Solution of an Open Problem Concerning the Augmented Zagreb Index and Chromatic Number of Graphs

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Abstract

Let G be a graph containing no component isomorphic to the path graph of order 2. Denote by d_w the degree of a vertex w in G. The augmented Zagreb index (AZI) of G is the sum of the quantities $(d_u d_v/(d_u + d_v - 2))^3$ over all edges uv of G. Denote by $\mathcal{G}(n, \chi)$ the class of all connected graphs of a fixed order n and with a fixed chromatic number χ, where $n \geq 5$ and $3 \leq \chi \leq n-1$. The problem of finding graph(s) attaining the maximum AZI in the class $\mathcal{G}(n, \chi)$ has been solved recently in [F. Li, Q. Ye, H. Broersma, R. Ye, MATCH Commun. Math. Comput. Chem. 85 (2021) 257–274] for the case when n is a multiple of χ. The present paper gives the solution of the aforementioned problem not only for the remaining case (that is, when n is not a multiple of χ) but also for the case considered in the aforesaid paper.

1 Introduction and statement of the main result

The (chemical) graph theoretical terminology and notation that are used in this paper but not defined here, can be found in some relevant well-known books, like [3, 4, 17].

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Graphs are being used to model chemical structures by replacing atoms and bonds of the structures with vertices and edges, respectively. In this way, it is possible to study the chemical structures using the concepts of graph theory. Such a field of study is usually referred to as the chemical graph theory. In chemical graph theory, the graph invariants that found some chemical applications are known as topological indices. The augmented Zagreb index (AZI), proposed by Furtula et al. [6] about a decade ago, has a better chemical applicability than several well-known other topological indices [6, 7, 9, 10]. For a graph G containing no component isomorphic to the path graph of order 2, the AZI is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u \, d_v}{d_u + d_v - 2} \right)^3,$$

where d_u, d_v are degrees of the vertices $u, v \in V(G)$, respectively, and $E(G)$ denotes the edge set of G. The AZI has been studied in mathematical point of view in various papers; for example, see some recent papers [1,5,8,12–16], recent survey [2] and related references given therein.

The chromatic number of a graph G is the minimum number of colors required to color the vertices of G such that no two adjacent vertices have the same color. Denote by $\mathcal{G}(n, \chi)$ the class of all connected graphs of a fixed order n and with a fixed chromatic number χ. Let us consider the following problem.

Problem 1 *Characterize the graph(s) attaining the maximum AZI from the class $\mathcal{G}(n, \chi)$.*

Note that $\mathcal{G}(n, 1)$ consists of only the edgeless graph $\overline{K}_n$ (the graph of order n and size zero) and $\mathcal{G}(n, n)$ contains also only one graph, that is the complete graph K_n. Thereby, the constraint $2 \le \chi \le n - 1$ should be imposed on Problem 1. Also, with the condition $2 \le \chi \le n - 1$, Problem 1 has been solved recently in [13] for the cases (i) when n is a multiple of χ, (ii) when $\chi = 2$. The primary aim of present paper is to give the solution of Problem 1 for the remaining case, that is, when n is not a multiple of χ and $3 \le \chi \le n-1$.

A graph whose vertex set can be partitioned into r sets $V_1, V_2, \ldots, V_r$ in such a way that all the vertices in every V_i (with $1 \le i \le r$) are pairwise non-adjacent is known as an r-partite graph, where $r \ge 2$ and the sets $V_1, V_2, \ldots, V_r$ are called the partite sets. If, in addition, every vertex of partite set V_i is adjacent to all the vertices of the other partite sets for $i = 1, 2, \ldots, r$, then the graph is called the complete r-partite graph. The main result of the present paper is given below, that is Theorem 1. This theorem not only gives the solution of the problem posed in [13] but also covers one of the main results of [13].

Theorem 1 *Among all connected graphs of a fixed order n and with a fixed chromatic number χ, only the graph $T_{n,\chi}$ has the maximum AZI, where $3 \le \chi \le n-1$, $n \ge 5$, and $T_{n,\chi}$ is the complete χ-partite graph of order n such that $|n_i - n_j| \le 1$, where n_i, with $i = 1, 2, \cdots, \chi$, is the number of vertices in the i-th partite set of $T_{n,\chi}$.*

The next result is a direct consequence of Theorem 1.

Corollary 2 *Let G be a connected graph of order n and with the chromatic number χ where $n \ge 5$ and $\chi \ge 3$. If $n = k\chi + r$, where k is a positive integer and r is an integer satisfying the inequality $0 \le r \le \chi - 1$, then*

$$AZI(G) \le \frac{r(r-1)(k+1)^2(n-k-1)^6}{16(n-k-2)^3} + \frac{r(\chi-r)(k^2+k)(n-k)^3(n-k-1)^3}{(2n-2k-3)^3} + \frac{(\chi-r)(\chi-r-1)k^2(n-k)^6}{16(n-k-1)^3},$$

with equality if and only if $G \cong T_{n,\chi}$.

2 Proof of Theorem 1

In order to prove Theorem 1, we need some lemmas first.

Lemma 3 *Let n_1 and n be fixed integers satisfying the inequalities $n \ge 3n_1 + 2$ and $n_1 \ge 1$. For $q \in \{0, 1\}$, define the function g_q as*

$$g_q(p) = \frac{(n_1+p)(n-n_1-p)^3}{(2n-2n_1-p-q-2)^3},$$

where p is any non-negative real number. Take

$$\alpha_q = 3n - 3n_1 - 2q - 4,$$

$$\beta_q = \sqrt{(n-n_1-q-2)(7n-4n_1-4q-8)}, \quad \text{and}$$

$$\gamma_q = 2n^2 - 4n_1 n + 2n_1^2 + 2n_1 q - nq + 4n_1 - 2n.$$

(The inequality $n \ge 3n_1 + 2$ gives $n - n_1 - q - 2 > 0$ and $7n - 4n_1 - 4q - 8 > 0$, and hence β_q is a (positive) real number.) The following statements hold.

(i) *The inequality $\alpha_q - \beta_q > 1$ holds. The function g_q is strictly increasing on the closed interval $[0, \alpha_q - \beta_q]$ and strictly decreasing on $[\alpha_q - \beta_q, \alpha_q + \beta_q]$.*

(ii) *The inequality $\alpha_q - \beta_q < \gamma_q/(\alpha_q + n_1)$ holds and the derivative function g'_q is strictly decreasing on $\left[0, \frac{\gamma_q}{\alpha_q+n_1}\right]$.*

(iii) *The function h_q defined as $h_q(p) = g_q(p) - g_q(p-1)$, is strictly decreasing on $\left[1, \frac{\gamma_q}{\alpha_q+n_1}\right]$.*

Proof: **(i)** Simple calculations yield

$$(\alpha_q - 1)^2 - \beta_q^2 = (2n - 5n_1 + q - 4)(n - n_1 - q - 2) + (q+1)^2,$$

which implies that

$$(\alpha_q - 1)^2 - \beta_q^2 > 0, \tag{1}$$

because $n \geq 3n_1 + 2$, $n_1 \geq 1$ and $q \in \{0, 1\}$. The inequalities $n \geq 3n_1 + 2$ and $n_1 \geq 1$ also imply that $\alpha_q > 1$ and consequently it holds that $(\alpha_q - 1) + \beta_q > 0$, which together with (1) imply that $\alpha_q - \beta_q > 1$. Next, the derivative function g'_q of g_q is given as

$$g'_q(p) = \frac{(n - n_1 - p)^2}{(2n - 2n_1 - p - q - 2)^4} \cdot \psi(p).$$

where

$$\psi(p) = p^2 - 2(3n - 3n_1 - 2q - 4)p + 2n^2 - 7n_1 n - 2n + 5n_1^2 + 8n_1 + 4n_1 q - nq.$$

Note that the graph of the function ψ is a parabola which opens upwards and it intersects p-axis at $p = \alpha_q \pm \beta_q$. Thereby, $\psi(p) > 0$ when $0 < p < \alpha_q - \beta_q$ and $\psi(p) < 0$ when $\alpha_q - \beta_q < p < \alpha_q + \beta_q$, and consequently we have $g'_q(p) > 0$ when $0 < p < \alpha_q - \beta_q$ and $g'_q(p) < 0$ when $\alpha_q - \beta_q < p < \alpha_q + \beta_q$. This completes the proof of part (i).

(ii) We note that $(\alpha_q + n_1)^2 - \beta_q^2 = n(2n - n_1 - q - 2) > 0$ and thus $\alpha_q + n_1 > \beta_q$, from which we have

$$\alpha_q - \frac{\gamma_q}{\alpha_q + n_1} = \frac{\beta_q^2}{\alpha_q + n_1} < \beta_q,$$

which gives the inequality mentioned in part (ii). Next, we prove the second conclusion of part (ii). In the remaining proof of part (ii), we assume that $p \in \left[0, \frac{\gamma_q}{\alpha_q+n_1}\right]$. Observe that $(n-n_1)(\alpha_q+n_1)-\gamma_q = n(n-n_1-q-2) > 0$, which implies that $\frac{\gamma_q}{\alpha_q+n_1} < n-n_1$ and thence we have $p < n-n_1$. Also, we have

$$g_q''(p) = \frac{6(n-n_1-p)(n-n_1-q-2)}{(2n-2n_1-p-q-2)^5} \cdot \phi(p),$$

where

$$\phi(p) = (3n-2n_1-2q-4)p - (2n^2-4n_1n+2n_1^2-2n+4n_1+2n_1q-nq).$$

Clearly, the inequality $g_q''(p) < 0$ holds when $\phi(p) < 0$, that is, when

$$p < \frac{2n^2-4n_1n+2n_1^2-2n+4n_1+2n_1q-nq}{3n-2n_1-2q-4} = \frac{\gamma_q}{\alpha_q+n_1},$$

which completes the proof of part (ii).

(iii) This statement is a direct consequence of part (ii). □

Lemma 4 *Let*

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

where $x, y > 2$. If y is fixed then the function Φ defined as $\Phi(x,y) = \Psi(x+1,y) - \Psi(x,y)$, is strictly decreasing in x when $x > y-2$.

Proof: The second order partial derivative function Ψ_{xx} of Ψ with respect to x is calculated as

$$\Psi_{xx}(x,y) = -\frac{6xy^3(y-2)(x-y+2)}{(x+y-2)^5},$$

which is negative for $x > y-2$ and hence Ψ_x is strictly decreasing in x when $x > y-2$. This implies that $\Phi_x(x,y) = \Psi_x(x+1,y) - \Psi_x(x,y) < 0$ when $x > y-2$. □

We also need the next two already known results.

Lemma 5 [11] *If y is a fixed real number greater than or equal to 3 then the function Ψ, defined in Lemma 4, is strictly increasing in x.*

Lemma 6 [11] *Let u and v be non-adjacent vertices in a connected graph G. If $G+uv$ is the graph obtained from G by adding the edge uv in G then $AZI(G+uv) > AZI(G)$.*

Now, we are in position to prove our main result, that is Theorem 1.

Proof of Theorem 1. Let G be a graph having the maximum AZI in the class of all connected graphs of a fixed order n and with a fixed chromatic number χ, where $3 \leq \chi \leq n-1$ and $n \geq 5$. Note that the vertex set $V(G)$ of G can be partitioned into χ independent subsets (a subset S of the vertex set of a graph is said to be independent if no two vertices of S are adjacent), say $V_1, V_2, \cdots, V_\chi$ such that $|V_i| = n_i$ for $i = 1, 2, \cdots, \chi$, provided that $n_1 \leq n_2 \leq \cdots \leq n_\chi$. Consequently, G is isomorphic to a χ-partite graph and hence, by Lemma 6, it must be isomorphic to the complete χ-partite graph $K_{n_1,n_2,\cdots,n_\chi}$. To complete the proof, we have to show that $n_\chi - n_1 \leq 1$. Contrarily, assume that $n_\chi - n_1 \geq 2$. In what follows, we construct a connected graph G' of order n and with a chromatic number χ satisfying the inequality $AZI(G') - AZI(G) > 0$, which gives a contradiction to the definition of G and hence our claim $n_\chi - n_1 \leq 1$ will be proved.

Let t be the least integer in the set $\{2, 3, \cdots, \chi\}$ satisfying the inequality $n_t - n_1 \geq 2$. Then, $n_i \in \{n_1, n_1 + 1\}$ for $i = 1, 2, \cdots, t-1$. It is possible that $n_i = n_1$ for every $i \in \{2, 3, \cdots, t-1\}$. However, if $n_i = n_1 + 1$ for some $i \in \{2, 3, \cdots, t-1\}$ then we assume that $s \in \{1, 2, \cdots, t-2\}$ is the largest integer satisfying $n_s = n_1$, which imply that $n_i = n_1$ for $i = 1, 2, \cdots, s$ and $n_i = n_1 + 1$ for $i = s+1, s+2, \cdots, t-1$. Take $A = \{2, 3, \cdots, \chi\} \setminus \{t\}$ and $G' \cong K_{n'_1,n'_2,\cdots,n'_\chi}$ where $n'_1 = n_1 + 1$, $n'_t = n_t - 1$, and $n'_i = n_i$ for every $i \in A$. Then, we have

$$\begin{aligned}
AZI(G') - AZI(G) &= (n_1+1)(n_t-1)\Psi(n-n_1-1, n-n_t+1) - n_1 n_t \Psi(n-n_1, n-n_t) \\
&\quad + \sum_{i\in A} [n_i(n_1+1)\Psi(n-n_1-1, n-n_i) - n_1 n_i \Psi(n-n_1, n-n_i)] \\
&\quad + \sum_{i\in A} [n_i(n_t-1)\Psi(n-n_t+1, n-n_i) - n_t n_i \Psi(n-n_t, n-n_i)] \\
&= \begin{cases} \Lambda_1 + n_1(t-2)\Lambda_2 + \sum_{i=t+1}^{\chi} n_i\Theta_i\,, & \text{if } n_1 = n_{t-1} \\ \Lambda_1 + n_1(s-1)\Lambda_2 + (n_1+1)(t-s-1)\Lambda_3 + \sum_{i=t+1}^{\chi} n_i\Theta_i\,, & \text{otherwise.} \end{cases}
\end{aligned} \tag{2}$$

where the function Ψ is defined in Lemma 4,

$$\Lambda_1 = (n_1+1)(n_t-1)\Psi(n-n_1-1, n-n_t+1) - n_1 n_t \Psi(n-n_1, n-n_t),$$

$$\begin{aligned}
\Lambda_2 &= (n_1+1)\Psi(n-n_1-1, n-n_1) - n_1\Psi(n-n_1, n-n_1) \\
&\quad + (n_t-1)\Psi(n-n_t+1, n-n_1) - n_t\Psi(n-n_t, n-n_1),
\end{aligned}$$

$$\Lambda_3 = (n_1+1)\Psi(n-n_1-1, n-n_1-1) - n_1\Psi(n-n_1, n-n_1-1)$$
$$+ (n_t-1)\Psi(n-n_t+1, n-n_1-1) - n_t\Psi(n-n_t, n-n_1-1),$$

and

$$\Theta_i = (n_1+1)\Psi(n-n_1-1, n-n_i) - n_1\Psi(n-n_1, n-n_i)$$
$$+ (n_t-1)\Psi(n-n_t+1, n-n_i) - n_t\Psi(n-n_t, n-n_i). \tag{3}$$

In order to prove that the right hand side of Equation (2) is positive, we will show that the quantities Λ_1, Λ_2, Λ_3, and Θ_i (when $i = t+1, \cdots, \chi$) are positive. First, let us prove that $\Lambda_1 > 0$. We note that the expression for Λ_1 can be rewritten as

$$\Lambda_1 = \frac{n_1 n_t \cdot \varphi(n, n_1, n_t) + (n_t - n_1 - 1)[(n-n_1-1)(n-n_t+1)]^3}{(2n-n_1-n_t-2)^3}, \tag{4}$$

where $\varphi(n, n_1, n_t) = [(n-n_1-1)(n-n_t+1)]^3 - [(n-n_1)(n-n_t)]^3$. Observe that the expression given on the right hand side of (4) is positive when $\varphi(n, n_1, n_t) > 0$, which is equivalent to $[(n-n_1)(n-n_t)+n_t-n_1-1]^3 - [(n-n_1)(n-n_t)]^3 > 0$, which is obviously true. Thus, we have

$$\Lambda_1 > 0. \tag{5}$$

Next, we show that $\Lambda_2 > 0$ and $\Lambda_3 > 0$. Note that the expressions for Λ_2 and Λ_3 can be rewritten as

$$\Lambda_{q+2} = (n-n_1-q)^3 \left[g_q(1) - g_q(0) + g_q(n_t-n_1-1) - g_q(n_t-n_1)\right], \tag{6}$$

where $q = 0, 1$ and the function g_q is defined in Lemma 3. By Lemma 3(i), it holds that

$$g_q(1) - g_q(0) > 0. \tag{7}$$

Let α_q, β_q, γ_q be the quantities defined in Lemma 3. Since $\chi \geq 3$, we get $\alpha_q \geq 3(n_t + 2n_1) - 3n_1 - 2q - 4 > n_t - n_1$ and hence

$$n_t - n_1 < \alpha_q + \beta_q. \tag{8}$$

In order to prove $\Lambda_{q+2} > 0$ (where $q = 0, 1$), we consider three cases. If $n_t - n_1 - 1 \geq \alpha_q - \beta_q$ then by (8) and Lemma 3(i), it holds that $g_q(n_t-n_1-1) - g_q(n_t-n_1) > 0$, which together with (7) and (6) yields $\Lambda_{q+2} > 0$. If $n_t - n_1 - 1 < \alpha_q - \beta_q$ and $n_t - n_1 \leq \alpha_q - \beta_q$ then by using Lemma 3(ii), we get $n_t - n_1 < \frac{\gamma_q}{\alpha_q + n_1}$, and hence by using Lemma 3(iii) we have $g_q(1) - g_q(0) = h_q(1) > h_q(n_t - n_1) = g_q(n_t - n_1) - g_q(n_t - n_1 - 1)$, which together with (6) gives $\Lambda_{q+2} > 0$. Lastly, if $n_t - n_1 - 1 < \alpha_q - \beta_q < n_t - n_1$ then by Lemma 3(i) it holds that $g_q(\alpha_q - \beta_q - 1) < g_q(n_t - n_1 - 1) < g_q(\alpha_q - \beta_q)$ and $g_q(n_t - n_1) < g_q(\alpha_q - \beta_q)$, which imply that

$$\begin{aligned} g_q(n_t - n_1) - g_q(n_t - n_1 - 1) &< g_q(\alpha_q - \beta_q) - g_q(n_t - n_1 - 1) \\ &< g_q(\alpha_q - \beta_q) - g_q(\alpha_q - \beta_q - 1) \\ &< g_q(1) - g_q(0), \end{aligned} \tag{9}$$

where the last inequality in (9) holds because of Lemma 3(iii) as $\alpha_q - \beta_q > 1$ (by Lemma 3(i)). From (6) and (9), it follows that $\Lambda_{q+2} > 0$. Thus, in all three possible cases, we have shown that

$$\Lambda_{q+2} > 0 \tag{10}$$

for $q = 0, 1$.

Observe that $\chi \geq t$. If $\chi = t$ then the term involving the summation symbol "$\sum$" in (2) becomes 0 and hence by using (5) and (10) in (2), we get $AZI(G') - AZI(G) > 0$, as desired. In what follows, we assume that $\chi > t$ and $i \in \{t + 1, \cdots, \chi\}$. To prove $AZI(G') - AZI(G) > 0$, it is enough to show that $\Theta_i > 0$. Because of $\sum_{j=1}^{\chi} n_j = n$ and $\chi > t$, the inequalities $n - n_1 - 1 > 3$, $n - n_i > 3$ and $n - n_1 - 1 \geq n - n_t + 1 > 3$ hold, and hence from Lemma 5, it follows that

$$\Psi(n - n_1, n - n_i) - \Psi(n - n_1 - 1, n - n_i) > 0$$

and

$$\Psi(n - n_1 - 1, n - n_i) - \Psi(n - n_t + 1, n - n_i) \geq 0,$$

which together with (3) imply that

$$\begin{aligned} \Theta_i &> n_t[\Psi(n - n_t + 1, n - n_i) - \Psi(n - n_t, n - n_i) \\ &\quad - (\Psi(n - n_1, n - n_i) - \Psi(n - n_1 - 1, n - n_i))] \\ &= n_t[\Phi(n - n_t, n - n_i) - \Phi(n - n_1 - 1, n - n_i)], \end{aligned} \tag{11}$$

where Φ is the function defined in Lemma 4. Since $n - n_1 - 1 > n - n_t > n - n_i - 2 \geq 2$, by using Lemma 4 we get $\Phi(n - n_t, n - n_i) - \Phi(n - n_1 - 1, n - n_i) > 0$ and hence (11) yields $\Theta_i > 0$. This completes the proof of Theorem 1.

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