j}{d_i+d_j-2}}\leqslant\sqrt{m(m+2^mPl(G)}\,.$$

From the above and inequality (3.26) we arrive at (3.25).

Equalities in (3.26) and (3.28) hold if and only if $\frac{d_i+d_j}{d_i+d_j-2}$ is constant for every two adjacent vertices $v_i$ and $v_j$ in $G$; that is, if and only if $d_i+d_j$ is constant for every two adjacent vertices $v_i$ and $v_j$ in $G$. This implies that equality in (3.25) holds if and only if $G$ is a regular or semiregular bipartite graph. □

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