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Sharp Upper Bounds for Augmented Zagreb Index of Graphs with Fixed Parameters

Fengwei Li[a,b,*] **, Qingfang Ye**[a] **, Hajo Broersma**[b] **, Ruixuan Ye**[c]

[a] *College of Basic Science, Ningbo University of Finance & Economics, Ningbo, Zhejiang 315175, P. R. China*

[b] *Faculty of EEMCS, University of Twente, P. O. Box 217, 7500 AE Enschede, The Netherlands*

[c] *School of Pharmacy, Wenzhou Medical University, Wenzhou, Zhejiang 325035, P. R. China*

fengwei.li@hotmail.com, fqy-y@163.com, h.j.broersma@utwente.nl, 1126253691@qq.com

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Abstract

The augmented Zagreb index (AZI index) is a degree-based molecular structure descriptor that can be used for modelling thermodynamic properties of organic chemical compounds. Motivated by its applicable potential, a series of investigations have been carried out in the past several years. In this paper, we present several sharp upper bounds on the AZI index of graphs with fixed parameters such as the independence number, edge-connectivity, chromatic number respectively, and characterize the corresponding extremal graphs.

1 Introduction

Topological indices (molecular structure descriptors) are numbers associated with chemical structures derived from their hydrogen–depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure–property correlations of organic compounds. Molecules and molecular compounds are often modeled by molecular graph. Topological indices of molecular graphs are one of the oldest and most widely used descriptors in QSPR/QSAR research [12, 16].

*The corresponding author.

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $N(u)$ denotes the set of its neighbors in G, and the degree of u is $d_u = |N(u)|$. The closed neighbourhood $N[u]$ of vertex u is given by $N[u] = N(u) \cup \{u\}$. A great variety of topological indices have been and are currently considered in theoretical chemistry [17, 21, 25, 26, 28, 29]. Among which the *augmented Zagreb index* (*AZI index* for short) is defined as

$$AZI(G) = \sum_{uv \in E(G)} f(d_u, d_v),$$

where $f(d_u, d_v) = (\frac{d_u d_v}{d_u + d_v - 2})^3$.

This graph invariant was firstly introduced by Furtula et al. [15] as a topological index, and it has been proven to be a valuable predictive index in the study of the heat of formation in octanes and heptanes (see [15]), whose prediction power is better than atom–bond connectivity index (please refer to [11, 14] for its research background). Moreover, Gutman and Tošovič [19] tested the correlation abilities of 20 vertex-degree-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers, and they found that the augmented Zagreb index yield the best results.

Furtula et al. [15] have studied extremal properties of AZI index of trees and chemical trees, they proved that among all trees the star has the minimum AZI index value. Huang et al. [20] and Wang et al. [30] gave sharp lower and upper bounds for various classes of connected graphs (e.g. trees, unicyclic graphs, bicyclic graphs, etc.) and characterized corresponding extremal graphs. Zhan et al. [31], determined the minimal and the second minimal AZI indices of the n-vertex unicyclic graphs. Additionally, they obtained the n-vertex bicyclic graphs in which the AZI index attains its minimal value. Cruz et al. [9] gave the maximal AZI index of trees with at most three branching vertices. Ali et al. [3] gave the maximum AZI index of graphs with given vertex connectivity and matching number.

The bounds of a descriptor are important information of a molecular graph in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters and many results concerning this topic can be found in [3, 4, 6–8, 10, 13, 18, 22–24, 27, 32]. So, we pay our attention to upper bounds for AZI index of graphs with some given parameter.

This paper is organized as follows. We first give some basic properties of AZI index in Section 2. In Section 3, we present sharp upper bounds for AZI index of connected graphs with given independence number, and determine graphs for which these bounds are best possible. In section 4, sharp upper bounds on the AZI index for connected graphs with given chromatic number are obtained, and the corresponding extremal graphs are characterized. In section 5, we determine sharp upper bounds for the AZI index for connected graphs with given edge-connectivity, and characterize the corresponding extremal graphs.

2 Preliminaries

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

For any $S \subset V(G)$, we use $G[S]$ to denote the *induced graph* of graph G. A set $S \subseteq E(G)$ is an *edge–cut set* of G, if $G - S$ is disconnected. The number of edges in a smallest edge–cut set of G is called the *edge connectivity* of a graph G and denoted by $\lambda(G)$. The *vertex connectivity* (commonly referred to as *connectivity*) $\kappa(G)$ of a graph G is the minimum number of vertices whose removal gives rise to a disconnected or trivial graph. Let K_n and $K_{n_1,n_2,\ldots,n_t}$ denote the complete graph of order n, the complete t-partite graph with $n_1, n_2, \ldots, n_t$ vertices in its t partite sets, respectively. $G+e$ denote the graph obtained from G by inserting an edge $e \notin E(G)$.

Now, we introduce the concept of the *complement* of a graph.

Definition 2.1 [5] *The complement of a graph G is a graph $\overline{G}$ on the same vertices such that two vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G.*

Definition 2.2 [5] *For two vertex-disjoint graphs G and H, the join of G and H, denoted by $G + H$, is a graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{xy|x \in V(G), y \in V(H)\}$.*

Lemma 2.3 [?] *Let G be a connected graph of order n $(n \geq 3)$, and $G \ncong K_n$. Then*

$$AZI(G) < AZI(G + e),$$

where $e \notin E(G)$.

Lemma 2.4 [?] *Let G be a connected graph of order n $(n \geq 3)$. Then*

$$AZI(G) \leq \frac{n(n-1)^7}{16(n-2)^3},$$

with equality holding if and only if $G \cong K_n$.

Lemma 2.5 [?] *Let G be a connected t-partite graph with $n_1, n_2, \ldots, n_t$ vertices in its t partite sets respectively, where $n = \sum_{i=1}^{t} n_i \geq 3$. Then*

$$AZI(G) \leq \sum_{1 \leq i < j \leq t} \frac{n_i n_j (n - n_i)^3 (n - n_j)^3}{(2n - n_i - n_j - 2)^3},$$

with equality holding if and only if $G \cong K_{n_1, n_2, \ldots, n_t}$.

Lemma 2.6 *Let*

$$f(x, y) = \left(\frac{xy}{x + y - 2}\right)^3$$

with positive integers x, y such that $x + y > 2$, then $f(x, y)$ is increasing with respect to x if $y \geq 2$; $f(x, y)$ is increasing with respect to y if $x \geq 2$.

Proof: If $y \geq 2$ is fixed, then it is easily seen that

$$\frac{\partial f(x, y)}{\partial x} = 3 \left(\frac{xy}{x + y - 2}\right)^2 \frac{y(y - 2)}{(x + y - 2)^2} \geq 0,$$

and thus $f(x, y)$ is increasing for x. By the symmetry of $f(x, y)$, we can prove $f(x, y)$ is increasing with respect to y if $x \geq 2$.

This completes the proof. ■

3 Sharp upper bounds for *AZI* index of graphs with given independence number

Let us denote by $\Gamma_{n,\alpha}$ the collection of all connected graphs with $n \geq 3$ vertices and independence number α. In this section, we will present upper bounds on the AZI index among all graphs in the collection $\Gamma_{n,\alpha}$.

Firstly, we introduce the concept of the *independence number* of a graph.

Definition 3.1 [5] *A subset $S \subset V(G)$ is called an independent set of G if no two vertices of S are adjacent in G. An independent set S is called a maximum independent set if G has no independent set S' with $|S'| > |S|$. The independence number of G, $\alpha(G)$, is the number of vertices in a maximum independent set of G.*

Theorem 3.2 *Let $G \in \Gamma_{n,\alpha}$. Then*

$$AZI(G) \leq \alpha(n - \alpha) \left(\frac{(n - \alpha)(n - 1)}{2n - \alpha - 3}\right)^3 + \frac{(n - \alpha)(n - \alpha - 1)}{16} \left(\frac{(n - 1)^2}{n - 2}\right)^3,$$

the equality holds if and only if $G \cong \overline{K_\alpha} + K_{n-\alpha}$.

Proof: Suppose that G^* is the graph with the maximum AZI index among all graphs in the collection $\Gamma_{n,\alpha}$. Let S be a maximum independent set in G^* satisfies that $|S| = \alpha$. By Lemmas 2.3, 2.4, we know that adding edges to a graph will increase its AZI index. Then, each vertex in S is adjacent to every vertex in $G^* - S$, and the induced graph $G[G^* - S]$ is the complete graph $K_{n-\alpha}$. Hence, we know that $G^* \cong \overline{K_\alpha} + K_{n-\alpha}$. So, we have

$$AZI(G^*) = \alpha(n-\alpha)f(n-1, n-\alpha) + \frac{(n-\alpha)(n-\alpha-1)}{2}f(n-1, n-1)$$
$$= \alpha(n-\alpha)\left(\frac{(n-\alpha)(n-1)}{2n-\alpha-3}\right)^3 + \frac{(n-\alpha)(n-\alpha-1)}{2}\left(\frac{(n-1)(n-1)}{2n-4}\right)^3.$$

This completes the proof. ■

4 Sharp upper bounds for AZI index of graphs with given chromatic number

Let us denote by $\Omega_{n,\chi}$ the collection of all connected graphs with $n \geq 3$ vertices and chromatic number $\chi(G) \geq 1$. In this section we consider the maximum AZI index of graphs over the set $\Omega_{n,\chi}$.

A (vertex) colouring of a graph G is a mapping $c : V(G) \to S$. The elements of S are called colours; the vertices of one colour form a colour class. If $|S| = k$, we say that c is a *k-colouring* (often we use $S = \{1, 2, \cdots, k\}$). A colouring is *proper* if adjacent vertices have different colours. A graph is *k-colourable* if it has a proper k-colouring. The *chromatic number* $\chi(G)$ is the least k such that G is k–colourable. A *p-clique* in G is a complete subgraph of G on p vertices.

Let $T_{n,l}$ denote a complete l-partite graph of order n with $|n_i - n_j| \leq 1$, where t_i, $i = 1, 2, \cdots, l$ is the number of vertices in the ith partition set of $T_{n,l}$.

The next inequality, known as Cauchy–Schwarz inequality [2], plays an important role in the next section.

Lemma 4.1 (Cauchy–Schwarz inequality) [2] *For all vectors $\overrightarrow{x}$ and $\overrightarrow{y}$ of a real inner product space,*

$$|\langle\overrightarrow{x}, \overrightarrow{y}\rangle| \leq \|\overrightarrow{x}\| \cdot \|\overrightarrow{y}\|$$

where $\langle\overrightarrow{x}, \overrightarrow{y}\rangle$ is the inner product. Equality hold if and only if the vectors $\overrightarrow{x}$ and $\overrightarrow{y}$ are linearly dependent.

Firstly, we give the sharp upper bound for AZI index of a graph with $\chi = 2$.

Theorem 4.2 *Let $G \in \Omega_{n,2}$ be a connected graph of order n with chromatic number $\chi = 2$. Then*

(i) *If n is even, then $AZI(G) \leq \frac{n^2}{4}\left(\frac{n^2}{4(n-2)}\right)^3$ if and only if $G \cong T_{n,2}$;*

(ii) *If n is odd, then $AZI(G) \leq \frac{n^2-1}{4}\left(\frac{n^2-1}{4(n-2)}\right)^3$ if and only if $G \cong T_{n,2}$.*

Proof: Assume that G^* is the graph with the maximum AZI index among all graphs of order n with chromatic number $\chi = 2$. It is obvious that the vertex set $V(G^*)$ can be divided into two independent sets V_1 and V_2. By Lemma 2.3, we know that adding edges to a graph will increase its AZI index. Then, each vertex in V_1 is adjacent to every vertex in V_2. Denote $|V_1| = n_1$, $|V_2| = n_2$, respectively. Consequently, we know that $G^* \cong \overline{K_{n_1}} + \overline{K_{n_2}}$. Assuming, without loss of generality, that $n_2 \geq n_1 \geq 1$, we claim that $|n_2 - n_1| \leq 1$ (note that in this case $G \cong T_{n,2}$).

Otherwise, if $n_2 \geq n_1 + 2$, let graph $G' \cong \overline{K_{n_1+1}} + \overline{K_{n_2-1}}$. Then

$$\begin{aligned} AZI(G') - AZI(G^*) &= (n_1+1)(n_2-1)f(n_1+1, n_2-1) - n_1n_2f(n_1,n_2) \\ &= \frac{((n_1+1)(n_2-1))^4}{(2n-n_1-n_2-2)^3} - \frac{(n_1n_2)^4}{(2n-n_1-n_2-2)^3} \\ &= \frac{[(n_1+1)^2(n_2-1)^2 - n_1^2n_2^2][(n_1+1)^2(n_2-1)^2 + n_1^2n_2^2]}{(2n-n_1-n_2-2)^3}. \end{aligned}$$

Combining the fact that $(n_1+1)(n_2-1) - n_1n_2 = n_2 - n_1 - 1 > 0$, we have

$$AZI(G') - AZI(G^*) > 0,$$

a contradiction. So, $G \cong T_{n,2}$.

This completes the proof. ■

In the following theorem, we give the maximum AZI index among all graphs of order n with chromatic number $\chi \geq 3$ such that the order n is divisible by χ.

Theorem 4.3 *Let $G \in \Omega_{n,\chi}$, the chromatic number $\chi \geq 3$ and χ divides n. Then*

$$AZI(G) \leq \frac{n^8(\chi-1)^7}{16\chi^4(n\chi-n-\chi)^3},$$

the equality holds if and only if $G \cong T_{n,\chi}$;

Proof: Assume that G^* is the graph with the maximum AZI index among all graphs of order n with chromatic number $\chi \geq 3$ and χ divides n. Let c be a proper colouring of G^* with colours $1, 2, \cdots, \chi$. For $1 \leq i \leq \chi$, let S_i be the independent set of vertices coloured i and let $n_i = |S_i|$. From Lemma 2.3 it is apparent that the AZI index gets increased if one adds edges between all pairs of nonadjacent vertices in the part of G^* induced by nonpendant vertices. Therefore, in this case the graph G^* is necessarily isomorphic to the connected χ-partite graph $K_{n_1,n_2,\dots,n_\chi}$ with $n_1, n_2, \dots, n_\chi$ vertices in its χ partite sets respectively, where $n = \sum_{i=1}^{\chi} n_i \geq 3$. Furthermore, by Lemma 2.5, we get

$$\begin{aligned} AZI(G) &\leq AZI(K_{n_1,n_2,\dots,n_\chi}) \\ &= \sum_{1\leq i<j\leq \chi} \frac{n_i n_j (n-n_i)^3 (n-n_j)^3}{(2n-n_i-n_j-2)^3} \\ &= \sum_{1\leq i<j\leq \chi} \frac{n_i n_j}{(2n-n_i-n_j-2)^3} (n-n_i)^3 (n-n_j)^3. \end{aligned} \tag{4.1}$$

Let

$$x_{ij} = \frac{n_i n_j}{(2n-n_i-n_j-2)^3}, \qquad y_{ij} = (n-n_i)^3 (n-n_j)^3$$

Note that the right-hand side of equation (4.1) is equivalent to the inner product $\langle \overrightarrow{x}, \overrightarrow{y} \rangle$ of vectors $\overrightarrow{x} := (x_{ij})_{i<j}$ and $\overrightarrow{y} := (y_{ij})_{i<j}$ of dimension $\binom{\chi}{2}$. Thus, by the Cauchy–Schwarz inequality,

$$AZI(G) \leq |\langle \overrightarrow{x}, \overrightarrow{y} \rangle| \leq \|\overrightarrow{x}\| \cdot \|\overrightarrow{y}\|, \tag{4.2}$$

and the equality $|\langle \overrightarrow{x}, \overrightarrow{y} \rangle| = \|\overrightarrow{x}\| \cdot \|\overrightarrow{y}\|$ in (4.2) holds if and only if $\overrightarrow{x}$ and $\overrightarrow{y}$ are linearly dependent, that is, if and only if $\overrightarrow{x} = \mu \overrightarrow{y}$ holds for some scalar $\mu \neq 0$. Hence, if and only if

$$\mu = \frac{x_{ij}}{y_{ij}} = \frac{n_i n_j}{(2n-n_i-n_j-2)^3} \cdot \frac{1}{(n-n_i)^3 (n-n_j)^3}$$

for each pair of indices $i < j$.

So, for any i, j, k such that $1 \leq i < j < k \leq \chi$, it follows from $\mu = \frac{x_{ij}}{y_{ij}} = \frac{x_{ik}}{y_{ik}}$ that

$$n_j (n-n_k)^3 (2n-n_i-n_k-2)^3 = n_k (n-n_j)^3 (2n-n_i-n_j-2)^3. \tag{4.3}$$

We claim that $n_j = n_k$ must hold. If not, without loss of generality, we assume that $n_j > n_k$, we have $n - n_k > n - n_j$ and

$$2n - n_i - n_k - 2 > 2n - n_i - n_j - 2.$$

Hence, the left-hand side of (4.3) is strictly greater than the right-hand side of it, a contradiction.

Since i, j, k were chosen arbitrarily, it follows that $n_1 = n_2 = \ldots = n_\chi$. Combining the fact that $n = \sum_{i=1}^{\chi} n_i$, we know that $n_i = \frac{n}{\chi}$ for all $i = 1, 2, \cdots, \chi$. In this case, we compute $\|\overrightarrow{x}\|$, $\|\overrightarrow{y}\|$ at $n_i = \frac{n}{\chi}$.

$$\|\overrightarrow{y}\| = \sqrt{\sum_{1\le i<j\le \chi} (n-n_i)^6(n-n_j)^6} = \sqrt{\sum_{1\le i<j\le \chi} (n-\frac{n}{\chi})^{12}}$$

$$= \sqrt{\binom{\chi}{2}\left(n-\frac{n}{\chi}\right)^{12}} = \frac{n^6(\chi-1)^6}{\chi^6}\sqrt{\frac{\chi(\chi-1)}{2}}.$$

$$\|\overrightarrow{x}\| = \sqrt{\sum_{1\le i<j\le \chi}\left(\frac{n_i n_j}{(2n-n_i-n_j-2)^3}\right)^2} = \sqrt{\sum_{1\le i\le j\le \chi}\frac{(\frac{n}{\chi})^4}{(2n-\frac{2n}{\chi}-2)^6}}$$

$$= \sqrt{\binom{\chi}{2}\frac{(\frac{n}{\chi})^4}{(2n-\frac{2n}{\chi}-2)^6}} = \frac{n^2\chi}{8(n\chi-n-\chi)^3}\sqrt{\frac{\chi(\chi-1)}{2}}.$$

Thus,

$$AZI(G) \le \|\overrightarrow{x}\|\cdot\|\overrightarrow{y}\| = \frac{n^8(\chi-1)^7}{16\chi^4(n\chi-n-\chi)^3},$$

as desired.

This completes the proof. ■

Next, we fix our attention on finding upper bound for AZI index of graphs with n vertices and any arbitrary chromatic number $\chi \ge 3$. To proceed, we need some known results.

Lemma 4.4 [20] *Let G be a connected graph with $m \ge 2$ edges and maximum degree $\Delta \ge 2$. Then*

$$AZI(G) \le \frac{m\Delta^6}{8(\Delta-1)^3}$$

with equality holding if and only if G is a path or a Δ-regular graph.

Lemma 4.5 (Turán's theorem) [1] *Let G be a graph of order n, size m, without p-clique, $p \ge 2$. Then*

$$m \le (1-\frac{1}{p-1})\frac{n^2}{2}.$$

Theorem 4.6 *Let G be a connected graph of order n with chromatic number $\chi \ge 3$, and the maximum degree $\Delta \ge 2$. Then*

$$AZI(G) \le \frac{n^2\Delta^6(\chi-1)}{16(\Delta-1)^3\chi}.$$

Proof: Using Lemma 4.5 on the maximum size of a graph with chromatic number $\chi \geq 3$, we get

$$m \leq \frac{n^2(\chi - 1)}{2\chi}.$$

Combing the above inequality and Lemma 4.4, we deduce

$$AZI(G) \leq \frac{n^2\Delta^6(\chi - 1)}{16(\Delta - 1)^3\chi}.$$

This completes the proof. ■

5 Sharp upper bounds for AZI index of graphs with given edge-connectivity

For convenience, we use $\Lambda_{n,\lambda}$ to denote the set of connected graphs of order $n \geq 3$ and edge-connectivity $\lambda \geq 1$. In this section, we determine the maximal values of AZI indices of graphs over the collection of graphs $\Lambda_{n,\lambda}$.

For positive integers $n(n \geq 3)$ and $k(k \geq 1)$, let $K_n(k)$ be the graph on n vertices obtained by attaching one vertex to exactly k vertices of K_{n-1}. It is easy to see that $K_n(k)$ has edge-connectivity k. An illustration of $K_7(3)$ is depicted in Figure 5.1.

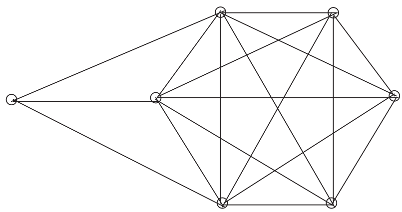

Figure 5.1. Graph $K_7(3)$ with edge-connectivity 3.

Firstly, we give a lemma which will be useful in our main result.

Lemma 5.1 *Let*

$$l(n,x) = \lambda f(x, n-1) + \frac{x(x-1)}{2} f(n-1, n-1) + x(n-x-1) f(n-1, n-2) + \frac{(n-x-1)(n-x-2)}{2} f(n-2, n-2)$$

be a function with positive integers $n(n \geq 6)$ and x such that $2 \leq x \leq \frac{n}{2} - 1$. Then

$$l(n,x) \geq l(n,2) = 16 + \frac{(n-1)^6}{2(n-2)^3} + \frac{2(n-3)(n-1)^3(n-2)^3}{(2n-5)^3} + \frac{(n-4)(n-2)^6}{16(n-3)^2}.$$

Proof: For fixed $n (n \geq 6)$, it is easily seen that

$$\frac{\partial l(n,x)}{\partial x} = \frac{x^3(4n+x-12)(n-1)^3}{(n+x-3)^4} + \frac{(2x-1)(n-1)^6}{16(n-2)^3}$$

$$+\frac{(n-2x-1)(n-1)^3(n-2)^3}{(2n-5)^3} + \frac{(3+2x-2n)(n-2)^6}{16(n-3)^3},$$

and

$$\frac{\partial^2 l(n,x)}{\partial x^2} = \frac{12x^2(n-3)^2(n-1)^3}{(n+x-3)^5}$$

$$+\frac{1}{8(n-2)^3(n-3)^3(2n-5)^3}((n-1)^6(n-3)^3(2n-5)^3$$

$$-16(n-1)^3(n-2)^6(n-3)^3 + (n-2)^9(2n-5)^3)$$

$$> \frac{1}{8(n-2)^3(n-3)^3(2n-5)^3}((n-1)^6(n-3)^3(2n-5)^3$$

$$-16(n-1)^3(n-2)^6(n-3)^3 + (n-2)^9(2n-5)^3) > 0.$$

Thus $\frac{\partial l(n,x)}{\partial x}$ is increasing for x, i.e.,

$$\frac{\partial l(n,x)}{\partial x} \geq \frac{\partial l(n,x)}{\partial x}|_{x=2} = \frac{16(2n-5)}{n-1} + \frac{3(n-1)^6}{16(n-2)^3}$$

$$+\frac{(n-5)(n-1)^3(n-2)^3}{(2n-5)^3} - \frac{(2n-7)(n-2)^6}{16(n-3)^3}$$

$$= \frac{1}{16(n-1)(n-2)^3(n-3)^3(2n-5)^3}(2^8(2n-5)^4(n-2)^3(n-3)^3+$$

$$3(n-1)^7(n-3)^3(2n-5)^3 + 16(n-5)(n-1)^4(n-2)^6(n-3)^3$$

$$-(n-1)(n-2)^9(2n-5)^3(2n-7)) > 0,$$

and thus $l(n,x)$ is increasing for x. So, we have

$$l(n,x) \geq l(n,2) = 16 + \frac{(n-1)^6}{8(n-2)^3} + \frac{2(n-3)(n-1)^3(n-2)^3}{(2n-5)^3}$$

$$+\frac{(n-4)(n-2)^6}{16(n-3)^2}.$$

This completes the proof. ∎

Theorem 5.2 *Let $G \in \Lambda_{n,\lambda}$. Then*

$$AZI(G) \leq \lambda^4 \left(\frac{n-1}{n+\lambda-3}\right)^3 + \lambda(n-\lambda-1)\left(\frac{(n-1)(n-2)}{2n-5}\right)^3$$

$$+\frac{\lambda(\lambda-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \frac{(n-\lambda-1)(n-\lambda-2)}{16}\left(\frac{(n-2)^2}{n-3}\right)^3,$$

the equality holds if and only if $G \cong K_n(\lambda)$.

Proof: Many thanks to the reviewer of this paper pointed out that this bound about the edge-connectivity is a special case of a more general result of Theorem 3.6 and Corollary 3.7 in [7]. We note the authors in [7] obtained the maximum AZI index of graphs with given $\lambda(G)$ via the well-known inequality that $\kappa(G) \leq \lambda(G)$ for any connected graph G. And we give a different way to get the maximum AZI index of graphs with given edge-connectivity $\lambda(G) \geq 1$, so, we here would like to retain the whole proof.

Assume that G^* is the graph with the maximum AZI index over the set $\Lambda_{n,\lambda}$. We distinguish two cases:

Case 1 If $\lambda = 1$, First, suppose G^* contains a vertex of degree 1, say v. Let $G' := G^* - \{v\}$. Then by Lemma 2.3 and by the assumption of G^*, we see that G' is the complete graph on $n-1$ vertices; for otherwise, there must exist two nonadjacent vertices x, y in G' such that the graph $G^* + \{xy\}$ has edge-connectivity 1 and $AZI(G^* + \{xy\}) > AZI(G^*)$, a contradiction. This implies that $G^* \cong K_n(1)$, and hence the assertion holds.

So we may assume that every vertex in G^* has degree at least 2. Let e be a cut-edge in G^*. Then $G^* - \{e\}$ has exactly two components, say G_1 and G_2. By Lemma 2.3 and by the assumption of G^*, we have both G_1 and G_2 as complete graphs. Let n_i be the number of vertices in G_i (for $i = 1, 2$), then $n = n_1 + n_2$. Without loss of generality, we may assume $n_2 \geq n_1$. Since G^* has minimum degree at least 2, we have $n_2 \geq n_1 \geq 3$ and hence $n \geq 6$. We now show that the maximum AZI index cannot be achieved in this case.

On one hand, by Lemma 2.6 and combining the fact that $n_2 \geq n_1 \geq 3$, we have

$$\begin{aligned} AZI(G^*) &= (n_1-1)f(n_1, n_1-1) + \frac{(n_1-1)(n_1-2)}{2} f(n_1-1, n_1-1) \\ &\quad + (n_2-1)f(n_2, n_2-1) + \frac{(n_2-1)(n_2-2)}{2} f(n_2-1, n_2-1) + f(n_1, n_2) \\ &\leq \frac{n_1(n_1-1)}{2} f(n_1, n_1-1) + \frac{n_2(n_2-1)}{2} f(n_2, n_2-1) + f(n_1, n_2) \\ &\leq \frac{n_2(n_2-1)}{2} f(n_2, n_2-1) + \frac{n_2(n_2-1)}{2} f(n_2, n_2-1) + f(n_1, n_2) \\ &= n_2(n_2-1)\left(\frac{n_2(n_2-1)}{2n_2-3}\right)^3 + f(n_1, n_2) \\ &\leq \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3} + \frac{n_2^6}{(n-2)^3}. \end{aligned}$$

On the other hand, from Lemma 2.6, we have

$$\begin{aligned}AZI(K_n(1)) &= f(1,n-1)+(n-2)f(n-1,n-2)+\frac{(n-2)(n-3)}{2}f(n-2,n-2)\\ &\geq f(1,n-1)+(n-2)f(n-2,n-2)+\frac{(n-2)(n-3)}{2}f(n-2,n-2)\\ &= f(1,n-1)+\frac{(n-1)(n-2)}{2}f(n-2,n-2)\\ &= \left(\frac{n-1}{n-2}\right)^3+\frac{(n-1)(n-2)^7}{16(n-3)^3}.\end{aligned}$$

In the next, we will prove that the inequality

$$\left(\frac{n-1}{n-2}\right)^3+\frac{(n-1)(n-2)^7}{16(n-3)^3} > \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3}+\frac{n_2^6}{(n-2)^3},$$

holds for $3 \leq n_2 \leq \frac{n}{2}$ and $n \geq 6$.

Let

$$h(n,n_2) = \left(\frac{n-1}{n-2}\right)^3+\frac{(n-1)(n-2)^7}{16(n-3)^3}-\frac{n_2^4(n_2-1)^4}{(2n_2-3)^3}-\frac{n_2^6}{(n-2)^3}$$

with $3 \leq n_2 \leq \frac{n}{2}$. Since

$$\frac{\partial h(n,n_2)}{\partial n_2} = -\frac{2n_2^3(n_2-1)^3(5n_2^3-13n_2+6)}{(2n_2-3)^4}-\frac{6n_2^5}{(n-2)^3} < 0,$$

we know that $h(n,n_2)$ is decreasing with respect to n_2 for $n \geq 6$ and $3 \leq n_2 \leq \frac{n}{2}$. We now discuss two subcases to finish the proof.

Subcase 1.1 If $n(n \geq 6)$ is even, then

$$h(n,n_2) \geq h(n,\frac{n}{2}) = \frac{1}{2^8(n-2)^3(n-3)^3}(2^8(n-1)^3(n-3)^3+$$

$$16(n-1)(n-2)^{10}-4n^6(n-3)^3-n^4(n-2)^7) > 0.$$

As a consequence we have

$$AZI(K_n(1))-AZI(G^*) \geq h(n,n_2) > 0,$$

a contradiction.

Subcase 1.2 If $n(n \geq 6)$ is odd, then

$$h(n,n_2) \geq h(n,\frac{n-1}{2}) = \frac{1}{2^8(n-2)^3(n-3)^3(n-4)^3}(2^8(n-1)^3(n-3)^3$$

$$(n-4)^3+16(n-1)(n-2)^{10}(n-3)^3(n-4)^3-(n-1)^3(n-3)^7$$

$$-4(n-1)^6(n-3)^3(n-4)^3) > 0.$$

So, we have

$$AZI(K_n(1)) - AZI(G^*) \geq h(n, n_2) > 0,$$

a contradiction.

From above discussions, we know that $G^* \cong K_n(1)$.

Case 2 If $\lambda \geq 2$, There exists an edge-cut set $S = \{e_1, e_2, \cdots, n_\lambda\}$ in G^*. Let G_1, G_2 be the two components in $G^* - S$. By Lemmas 2.3, 2.4, we know that G_1 and G_1 are both complete graphs. Let $n_i = |V(G_i)|$, $i = 1, 2$, then $n_1 + n_2 = n$.

Without loss of generality, let $n_2 \geq n_1$. If $n_1 = 1$, then $G^* \cong K_n$. Otherwise, $n_2 \geq n_1 \geq \lambda$ since G^* has minimum degree at least λ.

First, suppose G^* contains a vertex of degree λ, say v. Let $N(v) = \{v_1, v_2, \cdots, v_\lambda\}$. Denote $A = V(G^*) - N[v]$. If the induced subgraph $G[N(v) \cup A]$ is the complete graph K_{n-1}, then $G \cong K_n(\lambda)$ as claimed. Otherwise, there must exist two nonadjacent vertices $x, y \in V(G^*)$ such that $xy \in E(\overline{G[N(v) \cup A]})$ and the graph $G^* + xy$ has edge–connectivity λ, by Lemma 2.3, we know that $AZI(G^* + xy) > AZI(G^*)$, a contradiction.

So we may assume that every vertex in G^* has degree at least $\lambda + 1$. Then $n_2 \geq n_1 \geq \lambda + 1 \geq 3$. We now prove that maximum AZI index cannot be obtained in this case.

On one hand, by Lemma 2.6, we have

$$\begin{aligned}
AZI(G^*) &< \frac{n_1(n_1-1)}{2} f(n_1 - 1, n_1 - 1) + \frac{n_2(n_2-1)}{2} f(n_2 - 1, n_2 - 1) \\
&\qquad + \lambda f(n_1, n_2) \\
&\leq \frac{n_1(n_1-1)}{2} f(n_1, n_1 - 1) + \frac{n_2(n_2-1)}{2} f(n_2, n_2 - 1) + \lambda f(n_1, n_2) \\
&\leq \frac{n_2(n_2-1)}{2} f(n_2, n_2 - 1) + \frac{n_2(n_2-1)}{2} f(n_2, n_2 - 1) + \lambda f(n_1, n_2) \\
&= n_2(n_2-1) \left(\frac{n_2(n_2-1)}{2n_2 - 3} \right)^3 + \lambda f(n_1, n_2) \\
&\leq \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3} + \frac{\lambda n_2^6}{(n-2)^3}.
\end{aligned}$$

On the other hand, by Lemma 5.1 we have

$$AZI(K_n(\lambda)) = \lambda f(\lambda, n-1) + \frac{\lambda(\lambda-1)}{2} f(n-1, n-1)$$

$$+\lambda(n-\lambda-1) f(n-1, n-2) + \frac{(n-\lambda-1)(n-\lambda-2)}{2} f(n-2, n-2)$$

$$= l(n,\lambda) \geq l(n,2)$$
$$= 16 + \frac{(n-1)^6}{8(n-2)^3} + \frac{2(n-3)(n-1)^3(n-2)^3}{(2n-5)^3} + \frac{(n-4)(n-2)^6}{16(n-3)^2}.$$

By the assumption of G^*, to derive a contradiction, it suffices to show the inequality

$$l(n,2) > \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3} + \frac{\lambda n_2^6}{(n-2)^3} \tag{5.1}$$

holds for $3 \leq \lambda + 1 \leq n_2 \leq \frac{n}{2}$, $2 \leq \lambda \leq \frac{n}{2} - 1$.

Let

$$g(n,\lambda,n_2) = \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3} + \frac{\lambda n_2^6}{(n-2)^3}$$

with $2 \leq \lambda \leq \frac{n}{2} - 1$. Since

$$\frac{\partial g(n,\lambda,n_2)}{\partial \lambda} = \frac{n_2^6}{(n-2)^3} > 0,$$

we know that $g(n,\lambda,n_2)$ is increasing with respect to λ for $n \geq 6$ and $2 \leq \lambda \leq \frac{n}{2} - 1$.

We distinguish two subcases.

Subcase 2.1 If $n(n \geq 6)$ is even,

$$g(n,\lambda,n_2) \leq g(n,\frac{n}{2}-1,n_2) = \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3} + \frac{n_2^6}{2(n-2)^2}.$$

Since

$$\frac{\partial g(n,\frac{n}{2}-1,n_2)}{\partial n_2} = \frac{2n_2^3(n_2-1)^3(5n_2^2-13n_2+6)}{(2n_2-3)^4} + \frac{6n_2^5}{2(n-2)^2} > 0,$$

we know that $g(n,\frac{n}{2}-1,n_2)$ is increasing with respect to n_2 for $3 \leq \lambda+1 \leq n_2 \leq \frac{n}{2}$ and $n \geq 6$. It means that

$$g(n,\frac{n}{2}-1,n_2) \leq g(n,\frac{n}{2}-1,\frac{n}{2}) = \frac{n^4(n-2)^4}{2^8(n-3)^3} + \frac{n^6}{2^7(n-2)^2}.$$

It is easy to check that

$$\begin{aligned} l(n,2) - g(n,\frac{n}{2}-1,\frac{n}{2}) &= \frac{1}{2^8(n-2)^2(n-3)^3(2n-5)^3} \\ &(2^{12}(n-2)^2(n-3)^3(2n-5)^3 + 2^5(n-1)^6(n-3)^3(2n-5)^3 \\ &+2^9(n-3)^4(n-1)^3(n-2)^6 + 16(n-4)(n-3)(n-2)^9(2n-5)^3 \\ &-n^4(n-2)^7(2n-5)^3 - 2n^6(n-2)(n-3)^3(2n-5)^3) > 0. \end{aligned}$$

The above inequality implies that

$$l(n,\lambda) \geq l(n,2) > g(n,\frac{n}{2}-1,\frac{n}{2}) \geq g(n,\lambda,n_2).$$

Hence, we have

$$AZI(K_n(\lambda)) - AZI(G^*) \geq l(n,\lambda) - g(n,\lambda,n_2) > 0,$$

a contradiction.

Subcase 2.2 If $n(n \geq 6)$ is odd, as the same in the case 2.1, we know that $g(n, \lambda, n_2)$ is increasing with respect to λ for $n \geq 6$ and $2 \leq \lambda \leq \frac{n-1}{2} - 1$, i.e.,

$$g(n, \lambda, n_2) \leq g(n, \frac{n-1}{2} - 1, n_2) = \frac{n_2^4(n_2-1)^4}{(2n_2-3)^3} + \frac{(n-3)n_2^6}{2(n-2)^3}.$$

It is shown that $g(n, \frac{n-1}{2} - 1, n_2)$ is increasing with respect to n_2 for $3 \leq \lambda + 1 \leq n_2 \leq \frac{n-1}{2}$ and $n \geq 6$ from the fact that

$$\frac{\partial g(n, \frac{n-1}{2} - 1, n_2)}{\partial n_2} = \frac{2n_2^3(n_2-1)^3(5n_2^2 - 13n_2 + 6)}{(2n_2-3)^4} + \frac{6(n-3)n_2^5}{2(n-2)^2} > 0,$$

i.e.,

$$g(n, \frac{n-1}{2} - 1, n_2) \leq g(n, \frac{n-1}{2} - 1, \frac{n-1}{2}) = \frac{(n-1)^4(n-3)^4}{2^8(n-4)^3} + \frac{(n-3)(n-1)^6}{2^7(n-2)^2}.$$

It is easy to check that

$$l(n, 2) - g(n, \frac{n-1}{2} - 1, \frac{n-1}{2}) = \frac{1}{2^8(n-2)^3(n-3)^3(n-4)^3(2n-5)^3}$$

$$((n-4)^3(2^{12}(n-2)^2(n-3)^3(2n-5)^3 + 2^5(n-1)^6(n-3)^3(2n-5)^3$$

$$+2^9(n-3)^4(n-1)^3(n-2)^6 + 16(n-4)(n-3)(n-2)^9(2n-5)^3)$$

$$-(n-1)^4(n-2)^3(n-3)^7(2n-5)^3 - 2(n-1)^6(n-2)(n-3)^4(n-4)^3(2n-5)^3) > 0.$$

As a consequence we have

$$l(n, \lambda) \geq l(n, 2) > g(n, \frac{n-1}{2} - 1, \frac{n-1}{2}) \geq g(n, \lambda, n_2),$$

and hence

$$AZI(K_n(\lambda)) - AZI(G^*) \geq l(n, \lambda) - g(n, \lambda, n_2) > 0,$$

a contradiction.

From above two cases, we know that $G^* \cong K_n(\lambda)$, $\lambda \geq 1$.

This completes the proof. ■

It is well known that the class of k–vertex–connected graphs is a subclass of the class of k–edge–connected graphs where $k \geq 1$, and it is obvious that $K_n(k)$ is a k–vertex–connected graph, it can be concluded from Theorem 5.2 that a graph that maximizes the AZI index among all k–edge–connected graphs also maximizes the AZI index among all k–vertex–connected graphs.

Corollary 5.3 *Let G be a graph with the maximum AZI index among all graphs with n vertices and vertex–connectivity $\kappa \geq 1$. Then, $G \cong K_n(\kappa)$.*

6 Conclusion

In this paper, we give the sharp upper bounds for the AZI indices of graphs in terms of their fixed parameters such as independence number, chromatic number and edge-connectivity. As future work, it would be interesting to find the sharp upper bounds for AZI index among all graphs of order n with chromatic number $\chi \geq 3$ where n is not divisible by χ.

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