MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **88** (2022) 625–642
ISSN: 0340–6253
doi: 10.46793/match.88-3.625Z

On Bond Incident Degree Indices of Connected Graphs with Fixed Order and Number of Pendent Vertices

Wenliang Zhou[a], **Shumei Pang**[b,*], **Muhuo Liu**[c], **Akbar Ali**[d]

[a] *College of Economics and Management, and Research Center for Green Development of Agriculture, South China Agricultural University, Guangzhou, 510642, P.R. China*
[b] *International Business College, South China Normal University, Foshan, 528225, P.R. China*
[c] *Department of Mathematics, South China Agricultural University, Guangzhou, 510642, P.R. China*
[d] *Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia*

zhouwenliangscau@163.com, pangshumei1979@163.com, liumuhuo@163.com, akbarali.maths@gmail.com

(Received March 2, 2022)

Abstract

The graphs having the maximum value of certain bond incident degree indices (including the second Zagreb index, general sum-connectivity index, and general zeroth-order Randić index) in the class of all connected graphs with fixed order and number of pendent vertices are characterized in this paper. The problem of finding graphs having the minimum values of the second Zagreb index and general zeroth-order Randić index from the aforementioned class of connected graphs is also addressed. One of the obtained results

*Corresponding author.

about the first Zagreb index has already been proved in the papers [I. Gutman, M. Kamran Jamil, N. Akhter, *Trans. Combin.* **4** (2015) 43–48] and [M. Enteshari, B. Taeri, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 17–28]; however, it is proved here by another method with a short proof. Moreover, one of the obtained results concerning the second Zagreb index gives a partial solution to a problem attacked in the aforementiond paper of Enteshari and Taeri.

1 Introduction and statements of the main results

Throughout this paper, we consider only simple connected graphs. The edge set and vertex set of a graph G are denoted by $E(G)$ and $V(G)$, respectively. Let $d_G(u)$ denote the degree of a vertex u of G. We write $d(u)$ instead of $d_G(u)$ whenever there is no confusion about the graph under consideration. Those (chemical) graph theoretical terminology and notation that are used in this paper, but not defined here, can be found in some relevant books, like [5, 6, 24, 26].

A graph invariant is a function Φ defined on the set of all graphs such that the equation $\Phi(G) = \Phi(G')$ holds whenever the graphs G and G' are isomorphic. A graph invariant may be a numerical value (for example, size of a graph), a polynomial (for example, the matching polynomial of a graph), set of numbers (for example, the spectrum of a graph), etc. In chemical graph theory, a graph invariant assuming a single number for a graph is known as a topological index [26]. In the present paper, we are concerned with the topological indices defined in the following way [9, 13] for a graph G:

$$BID_{\varphi}(G) = \sum_{uv \in E(G)} \varphi\big(d(u), d(v)\big), \tag{1}$$

where φ is a real-valued symmetric function. Following Vukičević and Đurđević [25], we call the topological indices of the form (1) as **bond incident degree (BID) indices**. These indices are sometimes referred to as the **connectivity functions** [27] of G. If f is a real-valued function such that $\varphi\big(d(u),d(v)\big) = f\big(d(u)\big)/d(u) + f\big(d(v)\big)/d(v)$, then Equation (1) yields

$$BID_{\varphi}(G) = \sum_{uv\in E(G)} \left[\frac{f\big(d(u)\big)}{d(u)} + \frac{f\big(d(v)\big)}{d(v)}\right] = \sum_{v\in V(G)} f\big(d(v)\big). \qquad (2)$$

We remark here that the right equality of Equation (2) follows from a more general result reported in [7]. Following Yao et al. [29], we denote the rightmost expression of (2) by $H_f(G)$ and refer to such indices as the **vertex-degree-function indices** of G. It seems that these indices were first considered by Linial and Rozenman [18]. The vertex-degree-function indices H_f, being simple types of BID indices, have attracted considerable attention from researchers recently; for example, see the recent papers [1, 3, 14, 15, 22, 23, 29], recent review [16], and the related references listed therein.

The first and second Zagreb indices of a graph G, usually denoted by $M_1(G)$ and $M_2(G)$, respectively, are defined as

$$M_1(G) = \sum_{u\in V(G)} \big[d(u)\big]^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} d(u)d(v).$$

The first Zagreb index was appeared almost fifty years ago in [12] while the second Zagreb index was introduced in [11]. They were extended to **zeroth-order general Randić index** $R_{\alpha}^{0}(G)$ and **general Randić index** $R_{\alpha}(G)$ of G, respectively, where

$$R_{\alpha}^{0}(G) = \sum_{u\in V(G)} \big[d(u)\big]^{\alpha} \text{ and } R_{\alpha}(G) = \sum_{uv\in E(G)} \big(d(u)d(v)\big)^{\alpha},$$

where α is a real number. Denote by $\chi_{\alpha}(G)$ and $Pl_{\alpha}(G)$ the **general sum-connectivity index** and **general Platt index** of G, respectively, where

$$\chi_{\alpha}(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^{\alpha} \text{ and } Pl_{\alpha}(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)-2\big)^{\alpha}.$$

The concept of general Randić index was firstly proposed by Bollobás and

Erdős [4], the zeroth-order general Randić index was firstly put forward by Li and Zheng [17], the general sum-connectivity index was introduced by Zhou and Trinajstić [31], and the general Platt index of G was firstly studied by Ali and Dimitrov [2]. Actually, the topological indices $R_\alpha(G)$, $R^0_\alpha(G)$, $\chi_\alpha(G)$, and $Pl_\alpha(G)$ are special cases of (2) and general cases of many famous topological indices. For instance, $M_1(G) = R^0_2(G)$ is the first Zagreb index, $M_2(G) = R_1(G)$ is the second Zagreb index, $R^0_{-1}(G)$ is called the **inverse degree** $ID(G)$ of G $\big($see [28]$\big)$, $R_{-\frac{1}{2}}(G)$ is mostly referred to as the **Randić index** of G [21], $\chi_{-\frac{1}{2}}(G)$ is famous with the name **sum-connectivity index** of G [30], and $Pl_2(G)$ is known as the **reformulated first Zagreb index** of G [20].

As usual, the path, star, and complete graphs with n vertices are denoted by P_n, $K_{1,n-1}$, and K_n, respectively. As in [8], let $D_{n;s,t}$ be the tree obtained from the path graph P_{n-s-t} by attaching s pendent vertices to one of its end vertices and t pendent vertices to the other end vertex. Let $K^{(p)}_{n-p}$ be the graph obtained from the complete graph K_{n-p} by attaching p pendent vertices to one vertex of K_{n-p}. Denote by $\mathbb{C}^{(p)}_n$ the class of all connected graphs with n vertices and p pendent vertices. Let

$$G_0 = \begin{cases} D_{n;n-3,1} & \text{if } p = n-2, \\ \\ K^{(p)}_{n-p} & \text{if } 0 \le p \le n-3. \end{cases} \tag{3}$$

Theorem 1. *In the class $\mathbb{C}^{(p)}_n$ with $0 \le p \le n-2$ and $n \ge 4$, the graph G_0 uniquely attains the maximum values of χ_α, Pl_α and R^0_α for $\alpha > 1$ and maximum value of M_2.*

We note that each of the BID indices considered in Theorem 1 satisfies the inequality $BID_\varphi(G+uv) > BID_\varphi(G)$ for every pair of non-adjacent vertices u and v of a graph G. This observation implies that a graph attaining the minimum value of any of the aforementioned BID indices in the class $\mathbb{C}^{(p)}_n$, with $2 \le p \le n-2$ and $n \ge 4$, must be a tree. Denote by $\mathbb{T}^{(p)}_n$ the class of trees with n vertices and p pendent vertices, where $2 \le p \le n-2$.

Theorem 2. *Let F_0 be a tree having the minimum value of R^0_α in the* *class* $\mathbb{T}_n^{(p)}$*. If* $\alpha > 1$ *and* $s_0 = \left\lceil \frac{p-2}{n-p} \right\rceil + 2$*, then* F_0 *has the degree sequence*

$$\pi_{\mathbf{0}} = (\underbrace{s_0, \ldots, s_0}_{t_0}, \underbrace{s_0 - 1, \ldots, s_0 - 1}_{n-p-t_0}, \underbrace{1, \ldots, 1}_{p}), \tag{4}$$

where $t_0 = p(s_0 - 2) - n(s_0 - 3) - 2$*.*

The following result has been proved by Gutman and Kamran Jamil (see Theorem 4.1 of [10]) and Enteshari and Taeri [8] gave another proof using different method. Actually, it follows immediately from Theorem 2.

Corollary. [8, 10] *If* T^* *is a tree with the minimum first Zagreb index in the class* $\mathbb{T}_n^{(p)}$*, then* T^* *has the degree sequence* $\pi_{\mathbf{0}}$*, where* $\pi_{\mathbf{0}}$ *is as defined in* (4)

In [8], it has been shown that $D_{n;\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil}$ uniquely attains the minimum second Zagreb index among all trees of $\mathbb{T}_n^{(p)}$ for $p \in \{2, 3, 4, n-3, n-2\}$. Here, we extend this result to the case when $n \geq 3p - 5$ and $p \geq 4$ (by finding a lower bound on M_2 for nontrivial trees in terms of n and p for any n and p). By a **branching vertex** of a graph, we mean a vertex with degree at least three. Let $\mathcal{T}_0(n, p)$ be the class of all trees with n vertices, maximum degree 3 and p pendent vertices such that every pendent vertex is adjacent to a branching vertex and no two branching vertices are adjacent.

Theorem 3. *If* T *is a tree with* n *vertices and* p *pendent vertices, then*

$$M_2(T) \geq 4n + 3p - 16,$$

with equality if and only if $T \in \mathcal{T}_0(n, p) \cup \left\{K_{1,3}, K_{1,4}\right\}$*.*

For $n \geq 3p-5$ and $p \geq 4$, we can construct a tree T belonging to $\mathcal{T}_0(n, p)$ explained as follows: If $p = 4$ then $n \geq 7$ and hence $D_{n;2,2} \in \mathcal{T}_0(n, 4)$. If $p \geq 5$ then we obtain $T \in \mathcal{T}_0(n, p)$ by adding one edge between a pendent vertex pertaining to a tree of $\mathcal{T}_0(n-3, p-1)$ and the center of the star $K_{1,2}$. This observation leads to the next corollary of Theorem 3.

Corollary. *If* $4 \leq p \leq \frac{n+5}{3}$*, then the member(s) of* $\mathcal{T}_0(n, p)$ *is/are the only tree(s) with the minimum second Zagreb index in the class of trees with* n *vertices and* p *pendent vertices.*

2 Proofs of Theorems 1 and 2

We start this section with some definitions that are needed in the remaining part of this paper. A **k-vertex** of G is a vertex with degree k. A vertex adjacent to at least one pendent vertex is called a **quasi-pendent vertex**. Let $N_G(u)$ denote the set of neighbors of a vertex u of a graph G. Hereafter, let G be a connected graph, and let u and v be two vertices of G such that $\{w_1, w_2, \ldots, w_s\} \subseteq N_G(v) \setminus \big(N_G(u) \cup \{u\}\big)$, where $1 \le s \le d(v)$. Denote by

$$G^* = G - vw_1 - vw_2 - \cdots - vw_s + uw_1 + uw_2 + \cdots + uw_s.$$

Lemma 1. [19] *If $f(x)$ is a strictly convex and strictly increasing function, then $H_f(G^*) > H_f(G)$ when $d_G(u) \ge d_G(v)$ and $H_f(G) > H_f(F)$ when F is a proper subgraph of G.*

Proposition 4. *Let G be a graph with the maximum $H_f(G)$ in $\mathbb{C}_n^{(p)}$, where $0 \le p \le n-2$ and $n \ge 4$. If $f(x)$ is a strictly convex and strictly increasing function, then $G = G_0$, where G_0 is as defined in* (3).

Proof. By Lemma 1, $H_f(G) > H_f(F)$ holds for any proper subgraph F of G, which implies that G is obtained from K_{n-p} by adding p pendent vertices to some vertices of K_{n-p}.

The cases $p = 0, 1$, are trivial. When $2 \le p \le n-2$, we only prove the case of $p = n-2$, as the remaining cases can be proved similarly. Since $p = n-2$, $G = D_{n;s,n-2-s}$, where $n - s - 2 \ge s \ge 1$. If $s \ge 2$, then $G^* = G - vw_1 + uw_1$ is also a tree with $n-2$ pendent vertices, where $d_G(v) = s+1$, $d_G(u) = n-s-1$, and w_1 is a pendent neighbor of v. By Lemma 1, we have $H_f(G^*) > H_f(G)$, a contradiction. ■

A symmetric bivariate non-negative function $f(x, y)$ defined on positive real numbers is called a **special function** if the inequalities $\frac{\partial\varphi(x,y)}{\partial x} > 0$, $\varphi(x+1, z) + \varphi(y-1, z) \ge \varphi(x, z) + \varphi(y, z)$ and $\varphi(x+1, y-1) + \varphi(x+1, 1) \ge \varphi(x, y) + \varphi(y, 1)$ hold for any $x \ge y > 1$ and $z \ge 1$. Note that if $\varphi(x, y)$ is a special function and if G is a connected graph with $uv \notin E(G)$, then $BID_\varphi(G + uv) > BID_\varphi(G)$.

Proposition 5. *Let G be a graph with the maximum $BID_\varphi(G)$ in $\mathbb{C}_n^{(p)}$, where $0 \le p \le n-2$ and $n \ge 4$. If $\varphi(x,y)$ is a special function, then $G = G_0$, where G_0 is defined in* (3)*.*

Proof. Since $\varphi(x,y)$ is a special function, G is obtained from K_{n-p} by adding p pendent vertices to some vertices of K_{n-p}. If $0 \le p \le 1$ then the result trivially holds. In what follows, we assume that $2 \le p \le n-2$.

Case 1. $\boldsymbol{p = n-2}$.
Since $p = n-2$, $G = D_{n;s,n-2-s}$, where $n-s-2 \ge s \ge 1$. Contrarily, assume that $s \ge 2$. Note that $G^* = G - vw_1 + uw_1$ is also a tree with $n-2$ pendent vertices, where $d_G(v) = s+1$, $d_G(u) = n-s-1$, and w_1 is a pendent neighbor of $v \in V(G)$. Since $n \ge 2s+2$ and $\frac{\partial\varphi(x,y)}{\partial x} > 0$, we have

$$
\begin{aligned}
& BID_\varphi(G^*) - BID_\varphi(G) \\
=& \varphi(n-s,s) + (s-1)\varphi(s,1) + (n-s-1)\varphi(n-s,1) \\
& - \varphi(n-1-s,s+1) - s\varphi(s+1,1) - (n-s-2)\varphi(n-s-1,1) \\
=& s\big(\varphi(s,1) + \varphi(n-s,1) - \varphi(n-1-s,1) - \varphi(s+1,1)\big) \\
& + (n-2s-2)\big(\varphi(n-s,1) - \varphi(n-1-s,1)\big) \\
& + \varphi(n-s,s) + \varphi(n-s,1) - \varphi(n-s-1,s+1) - \varphi(s,1) \\
\ge& \varphi(n-s,s) + \varphi(n-s,1) - \varphi(n-1-s,s+1) - \varphi(s,1) \\
\ge& \varphi(s+1,1) - \varphi(s,1) > 0,
\end{aligned}
$$

contrary with the choice of G.

Case 2. $\boldsymbol{2 \le p \le n-3}$.
Recall that G is obtained from K_{n-p} by adding p pendent vertices to some vertices of K_{n-p}. It suffices to show that all of these p pendent vertices are adjacent to the same vertex of K_{n-p}. Suppose to the contrary that u and v are two quasi-pendent vertices of K_{n-p} adjacent to t and s pendent vertices, respectively, where $t \ge s \ge 1$. This implies that $d_G(u) = n-p-1+t \ge n-p-1+s = d_G(v) \ge 3$. Let $u_1, u_2, \ldots, u_{n-p-2}$ be the non-pendent vertices of G different from u and v. Let $G^* = G - vw_1 + uw_1$, where w_1 is

a pendent vertex adjacent to v. From the definition of $BID_\varphi(G)$, we have

$$\begin{aligned}
& BID_\varphi(G^*) - BID_\varphi(G) \\
=& \varphi(d_G(u)+1, d_G(v)-1) + (s-1)\varphi(d_G(v)-1, 1) \\
& + (t+1)\varphi(d_G(u)+1, 1) - \varphi(d_G(u), d_G(v)) - s\varphi(d_G(v), 1) \\
& - t\varphi(d_G(u), 1) + \sum_{i=1}^{n-p-2} \big[\varphi(d_G(u)+1, d_G(u_i)) + \varphi(d_G(v)-1, d_G(u_i)) \\
& - \varphi(d_G(u), d_G(u_i)) - \varphi(d_G(v), d_G(u_i))\big] \\
\geq& (s-1)\big[\varphi(d_G(v)-1, 1) + \varphi(d_G(u)+1, 1) - \varphi(d_G(u), 1) - \varphi(d_G(v), 1)\big] \\
& + (t+1-s)\big[\varphi(d_G(u)+1, 1) - \varphi(d_G(u), 1)\big] + \varphi(d_G(u)+1, d_G(v)-1) \\
& + \varphi(d_G(u)+1, 1) - \varphi(d_G(u), d_G(v)) - \varphi(d_G(v), 1) \\
\geq& (t+1-s)\big[\varphi(d_G(u)+1, 1) - \varphi(d_G(u), 1)\big] > 0,
\end{aligned}$$

a contradiction. ■

Proof of Theorem 1. Let $f(x) = x^\alpha$, $\varphi_0(x,y) = (x+y-2)^\alpha$, $\varphi_1(x,y) = (x+y)^\alpha$, and $\varphi_2(x,y) = xy$, where $\alpha > 1$. The function f is strictly convex as well as strictly increasing because $f''(x) = \alpha(\alpha-1)x^{\alpha-2} > 0$ and $f'(x) = \alpha x^{\alpha-1} > 0$. By Proposition 4, G_0 uniquely attains the maximum value of R_α^0 among all the members of $\mathbb{C}_n^{(p)}$ for $\alpha > 1$.

In what follows, we prove that each of the functions $\varphi_0, \varphi_1, \varphi_2$, is a special function and hence by using Proposition 5 we arrive at the desired conclusion.

Since $\alpha > 1$, we conclude that $\varphi_1(x+1,z) + \varphi_1(y-1,z) = (x+1+z)^\alpha + (y+z-1)^\alpha \geq (x+z)^\alpha + (y+z)^\alpha = \varphi_1(x,z) + \varphi_1(y,z)$, $\frac{\partial \varphi_1(x,y)}{\partial x} = \alpha(x+y)^{\alpha-1} > 0$, $\varphi_1(x+1, y-1) + \varphi_1(x+1, 1) = (x+y)^\alpha + (x+2)^\alpha > (x+y)^\alpha + (y+1)^\alpha = \varphi_1(x,y) + \varphi_1(y,1)$ hold for $x \geq y > 1$ and $z \geq 1$. Thus, φ_1 is a special function. In a similar way, we can verify that φ_0 is also a special function.

Finally, we note that $\varphi_2(x+1,z) + \varphi_2(y-1,z) = z(x+y) = \varphi_2(x,z) + \varphi_2(y,z)$, $\frac{\partial \varphi_2(x,y)}{\partial x} = y > 0$, and $\varphi_2(x+1,y-1) + \varphi_2(x+1,1) = \varphi_2(x,y) + \varphi_2(y,1)$ hold for $x \geq y > 1$ and $z \geq 1$. Thus, φ_2 is also a special function. ■

Let $\mathbf{D} = (d_1, d_2, \ldots, d_n)$ and $\mathbf{D}^* = (d_1^*, d_2^*, \ldots, d_n^*)$ be two different degree sequences of two graphs where $d_i \geq d_j$ and $d_i^* \geq d_j^*$ whenever $i \leq j$. We write $\mathbf{D} \lhd \mathbf{D}^*$ if and only if $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d_i^*$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d_i^*$ for all $j = 1, 2, \ldots, n$, provided that the inequality $\sum_{i=1}^{j} d_i < \sum_{i=1}^{j} d_i^*$ holds for at least one $j \in \{1, 2, \ldots, n\}$. In [19], the next lemma has been proven.

Lemma 2. [19] *Let G and G^* be two graphs with the degree sequences $\mathbf{D}$ and $\mathbf{D}^*$, respectively. If $\mathbf{D} \lhd \mathbf{D}^*$ and $f(x)$ is a strictly convex function on $x \geq 1$, then $H_f(G) < H_f(G^*)$.*

As shown in Theorem 4.2 of [29], if $f(x)$ is a strictly convex function defined on $x \geq 1$, then the trees with the degree sequence

$$(p, \underbrace{2, \ldots, 2}_{n-p-1}, \underbrace{1, \ldots, 1}_{p})$$

has the maximum value of H_f among all trees of $\mathbb{T}_n^{(p)}$; the following theorem can be considered as the minimal version of this result.

Theorem 6. *Let T^* be a tree having the minimum value of H_f in $\mathbb{T}_n^{(p)}$. If $s_0 = \left\lceil \frac{p-2}{n-p} \right\rceil + 2$ and $f(x)$ is a strictly convex function on $x \geq 1$, then T^* is a tree with the degree sequence $\pi_{\mathbf{0}}$, where $\pi_{\mathbf{0}}$ is defined in (4).*

Proof. Because of Lemma 2, it suffices to show that $\pi_{\mathbf{0}}$ is minimum with respect to the relation '$\lhd$'. Let $\mathbf{D}^* = (d_1^*, d_2^*, \ldots, d_n^*)$ be the degree sequence of a tree belonging to the class $\mathbb{T}_n^{(p)}$ such that $\mathbf{D}^* \neq \pi_{\mathbf{0}}$. Denote by $t_0 = p(s_0 - 2) - n(s_0 - 3) - 2$ and $\pi_{\mathbf{0}} = (d_1, d_2, \ldots, d_n)$, that is, $d_1 = d_2 = \cdots = d_{t_0} = s_0$ and $d_{t_0+1} = d_{t_0+2} = \cdots = d_{n-p} = s_0 - 1$. To complete the proof, it suffices to show that

$$\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d_i^* \tag{5}$$

for all $1 \leq j \leq n - p$.

If $d_1^* \le s_0 - 1$, then

$$\begin{aligned} 2(n-1) &= d_1^* + d_2^* + \cdots + d_n^* \\ &\le (n-p)(s_0-1) + p = (n-p)\left(\left\lceil \frac{p-2}{n-p} \right\rceil + 1\right) + p \\ &< (n-p)\left(\frac{p-2}{n-p} + 2\right) + p = 2(n-1), \end{aligned}$$

a contradiction. Thus, $d_1^* \ge s_0$. If $d_{n-p}^* \ge s_0$, then (5) holds and we are done. In what follows, we suppose that there exists k with $1 \le k \le n-p-1$ such that $d_1^* \ge \cdots \ge d_k^* \ge s_0$ and $d_{k+1}^* \le s_0 - 1$.

Since (5) already holds for $1 \le j \le k$, we take j satisfying $k+1 \le j \le n-p$. Since $d_{n-p}^* \le d_{n-p-1}^* \le \cdots \le d_{j+1}^* \le d_j^* \le \cdots \le d_{k+1}^* \le s_0 - 1 = d_{n-p} = d_{n-p-1} = \cdots = d_{t_0+1} < s_0 = d_{t_0} = d_{t_0-1} = \cdots = d_1$ and $k+1 \le j \le n-p$, we have

$$\begin{aligned} d_1^* + d_2^* + \cdots + d_j^* &= 2(n-1) - p - d_{n-p}^* - \cdots - d_{j+1}^* \\ &\ge 2(n-1) - p - (n-p-j)(s_0-1) \\ &\ge 2(n-1) - d_{j+1} - d_{j+2} - \cdots - d_n \\ &= d_1 + d_2 + \cdots + d_j, \end{aligned}$$

which implies that (5) holds. This completes the proof. ■

One can easily checked that Theorem 2 follows from Theorem 6, as $f(x) = x^\alpha$ is a strictly convex function defined on $x \ge 1$ for $\alpha > 1$.

3 Proof of Theorem 3

This section is dedicated to the proof of Theorem 3. Recall that a **branching vertex** of G is a vertex with degree at least three. Let $q(G)$ be the **branching number**, that is, the number of branching vertices of G.

Lemma 3. [8] *Let T be a tree of $\mathbb{T}_n^{(p)}$, where $2 \le p \le n-2$. If $1 \le q(T) \le 2$ and $T \ne D_{n;\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil}$, then $M_2(T) > M_2\big(D_{n;\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil}\big)$.*

A **special vertex** is a quasi-pendent vertex having at most one non-pendent neighbor. For any two vertices x and y of a tree T, let P_{xy} be the unique path connecting the vertices x and y.

Lemma 4. *Let x, y be two non-pendent vertices of a tree T such that x is a quasi-pendent vertex of T. If y is not a special vertex and $d_T(y) > d_T(x)$, then there exists another tree T' such that $M_2(T') < M_2(T)$, where T and T' have the same degree sequence.*

Proof. Suppose that w_1 is a pendent vertex adjacent to x. Since y is not a special vertex, y is adjacent to some non-pendent vertex y_1 such that $y_1 \notin P_{xy}$. Let $T' = T + xy_1 + yw_1 - xw_1 - yy_1$. Since $d_T(y_1) > 1 = d_T(w_1)$ and $d_T(x) < d_T(y)$, we have $M_2(T') - M_2(T) = \big(d_T(y) - d_T(x)\big)\big(d_T(w_1) - d_T(y_1)\big) < 0$. Now, it is easily checked that T' is a tree containing the same degree sequence as T. ■

Recall that $\mathcal{T}_0(n, p)$ is the class of trees with n vertices, maximum degree 3 and p pendent vertices such that every pendent vertex is adjacent to a branching vertex and no two branching vertices are adjacent. If $T \in \mathcal{T}_0(n, p)$, then let n_i be the number of vertices of degree i of T and let $m_{i,j}(T)$ be the number of those edges of T whose one end-vertex is an i-vertex and the other one is a j-vertex. By a fact reported in [8], it holds that

$$\sum_{i=3}^{p}(i-2)n_i = p - 2,$$

which gives $n_3 = p - 2$. Since $m_{1,3}(T) = p$, we have $m_{2,3}(T) = 3n_3 - m_{1,3}(T) = 2(p-3)$. Combining this with $|E(T)| = n - 1$, we can conclude that

$$m_{1,3}(T) = p, \quad m_{2,2}(T) = n - 3p + 5, \quad \text{and} \quad m_{2,3}(T) = 2(p-3),$$

which implies that

$$M_2(T) = 4n + 3p - 16.$$

Proof of Theorem 3. For $n = 1, 2, 3$, the result trivially holds, as T must be a star. If $p = n - 1 \geq 3$, then $T = K_{1,n-1}$ and thus $M_2(T) = (n-1)^2 \geq 4n + 3(n-1) - 16 = 4n + 3p - 16$, with equality if and only if $T \in \big\{K_{1,3}, K_{1,4}\big\}$. Next, we prove the theorem by induction on p, where $2 \leq p \leq n - 2$. The result is trivial for $p = 2$, because $n \geq 4$ and

$M_2(P_n) = 4n - 8 > 4n - 10$. Also, if $p = 3$ and $n \geq 5$, then from Lemma 3 it follows that $M_2(T) \geq M_2\big(D_{n;\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil}\big) = 4n - 6 > 4n - 7$. Hence, the induction starts. Assume that $p \geq 4$. Then, $n \geq p + 2 \geq 6$. Take T as a tree belonging to $\mathbb{T}_n^{(p)}$ such that $M_2(T)$ is as small as possible. To complete the proof, it suffices to show that $M_2(T) \geq 4n + 3p - 16$ with equality if and only if $T \in \mathcal{T}_0(n, p)$.

We first suppose that **at least one quasi-pendent vertex, say x_0, of T is a 2-vertex**. Since $p \geq 4$, T contains at least one branching vertex. By Lemma 4, we can conclude that each branching vertex of T must be a special vertex. Now, let y_0 be a branching vertex of T such that the distance between x_0 and y_0 is as small as possible. Since each branching vertex of T must be a special vertex, y_0 is a special vertex and it is the unique branching vertex of T. Now, we can conclude that $T = D_{n;p-1,1}$. Combining this with $p \geq 4$, it follows that $M_2(T) = p(p-1) + 2p + 2 + 4(n - 2 - p) = p(p-3) + 4n - 6 > 4n + 3p - 16$, as required.

Next, we suppose that **each quasi-pendent vertex of T is a branching vertex.**

Case 1. T contains at least one quasi-pendent vertex with degree greater than 3.

Let $u_0 \in V(T)$ be a pendent vertex adjacent to an s-vertex u, where $s \geq 4$. Take $N_T(u) = \{u_0, u_1, \ldots, u_{r-1}, u_r, u_{r+1}, \ldots, u_{s-1}\}$ where $d_T(u_i) = 1$ for all $i \in \{0, 1, \ldots, r-1\}$ and $d_T(u_j) \geq 2$ for all $j \in \{r, r+1, \ldots, s-1\}$, with $r \geq 1$. Certainly, $T - u_0$ is a tree with $n - 1$ vertices and $p - 1$ pendent vertices. By using the inductive hypothesis, we have $M_2(T - u_0) \geq 4(n-1) + 3(p-1) - 16$. Combining this with $s > r$ and $s \geq 4$, we have

$$\begin{aligned}
M_2(T) &= M_2(T - u_0) + s + r - 1 + \sum_{j=r}^{s-1} d_T(u_j) \\
&\geq 4(n-1) + 3(p-1) - 16 + s + r - 1 + 2(s - r) \\
&= (4n + 3p - 16) + (s - r) + (2s - 8) \\
&> 4n + 3p - 16,
\end{aligned}$$

as desired.

Case 2. Every quasi-pendent vertex of T is a 3-vertex and T contains at least one quasi-pendent vertex having only one pendent neighbor.

Let $u \in V(T)$ such that $N_T(u) = \{u_0, u_1, u_2\}$ where $d_T(u_0) = 1$ and $2 \le d_T(u_1) \le d_T(u_2)$. Certainly, $T - u_0$ is also a tree with $n-1$ vertices and $p-1$ pendent vertices. By using the inductive hypothesis, we have

$$\begin{aligned} M_2(T) &= M_2(T - u_0) + d_T(u_1) + d_T(u_2) + 3 \\ &\ge (4n + 3p - 16) + d_T(u_1) + d_T(u_2) - 4 \\ &\ge 4n + 3p - 16, \end{aligned}$$

where the equation $M_2(T - u_0) = 4(n-1) + 3(p-1) - 16$ holds if and only if $T - u_0 \in \mathcal{T}_0(n-1, p-1)$ and $d_T(u_1) = d_T(u_2) = 2$; that is, if and only if $T \in \mathcal{T}_0(n, p)$.

Case 3. Every quasi-pendent vertex of T is a 3-vertex and T contains at least one quasi-pendent vertex having two pendent neighbors and a neighbor of degree greater than 2.

Let $u \in V(T)$ such that $N_T(u) = \{u_0, u_1, u_2\}$ where $d_T(u_0) = d_T(u_1) = 1$ and $d_T(u_2) \ge 3$. Let T_1 be the tree formed from T by deleting the vertices u_0 and u_1. Then, T_1 is a tree with $n-2$ vertices and $p-1$ pendent vertices. Since $n - 2 \ge 4$, by using the inductive hypothesis, we have

$$\begin{aligned} M_2(T) &= M_2(T_1) + 2d_T(u_2) + 6 \\ &\ge (4n + 3p - 16) + 2d_T(u_2) - 5 \\ &> 4n + 3p - 16, \end{aligned}$$

as desired.

Case 4. Every quasi-pendent vertex of T is a 3-vertex, which has two pendent neighbors and a neighbor of degree 2.

We first assume that the maximum degree of T is at least 4. By our hypothesis, the vertex with maximum degree of T is not a quasi-pendent vertex and thus it is not a special vertex, which is contrary with the choice of T and Lemma 4. Next, we suppose that the maximum degree of T is equal to 3.

If the maximum degree of T is 3 and no two branching vertices of T are adjacent, then $T \in \mathcal{T}_0(n,p)$ and hence $M_2(T) = 4n + 3p - 16$.

Next, we suppose that the maximum degree of T is 3 and it contains at least one pair of adjacent branching vertices. Let u_0v_0 be an edge of T with $d_T(u_0) = d_T(v_0) = 3$. Let w_0 be a pendent vertex of T such that w_0 is connected with v_0 in $T - u_0v_0$. Let T_2 be the tree formed from T by deleting the edge u_0v_0 and then adding the edge u_0w_0. Then, T_2 is a tree with n vertices and $p-1$ pendent vertices. Suppose that $N_T(v_0) = \{u_0, u_1, u_2\}$. Since every quasi-pendent vertex of T is a 3-vertex, which has two pendent neighbors and a neighbor of degree 2, $d_T(u_1) \geq d_T(u_2) \geq 2$. By using the inductive hypothesis, we have

$$\begin{aligned} M_2(T) = M_2(T_2) + d_T(u_1) + d_T(u_2) &\geq 4n + 3(p-1) - 16 + 4 \\ &> 4n + 3p - 16, \end{aligned}$$

as desired. ■

4 Further discussion

As indicated in Corollary 1, the bound on M_2 for trees of $\mathbb{T}_n^{(p)}$ given in Theorem 3 is best possible when $4 \leq p \leq \frac{n+5}{3}$. The following result gives the best possible bound on M_2 for members of $\mathbb{T}_n^{(p)}$ when $p \in \{2, 3, 4, n-3, n-2\}$.

Lemma 5. [8] *If $p \in \{2, 3, 4, n-3, n-2\}$, then $D_{n;\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil}$ uniquely attains the minimum second Zagreb index among all trees in the class $\mathbb{T}_n^{(p)}$.*

Thus, it seems to be an interesting problem to characterize the trees having minimum value of M_2 in the class $\mathbb{T}_n^{(p)}$ when $\frac{n+5}{3} < p \leq n-4$.

In what follows, we take $T_0 \in \mathbb{T}_n^{(p)}$ such that $M_2(T_0)$ is as small as possible. We may suppose that $q(T_0) \geq 3$ by Lemma 3. With the similar argument as Lemma 4, we have

Lemma 6. *Let x_0, y_0 be two non-pendent vertices of T_0 such that x_0 is a quasi-pendent vertex. If y_0 is not a special vertex, then $d_{T_0}(y_0) \leq d_{T_0}(x_0)$.*

In what follows, we give more properties of T_0. Firstly, from Lemma 6, we conclude that the following claim holds.

Claim 1. *Let x_0 and y_0 be two non-pendent vertices of T_0.*
(i) If they are quasi-pendent vertices and they are not special vertices, then $d_{T_0}(x_0) = d_{T_0}(y_0)$;
(ii) If x_0 is a special vertex and y_0 is not a special vertex, then $d_{T_0}(x_0) \geq d_{T_0}(y_0)$;
(iii) If x_0 is a quasi-pendent vertex and y_0 is not a quasi-pendent vertex, then $d_{T_0}(x_0) \geq d_{T_0}(y_0)$;
(iv) T_0 must contain a special vertex with maximum degree Δ.

Claim 2. *Let x_0 and y_0 be two branching vertices of T_0. If $x_0y_0 \in E(T_0)$, then T_0 contains no edge u_0v_0 with $d_{T_0}(u_0) = d_{T_0}(v_0) = 2$.*

Proof. By contradiction, we assume that $u_0v_0 \in E(T_0)$ with $d_{T_0}(u_0) = d_{T_0}(v_0) = 2$. We may suppose that $v_0, x_0 \notin P_{y_0u_0}$. Let $T_2 = T_0 + x_0u_0 + y_0v_0 - x_0y_0 - u_0v_0$. Then, T_2 is also a tree with n vertices and p pendent vertices such that $M_2(T_2) - M_2(T_0) = \big(d_{T_0}(x_0) - 2\big)\big(2 - d_{T_0}(y_0)\big) < 0$, contrary with the choice of T_0. ■

Claim 3. *Let x_0 and y_0 be two special vertices of T_0 and x, y be two non-pendent vertices adjacent to x_0 and y_0, respectively. Then, $d_{T_0}(x_0) \geq d_{T_0}(y)$. Furthermore, if $d_{T_0}(x_0) < d_{T_0}(y_0)$ and $yx_0 \notin E(T_0)$, then $d_{T_0}(x) \geq d_{T_0}(y)$.*

Proof. Let x_1 be a pendent vertex adjacent to x_0 and $T_3 = T_0 + x_0y_0 + yx_1 - yy_0 - x_0x_1$. Then,

$$\begin{aligned} M_2(T_3) - M_2(T_0) =& d_{T_0}(x_0)d_{T_0}(y_0) + d_{T_0}(y) - d_{T_0}(x_0) - d_{T_0}(y)d_{T_0}(y_0) \\ =& \big(d_{T_0}(y_0) - 1\big)\big(d_{T_0}(x_0) - d_{T_0}(y)\big) \geq 0 \end{aligned}$$

and thus $d_{T_0}(x_0) \geq d_{T_0}(y)$.

Let $T_4 = T_0 + x_0y + y_0x - yy_0 - x_0x$. Then, $M_2(T_4) - M_2(T_0) = \big(d_{T_0}(y_0) - d_{T_0}(x_0)\big)\big(d_{T_0}(x) - d_{T_0}(y)\big)$. By the choice of T_0, we have $d_{T_0}(x) \geq d_{T_0}(y)$ when $d_{T_0}(x_0) < d_{T_0}(y_0)$. ■

Claim 4. *Let x_0 and y_0 be two special vertices of T_0 and x, y be two non-pendent vertices adjacent to x_0 and y_0, respectively. If $d_{T_0}(x) \geq d_{T_0}(y)$, then $d_{T_0}(y_0) \geq d_{T_0}(x_0) - 1$. Furthermore, if $d_{T_0}(x) > d_{T_0}(y)$, then $d_{T_0}(y_0) \geq d_{T_0}(x_0)$.*

Proof. Since x_0 and y_0 are two special vertices of T_0, x_0 and y_0 are adjacent to exactly $d_{T_0}(x_0) - 1$ and $d_{T_0}(y_0) - 1$ pendent vertices, respectively. Assume that $d_{T_0}(x_0) - 2 \geq d_{T_0}(y_0) \geq 2$. Denote by $T_5 = T_0 + y_0x_1 - x_0x_1$, where x_1 is a pendent vertex adjacent to x_0. Then,

$$
\begin{aligned}
& M_2(T_5) - M_2(T_0) \\
&= \big(d_{T_0}(x_0) - 1\big)\big(d_{T_0}(x) + d_{T_0}(x_0) - 2\big) + \big(d_{T_0}(y_0) + 1\big)\big(d_{T_0}(y_0) + d_{T_0}(y)\big) \\
&\quad - d_{T_0}(x_0)\big(d_{T_0}(x) + d_{T_0}(x_0) - 1\big) - d_{T_0}(y_0)\big(d_{T_0}(y) + d_{T_0}(y_0) - 1\big) \\
&= d_{T_0}(y) - d_{T_0}(x) + 2\big(d_{T_0}(y_0) - d_{T_0}(x_0)\big) + 2 < 0,
\end{aligned}
\tag{6}
$$

contrary with the choice of T_0. By (6), with the similar reason, we can show the Furthermore part. ■

***Acknowledgment*:** Comments from three anonymous referees are gratefully acknowledged. The first author is supported by the 2019 project of the 13th five year plan for the development of philosophy and Social Sciences in Guangzhou (No. 2019GZYB41): Research on the innovation of floating population management and service in Guangzhou; The third author is supported by the Natural Science Foundation of Guangdong Province (No. 2022A1515011786).

References

[1] A. Ali, A. A. Bhatti, N. Iqbal, T. Alraqad, J. P. Mazorodze, H. Saber, A. M. Alanazi, Some bond incident degree indices of cactus graphs, *J. Math.* **2022** (2022) #8325139.

[2] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, *Discr. Appl. Math.* **238** (2018) 32–40.

[3] A. Ali, I. Gutman, H. Saber, A. M. Alanazi, On bond incident degree indices of (n, m)-graphs, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 89–96.

[4] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Comb.* **50** (1998) 225–233.

[5] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[6] G. Chartrand, L. Lesniak, P. Zhang, *Graphs & Digraphs*, CRC Press, Boca Raton, 2016.

[7] T. Došlić, T. Réti, D. Vukičević, On the vertex degree indices of connected graphs, *Chem. Phys. Lett.* **512** (2011) 283–286.

[8] M. Enteshari, B. Taeri, Extremal Zagreb indices of graphs of order n with p pendent vertices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 17–28.

[9] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361

[10] I. Gutman, M. K. Jamil, N. Akhter, Graphs with fixed number of pendent vertices and minimal first Zagreb index, *Trans. Comb.* **4** (2015) 43–48.

[11] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[12] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi-$electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[13] B. Hollas, The covariance of topological indices that depend on the degree of a vertex, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 177–187.

[14] Z. Hu, L. Li, X. Li, D. Peng, Extremal graphs for topological index defined by a degree-based edge-weight function, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 505–520.

[15] Z. Hu, X. Li, D. Peng, Graphs with minimum vertex-degree function-index for convex functions, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 521–533.

[16] X. Li, D. Peng, Extremal problems for graphical function-indices and f-weighted adjacency matrix, *Discr. Math. Lett.* **9** (2022) 57–66.

[17] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.

[18] N. Linial, E. Rozenman, An extremal problem on degree sequences of graphs, *Graphs Comb.* **18** (2002) 573–582

[19] M. Liu, Y. Yao, K. Ch. Das, Extremal results for cacti, *Bull. Malays. Math. Sci. Soc.* **43** (2020) 2783–2798.

[20] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, *Mol. Diversity* **8** (2004) 393–399.

[21] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[22] I. Tomescu, Properties of connected (n, m)-graphs extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 285–294.

[23] I. Tomescu, Graphs with given cyclomatic number extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 109–114.

[24] N. Trinajstić. *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[25] D. Vukičević, J. Đurđević, Bond additive modelling 10. Upper and lower bounds of bond incident degree indices of catacondensed fluoranthenes, *Chem. Phys. Lett.* **515** (2011) 186–189.

[26] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, 2018.

[27] H. Wang, Functions on adjacent vertex degrees of trees with given degree sequence, *Cent. Eur. J. Math.* **12** (2014) 1656–1663.

[28] K. Xu, K. C. Das, Some extremal graphs with respect to inverse degree, *Discr. Appl. Math.* **203** (2016) 171–183.

[29] Y. Yao, M. Liu, F. Belardo, C. Yang, Unified extremal results of topological index and graph spectrum, *Discr. Appl. Math.* **271** (2019) 218–232.

[30] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.

[31] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.