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The Extremal Graphs of Some Topological Indices with Given Vertex k-Partiteness

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Abstract: The vertex k-partiteness of graph G is defined as the fewest number of vertices whose deletion from G yields a k-partite graph. In this paper, we characterize the extremal value of the reformulated first Zagreb index, the multiplicative-sum Zagreb index, the general Laplacian-energy-like invariant, the general zeroth-order Randić index, and the modified-Wiener index among graphs of order n with vertex k-partiteness not more than m.

Keywords: topological index; vertex k-partiteness; extremal graph

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1. Introduction

All graphs considered in this paper are simple, undirected, and connected. Let G be a graph with vertex set $V(G) = \{v_1, \cdots, v_n\}$ and edge set $E(G) = \{e_1, \cdots, e_m\}$. The degree of a vertex $u \in V(G)$ is the number of edges incident to u, denoted by $d_G(u)$. The distance between two vertices u and v is the length of the shortest path connecting u and v, denoted by $d_G(u, v)$. The complement of G, denoted by $\overline{G}$, is the graph with vertex set $V(\overline{G}) = V(G)$ and edge set $E(\overline{G}) = \{uv : uv \notin E(G)\}$. A subgraph of G induced by H, denoted by $\langle H \rangle$, is the subgraph of G that has the vertex set H, and for any two vertices $u, v \in V(H)$, they are adjacent in H iff they are adjacent in G. The adjacency matrix of G is a square $n \times n$ matrix such that its element a_{ij} is one when there is an edge from vertex u_i to vertex u_j, and zero when there is no edge, denoted by $A(G)$. Let $D(G) = diag(d_1, d_2, \cdots, d_n)$ be the diagonal matrix of vertex degrees of G. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$, and the eigenvalues of $L(G)$ are called Laplacian eigenvalues of G, denoted by $\mu_1, \cdots, \mu_n$ with $\mu_1 \geq \cdots \geq \mu_n$. It is well known that $\mu_n = 0$, and the multiplicity of zero corresponds to the number of connected components of G.

A bipartite graph is a graph whose vertex set can be partitioned into two disjoint sets U_1 and U_2, such that each edge has an end vertex in U_1 and the other one in U_2. A complete bipartite graph, denoted by $K_{s,t}$, is a bipartite graph with $|U_1| = s$ and $|U_2| = t$, where any two vertices $u \in U_1$ and $v \in U_2$ are adjacent. If every pair of distinct vertices in G is connected by a unique edge, we call G a complete graph. The complete graph with n vertices is denoted by K_n. An independent set of G is a set of vertices, no two of which are adjacent. A graph G is called k-partite if its vertex-set can be partitioned into k different independent sets $U_1, \cdots, U_k$. When $k = 2$, they are the bipartite graphs, and $k = 3$ the tripartite graphs. The vertex k-partiteness of graph G, denoted by $v_k(G)$, is the fewest number of vertices whose deletion from G yields a k-partite graph. A complete k-partite graph, denoted by $K_{s_1, \cdots, s_k}$, is a k-partite graph with k different independent sets $|U_1| = s_1, \cdots, |U_k| = s_k$, where there is an edge between every pair of vertices from different independent sets.

A topological index is a numerical value that can be used to characterize some properties of molecule graphs in chemical graph theory. Recently, many researchers have paid much attention to studying different topological indices. Dimitrov [1] studied the structural properties of trees with minimal atom-bond connectivity index. Li and Fan [2] obtained the extremal graphs of the Harary index. Xu et al. [3] determined the eccentricity-based topological indices of graphs. Hayat et al. [4] studied the valency-based topological descriptors of chemical networks and their applications. Let $G+uv$ be the graph obtained from G by adding an edge $uv \in E(\overline{G})$. Let $I(G)$ be a graph invariant, if $I(G+uv) > I(G)$ (or $I(G+uv) < I(G)$, respectively) for any edge $uv \in E(\overline{G})$, then we call $I(G)$ a monotonic increasing (or decreasing, respectively) graph invariant with the addition of edges [5]. Let $\mathscr{G}_{n,m,k}$ be the set of graphs with order n and vertex k-partiteness $v_k(G) \leq m$, where $1 \leq m \leq n-k$. In [5–7], the authors have researched several monotonic topological indices in $\mathscr{G}_{n,m,2}$, such as the Kirchhoff index, the spectral radius, the signless Laplacian spectral radius, the modified-Wiener index, the connective eccentricity index, and so on. Inspired by these results, we extend the parameter of graph partition from two-partiteness to arbitrary k-partiteness. Moreover, we study some monotonic topological indices and characterize the graphs with extremal monotonic topological indices in $\mathscr{G}_{n,m,k}$.

2. Preliminaries

The join of two-vertex-disjoint graphs G_1, G_2, denoted by $G = G_1 \vee G_2$, is the graph obtained from the disjoint union $G_1 \cup G_2$ by adding edges between each vertex of G_1 and each of G_2. It is to say that $V(G) = V(G_1) \cup V(G_2)$ and $E(G) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}$.

The join operation can be generalized as follows. Let $F = \{G_1, \cdots, G_k\}$ be a set of vertex-disjoint graphs and H be an arbitrary graph with vertex set $V(H) = \{1, \cdots, k\}$. Each vertex $i \in V(H)$ is assigned to the graph $G_i \in F$.

The H-join of the graphs $G_1, \cdots, G_k$ is the graph $G = H[G_1, \cdots, G_k]$, such that $V(G) = \bigcup\limits_{j=1}^{k} V(G_j)$ and:

$$E(G) = \bigcup_{j=1}^{k} E(G_j) \bigcup \Big(\bigcup_{ij \in E(H)} \{uv : u \in V(G_i), v \in V(G_j)\} \Big).$$

If $H = K_2$, the H-join is the usual join operation of graphs, and the complete k-partite graph $K_{s_1,\cdots,s_k}$ can be seen as the K_k-join graph $K_k[O_{s_1}, \cdots, O_{s_k}]$, where O_{s_i} is an empty graph of order s_i, $1 \leq i \leq k$.

For $U \subseteq V(G)$, let $G-U$ be the graph obtained from G by deleting the vertices in U and the edges incident with them.

Lemma 1. *Let G be an arbitrary graph in $\mathscr{G}_{n,m,k}$ and $I(G)$ be a monotonic increasing graph invariant. Then, there exists k positive integers $s_1, \cdots, s_k$ satisfying $\sum\limits_{i=1}^{k} s_i = n-m$, such that $I(G) \leq I(\widehat{G})$ holds for all graphs $G \in \mathscr{G}_{n,m,k}$, where $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}]) \in \mathscr{G}_{n,m,k}$, with equality holds if and only if $G \cong \widehat{G}$.*

Proof. Choose $\widehat{G} \in \mathscr{G}_{n,m,k}$ with the maximum value of a monotonic increasing graph invariant such that $I(G) \leq I(\widehat{G})$ for all $G \in \mathscr{G}_{n,m,k}$. Assume that the k-partiteness of graph $\widehat{G}$ is m', then there exists a vertex set U of graph $\widehat{G}$ with order m' such that $\widehat{G}-U$ is a k-partite graph with k-partition $\{U_1, \cdots, U_k\}$. For $1 \leq i \leq k$, let s_i be the order of U_i; hence, $n = \sum\limits_{i=1}^{k} s_i + m'$.

Firstly, we claim that $\widehat{G} - U = K_k[O_{s_1}, \cdots, O_{s_k}]$. Otherwise, there exists at least two vertices $u \in U_{s_i}$ and $v \in U_{s_j}$ for some $i \neq j$, which are not adjacent in $\widehat{G}$. By joining the vertices u and v, we get a new graph $\widehat{G}+uv$, obviously, $\widehat{G}+uv \in \mathscr{G}_{n,m,k}$. Then, $I(\widehat{G}) < I(\widehat{G}+uv)$, which is a contradiction.

Secondly, we claim that U is the complete graph $K_{m'}$. Otherwise, there exists at least two vertices $u, v \in U$, which are not adjacent. By connecting the vertices u and v, we arrive at a new graph $\widehat{G}+uv$, obviously, $\widehat{G}+uv \in \mathscr{G}_{n,m,k}$. Then, we have $I(\widehat{G}) < I(\widehat{G}+uv)$, a contradiction again.

Using a similar method, we can get $\widehat{G} = K_{m'} \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$.

Finally, we prove that $m' = m$. If $m' \leq m-1$, then $\sum_{i=1}^{k} s_i = n - m' \geq n - m + 1 > n - m \geq k$; thus, $\sum_{i=1}^{k} s_i > k$. Without loss of generality, we assume that $s_1 \geq 2$. By moving a vertex $u \in O_{s_1}$ to the set of U and adding edges between u and all the other vertices in O_{s_1}, we get a new graph $\widetilde{G} = K_{m'+1} \vee (K_k[O_{s_1-1}, O_{s_2}, \cdots, O_{s_k}])$. It is easy to check that $\widetilde{G} \in \mathscr{G}_{n,m,k}$ has $s_1 - 1$ edges more than the graph $\widehat{G}$. By the definition of the monotonic increasing graph invariant, we get $I(\widehat{G}) < I(\widetilde{G})$, which is obviously another contradiction.

Therefore, $\widehat{G}$ is the join of a complete graph with order m and a complete k-partite graph with order $n - m$. That is to say $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$.

The proof of the lemma is completed. □

Lemma 2. *Let G be an arbitrary graph in $\mathscr{G}_{n,m,k}$ and $I(G)$ be a monotonic decreasing graph invariant. Then, there exists k positive integers $s_1, \cdots, s_k$ satisfying $\sum_{i=1}^{k} s_i = n - m$, such that $I(G) \geq I(\widehat{G})$ holds for all graphs $G \in \mathscr{G}_{n,m,k}$, where $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}]) \in \mathscr{G}_{n,m,k}$, with equality holds if and only if $G \cong \widehat{G}$.*

3. Main Results

In this section, we will characterize the graphs with an extremal monotonic increasing (or decreasing, respectively) graph invariant in $\mathscr{G}_{n,m,k}$. Assume that $n - m = sk + t$, where s is a positive integer and t is a non-negative integer with $0 \leq t < k$.

3.1. The Reformulated First Zagreb Index, Multiplicative-Sum Zagreb Index, and k-Partiteness

The first Zagreb index is used to analyze the structure-dependency of total π-electron energy on the molecular orbitals, introduced by Gutman and Trinajstć [8]. It is denoted by:

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)),$$

which can be also calculated as:

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2.$$

Todeschini and Consonni [9] considered the multiplicative version of the first Zagreb index in 2010, defined as:

$$\Pi_1(G) = \prod_{u \in V(G)} d_G(u)^2.$$

For an edge $e = uv \in E(G)$, we define the degree of e as $d_G(e) = d_G(u) + d_G(v) - 2$. Milličević et al. [10] introduced the reformulated first Zagreb index, defined as:

$$\widetilde{M}_1(G) = \sum_{e \in E(G)} d_G(e)^2 = \sum_{uv \in E(G)} (d_G(u) + d_G(v) - 2)^2.$$

Eliasi et al. [11] introduced another multiplicative version of the first Zagreb index, which is called the multiplicative-sum Zagreb index and defined as:

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d_G(u) + d_G(v)).$$

They are widely used in chemistry to study the heat information of heptanes and octanes. For some recent results on the fourth Zagreb indices, one can see [12–17].

Lemma 3. *Let G be a graph with $u, v \in V(G)$. If $uv \in E(\overline{G})$, then $\widetilde{M}_1(G) < \widetilde{M}_1(G+uv)$.*

Lemma 4. *Let G be a graph with $u, v \in V(G)$. If $uv \in E(\overline{G})$, then $\Pi_1^*(G) < \Pi_1^*(G+uv)$.*

Note that $s_1, \cdots, s_k$ are k positive integers with $\sum\limits_{i=1}^{k} s_i = n - m$.

Theorem 1. *Let $\widehat{G}$ be a graph of order $n > 2$, and the join of a complete graph with order m and a complete k-partite graph with order $n-m$ in $\mathscr{G}_{n,m,k}$, i.e., $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$. By moving one vertex from the part of O_{s_1} to the part of O_{s_2}, we get a new graph $\widetilde{G} = K_m \vee (K_k[O_{s_1-1}, O_{s_2+1}, \cdots, O_{s_k}])$. If $s_1 - 1 \geq s_2 + 1$, then $\widetilde{M}_1(\widetilde{G}) > \widetilde{M}_1(\widehat{G})$.*

Proof. By the definition of the reformulated first Zagreb index $\widetilde{M}_1(G)$, we can calculate as follows:

$$\widetilde{M}_1(\widehat{G}) = \frac{m(m-1)}{2}(2n-4)^2 + \sum_{i=1}^{k} ms_i(2n-s_i-3)^2 + \sum_{1\leq i<j\leq k} s_i s_j (2n-s_i-s_j-2)^2.$$

Therefore,

$$\begin{aligned}
\widetilde{M}_1(\widetilde{G}) - \widetilde{M}_1(\widehat{G}) &= m(s_1-1)(2n-s_1-2)^2 + m(s_2+1)(2n-s_2-4)^2 \\
&+ (s_1-1)(s_2+1)(2n-s_1-s_2-2)^2 - ms_1(2n-s_1-3)^2 \\
&- ms_2(2n-s_2-3)^2 - s_1s_2(2n-s_1-s_2-2)^2 \\
&+ \sum_{i=3}^{k}(s_1-1)s_i(2n-s_1-s_i-1)^2 + \sum_{i=3}^{k}(s_2+1)s_i(2n-s_2-s_i-3)^2 \\
&- \sum_{i=3}^{k} s_1s_i(2n-s_1-s_i-2)^2 - \sum_{i=3}^{k} s_2s_i(2n-s_2-s_i-2)^2 \\
&= (s_1-s_2-1)[(5n+3p-12)p + (n+p-2)^2 \\
&+ (7n+8m-12)\sum_{i=3}^{k} s_i + (\sum_{i=3}^{k} s_i)^2 + \sum_{i=3}^{k} s_i(3\sum_{i=3}^{k} s_i - 4s_i) \\
&= (s_1-s_2-1)[(n-2)^2 + (7n-16)m + 4m^2 \\
&+ (7n+8m-12)\sum_{i=3}^{k} s_i + 4(\sum_{i=3}^{k} s_i)^2 - 4\sum_{i=3}^{k} s_i^2] \\
&> (s_1-s_2-1)[(n-2)^2 + (4n-8)m + 4m^2] \\
&= (s_1-s_2-1)(n-2+2m)^2 > 0. \quad \square
\end{aligned}$$

Note that we have $n - m = sk + t = (k-t)s + t(s+1)$, where s is a positive integer and t is a non-negative integer with $0 \leq t < k$. For simplicity, we write $K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}]) = K_m \vee (K_k[\underbrace{O_s, \cdots, O_s}_{k-t}, \underbrace{O_{s+1}, \cdots, O_{s+1}}_{t}])$. Then, the extremal value and the corresponding graph of the reformulated first Zagreb index $\widetilde{M}_1(G)$ can be shown as follows.

Theorem 2. *Let G be an arbitrary graph in $\mathscr{G}_{n,m,k}$. Then:*

$$\begin{aligned}
\widetilde{M}_1(G) \leq \frac{m(m-1)}{2}&(2n-4)^2 + m(n-m)(6n-3s-11) \\
&+ 2(n-m)(n-m-s)(n-s-1)^2 \\
&+ t(s+1)[-6(n-s-1)^2 + n + 2m(5-2n+s) + (t-2)(s+1)],
\end{aligned}$$

with the equality holding if and only if $G \cong K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Proof. By Lemmas 1, 3, and Theorem 1, the extremal graph having the maximum reformulated first Zagreb index in $\mathscr{G}_{n,m,k}$ is the graph $K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Let $\widehat{G} = K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Then, we obtain that:

$$\begin{aligned}\widetilde{M}_1(\widehat{G}) &= \frac{m(m-1)}{2}(2n-4)^2 + (k-t)ms(2n-s-3)^2 \\ &+ tm(s+1)(2n-s-4)^2 + \frac{t(t-1)}{2}(s+1)^2(2n-2s-4)^2 \\ &+ \frac{(k-t)(k-t-1)}{2}s^2(2n-2s-2)^2 + t(k-t)s(s+1)(2n-2s-3)^2 \\ &= \frac{m(m-1)}{2}(2n-4)^2 + m(n-m)(6n-3s-11) \\ &+ 2(n-m)(n-m-s)(n-s-1)^2 \\ &+ t(s+1)[-6(n-s-1)^2 + n + 2m(5-2n+s) + (t-2)(s+1)]. \quad \square\end{aligned}$$

Theorem 3. *Let* $\widehat{G}$ *be a graph of order* $n > 2$, *and the join of a complete graph with order* m *and a complete* k*-partite graph with order* $n-m$ *in* $\mathscr{G}_{n,m,k}$, *i.e.,* $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$. *If* $s_1 - 1 \geq s_2 + 1$, *by moving one vertex from the part of* O_{s_1} *to the part of* O_{s_2}, *we get a new graph* $\widetilde{G} = K_m \vee (K_k[O_{s_1-1}, O_{s_2+1}, \cdots, O_{s_k}])$. *Then,* $\Pi_1^*(\widetilde{G}) > \Pi_1^*(\widehat{G})$.

Proof. By the definition of the multiplicative-sum Zagreb index $\Pi_1^*(G)$, it is easy to see that:

$$\Pi_1^*(\widehat{G}) = (2n-2)^{\frac{m(m-1)}{2}} \Pi_{i=1}^k (2n-s_i-1)^{ms_i} \Pi_{1 \leq i < j \leq k} (2n-s_i-s_j)^{s_i s_j}.$$

Hence,

$$\begin{aligned}\frac{\Pi_1^*(\widetilde{G})}{\Pi_1^*(\widehat{G})} &= (2n-s_1-s_2)^{(s_1-s_2-1)} \frac{2n-s_2-2}{2n-s_1-1} a^{m(s_1-1)} b^{ms_2} \\ &\quad \Pi_{i=3}^k c^{(s_1-1)s_i} \Pi_{i=3}^k d^{s_2 s_i} \Pi_{i=3}^k \left(\frac{2n-s_2-s_i-1}{2n-s_1-s_i}\right)^{s_i} \\ &\quad > (ab)^{ms_2} \Pi_{i=3}^k (cd)^{s_2 s_i},\end{aligned}$$

where $a = \frac{2n-s_1}{2n-s_1-1}, b = \frac{2n-s_2-2}{2n-s_2-1}, c = \frac{2n-s_1-s_i+1}{2n-s_1-s_i}, d = \frac{2n-s_2-s_i-1}{2n-s_2-s_i}$.

By a simple calculation, we have:

$$(2n-s_1)(2n-s_2-2) - (2n-s_1-1)(2n-s_2-1) = s_1 - s_2 - 1 > 0,$$

$$(2n-s_1-s_i+1)(2n-s_2-s_i-1) - (2n-s_1-s_i)(2n-s_2-s_i) = s_1 - s_2 - 1 > 0.$$

Therefore, $\frac{\Pi_1^*(\widetilde{G})}{\Pi_1^*(\widehat{G})} > 1$. $\square$

Theorem 4. *Let* G *be an arbitrary graph in* $\mathscr{G}_{n,m,k}$. *Then:*

$$\begin{aligned}\Pi_1^*(G) &\leq (2n-2)^{\frac{m(m-1)}{2}} (2n-s-1)^{ms(k-t)} (2n-s-2)^{m(s+1)t} \\ &\quad (2n-2s)^{\frac{s^2(k-t)(k-t-1)}{2}} (2n-2s-2)^{\frac{(s+1)^2 t(t-1)}{2}} (2n-2s-1)^{s(s+1)t(k-t)},\end{aligned}$$

with the equality holding if and only if $G \cong K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Proof. By Lemmas 1, 4, and Theorem 3, the extremal graph having the maximum multiplicative-sum Zagreb index in $\mathscr{G}_{n,m,k}$ should be the graph $K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Let $\widehat{G} = K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$. We get that,

$$\Pi_1^*(\widehat{G}) = (2n-2)^{\frac{m(m-1)}{2}}(2n-s-1)^{ms(k-t)}(2n-s-2)^{m(s+1)t}$$
$$(2n-2s)^{\frac{s^2(k-t)(k-t-1)}{2}}(2n-2s-2)^{\frac{(s+1)^2 t(t-1)}{2}}(2n-2s-1)^{s(s+1)t(k-t)}. \quad \square$$

3.2. The General Laplacian-Energy-Like Invariant and k-Partiteness

The general Laplacian-energy-like invariant (also called the sum of powers of the Laplacian eigenvalues) of a graph G is defined by Zhou [18] as:

$$S_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha,$$

where α is an arbitrary real number.

$S_\alpha(G)$ is the Laplacian-energy-like invariant [19], and the Laplacian energy [20] when $\alpha = \frac{1}{2}$ and $\alpha = 2$, respectively. For $\alpha = -1$, $nS_{-1}(G)$ is equal to the Kirchhoff index [21], and $\alpha = 1$, $\frac{1}{2}S_1(G)$ is equal to the number of edges in G. For some recent results on the general Laplacian-energy-like invariant, one can see [22–25].

Lemma 5. *[18] Let G be a graph with $u, v \in V(G)$. If $uv \in E(\overline{G})$, then $S_\alpha(G) > S_\alpha(G+uv)$ for $\alpha < 0$, and $S_\alpha(G) < S_\alpha(G+uv)$ for $\alpha > 0$.*

Lemma 6. *[26] If $\mu_1 \geq \cdots \geq \mu_{i-1} \geq \mu_i = 0$ are the Laplacian eigenvalues of graph G and $\mu_1' \geq \cdots \geq \mu_{j-1}' \geq \mu_j' = 0$ are the Laplacian eigenvalues of graph G', then the Laplacian eigenvalues of $G \vee G'$ are:*

$$i+j, \mu_1+j, \mu_2+j, \cdots, \mu_{i-1}+j, \mu_1'+i, \mu_2'+i, \cdots, \mu_{j-1}'+i, 0.$$

It is well known that Laplacian eigenvalues of the complete graph K_p are $0, p, \cdots, p$, and Laplacian eigenvalues of O_p are $0, 0, \cdots, 0$. Then, the Laplacian eigenvalues of $K_{s_1,s_2} = O_{s_1} \vee O_{s_2}$ are $s_1 + s_2, s_2, \cdots, s_2, s_1, \cdots, s_1, 0$, where the multiplicity of s_2 is $s_1 - 1$ and the multiplicity of s_1 is $s_2 - 1$. The Laplacian eigenvalues of $K_{s_1,s_2,s_3} = K_{s_1,s_2} \vee O_{s_3}$ are $s_1+s_2+s_3, s_1+s_2+s_3, s_2+s_3, \cdots, s_2+s_3, s_1+s_3, \cdots, s_1+s_3, 0$, where the multiplicity of s_2+s_3 is $s_1 - 1$ and the multiplicity of s_1+s_3 is $s_2 - 1$.

By induction, we have that the Laplacian eigenvalues of $K_{s_1,\cdots,s_k}$ are $\sum_{i=1}^k s_i, \cdots, \sum_{i=1}^k s_i, \sum_{i=1}^k s_i - s_1, \cdots, \sum_{i=1}^k s_i - s_1, \cdots, \sum_{i=1}^k s_i - s_k, \cdots, \sum_{i=1}^k s_i - s_k, 0$, where the multiplicity of $\sum_{i=1}^k s_i$ is $k-1$ and the multiplicity of $\sum_{i=1}^k s_i - s_j$ is $s_j - 1$, for $1 \leq j \leq k$.

From Lemma 6 and the above analysis, we obtain the following lemma.

Lemma 7. *Let $\widehat{G}$ be a graph of order n, and the join of a complete graph with order m and a complete k-partite graph with order $n-m$ i.e., $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$. Then, the Laplacian eigenvalues of $\widehat{G}$ are $n, \cdots, n, n-s_1, \cdots, n-s_1, \cdots, n-s_k, \cdots, n-s_k, 0$, where the multiplicity of n is $m+k-1$ and the multiplicity of $n-s_j$ is $s_j - 1$, for $1 \leq j \leq k$.*

Theorem 5. *Let $\widehat{G}$ be a graph of order $n > 2$, and the join of a complete graph with order m and a complete k-partite graph with order $n-m$ in $\mathscr{G}_{n,m,k}$, i.e., $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$. If $s_1 - 1 \geq s_2 + 1$, by moving* *one vertex from the part of* O_{s_1} *to the part of* O_{s_2}*, we get a new graph* $\widetilde{G} = K_m \vee (K_k[O_{s_1-1}, O_{s_2+1}, \cdots, O_{s_k}])$*. Then,* $S_\alpha(\widetilde{G}) < S_\alpha(\widehat{G})$ *for* $\alpha < 0$*, and* $S_\alpha(\widetilde{G}) > S_\alpha(\widehat{G})$ *for* $0 < \alpha < 1$*.*

Proof. By the definition of the general Laplacian-energy-like invariant $S_\alpha(G)$ and Lemma 7, we conclude that:

$$S_\alpha(\widehat{G}) = (m+k-1)n^\alpha + \sum_{i=1}^{k}(s_i-1)(n-s_i)^\alpha.$$

Therefore:

$$\begin{aligned} S_\alpha(\widetilde{G}) - S_\alpha(\widehat{G}) &= (s_1-2)(n-s_1+1)^\alpha + s_2(n-s_2-1)^\alpha \\ &\quad - (s_1-1)(n-s_1)^\alpha - (s_2-1)(n-s_2)^\alpha \\ &= (s_1-2)[(n-s_1+1)^\alpha - (n-s_1)^\alpha] \\ &\quad + (s_2-1)[(n-s_2-1)^\alpha - (n-s_2)^\alpha] + (n-s_2-1)^\alpha - (n-s_1)^\alpha. \end{aligned}$$

For $\alpha < 0$, we have:

$$\begin{aligned} S_\alpha(\widetilde{G}) - S_\alpha(\widehat{G}) &< (s_1-2)[(n-s_1+1)^\alpha - (n-s_1)^\alpha] + (s_2-1)[(n-s_2-1)^\alpha - (n-s_2)^\alpha] \\ &< (s_1-2)[(n-s_1+1)^\alpha - (n-s_1)^\alpha + (n-s_2-1)^\alpha - (n-s_2)^\alpha] \\ &= (s_1-2)[f(n-s_1) - f(n-s_2-1)], \end{aligned}$$

where $f(x) = (x+1)^\alpha - x^\alpha$, $f'(x) = \alpha(x+1)^{\alpha-1} - \alpha x^{\alpha-1} > 0$.

Then, $f(n-s_1) < f(n-s_2-1)$, and $S_\alpha(\widetilde{G}) < S_\alpha(\widehat{G})$.

For $0 < \alpha < 1$, we have:

$$\begin{aligned} S_\alpha(\widetilde{G}) - S_\alpha(\widehat{G}) &> (s_1-2)[(n-s_1+1)^\alpha - (n-s_1)^\alpha] + (s_2-1)[(n-s_2-1)^\alpha - (n-s_2)^\alpha] \\ &> (s_2-1)[(n-s_1+1)^\alpha - (n-s_1)^\alpha + (n-s_2-1)^\alpha - (n-s_2)^\alpha] \\ &= (s_2-1)[f(n-s_1) - f(n-s_2-1)], \end{aligned}$$

where $f(x) = (x+1)^\alpha - x^\alpha$, $f'(x) = \alpha(x+1)^{\alpha-1} - \alpha x^{\alpha-1} < 0$.

Then, $f(n-s_1) > f(n-s_2-1)$, and $S_\alpha(\widetilde{G}) > S_\alpha(\widehat{G})$. □

Theorem 6. *Let G be an arbitrary graph in* $\mathscr{G}_{n,m,k}$*. Then,*
for $\alpha < 0, S_\alpha(G) \geq (m+k-1)n^\alpha + (k-t)(s-1)(n-s)^\alpha + ts(n-s-1)^\alpha$*,*
for $0 < \alpha < 1, S_\alpha(G) \leq (m+k-1)n^\alpha + (k-t)(s-1)(n-s)^\alpha + ts(n-s-1)^\alpha$*,*
with the equality holding if and only if $G \cong K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$*.*

Proof. By Lemmas 1, 2, and Theorem 5, the extremal graph having the extremal value of the general Laplacian-energy-like invariant in $\mathscr{G}_{n,m,k}$ should be the graph $K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Let $\widehat{G} = K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$, then we can verify that
$S_\alpha(\widehat{G}) = (m+k-1)n^\alpha + (k-t)(s-1)(n-s)^\alpha + ts(n-s-1)^\alpha$. □

3.3. The General Zeroth-Order Randić Index and k-Partiteness

The general zeroth-order Randić index is introduced by Li [27] as:

$$^0R_\alpha(G) = \sum_{u \in V(G)} (d_G(u))^\alpha,$$

where α is a non-zero real number.

${}^0R_\alpha(G)$ is the inverse degree [28], the zeroth-Randić index [29], the first Zagreb index [30], and the forgotten index [31] when $\alpha = -1, \alpha = -\frac{1}{2}, \alpha = 2$, and $\alpha = 3$, respectively. For some recent results on the general zeroth-order Randić index, one can see [32–34].

Lemma 8. *Let G be a graph with $u, v \in V(G)$. If $uv \in E(\overline{G})$, then ${}^0R_\alpha(G) > {}^0R_\alpha(G+uv)$ for $\alpha < 0$, and ${}^0R_\alpha(G) < {}^0R_\alpha(G+uv)$ for $\alpha > 0$.*

Theorem 7. *Let $\widehat{G}$ be a graph of order $n > 2$, and the join of a complete graph with order m and a complete k-partite graph with order $n-m$ in $\mathcal{G}_{n,m,k}$, i.e., $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$. If $s_1 - 1 \geq s_2 + 1$, by moving one vertex from the part of O_{s_1} to the part of O_{s_2}, we get a new graph $\widetilde{G} = K_m \vee (K_k[O_{s_1-1}, O_{s_2+1}, \cdots, O_{s_k}])$. Then, ${}^0R_\alpha(\widetilde{G}) < {}^0R_\alpha(\widehat{G})$ for $\alpha < 0$, and ${}^0R_\alpha(\widetilde{G}) > {}^0R_\alpha(\widehat{G})$ for $0 < \alpha < 1$.*

Proof. By the definition of the general zeroth-order Randić index ${}^0R_\alpha(G)$, we have:

$$ {}^0R_\alpha(\widehat{G}) = m(n-1)^\alpha + \sum_{i=1}^{k} s_i(n-s_i)^\alpha $$

Then,

$$ \begin{aligned} {}^0R_\alpha(\widetilde{G}) - {}^0R_\alpha(\widehat{G}) &= (s_1-1)(n-s_1+1)^\alpha - s_1(n-s_1)^\alpha \\ &\quad + (s_2+1)(n-s_2-1)^\alpha - s_2(n-s_2)^\alpha \\ &= (n-s_2-1)^\alpha - (n-s_1)^\alpha \\ &\quad + (s_1-1)[(n-s_1+1)^\alpha - (n-s_1)^\alpha] + s_2[(n-s_2-1)^\alpha - (n-s_2)^\alpha]. \end{aligned} $$

For $\alpha < 0$, we have:

$$ \begin{aligned} {}^0R_\alpha(\widetilde{G}) - {}^0R_\alpha(\widehat{G}) &< (s_1-1)[(n-s_1+1)^\alpha - (n-s_1)^\alpha + (n-s_2-1)^\alpha - (n-s_2)^\alpha] \\ &= (s_1-1)[f(n-s_1) - f(n-s_2-1)], \end{aligned} $$

where $f(x) = (x+1)^\alpha - x^\alpha$, $f'(x) = \alpha(x+1)^{\alpha-1} - \alpha x^{\alpha-1} > 0$. Then, $f(n-s_1) < f(n-s_2-1)$, ${}^0R_\alpha(\widetilde{G}) < {}^0R_\alpha(\widehat{G})$.

For $0 < \alpha < 1$, we have:

$$ \begin{aligned} {}^0R_\alpha(\widetilde{G}) - {}^0R_\alpha(\widehat{G}) &> s_2[(n-s_1+1)^\alpha - (n-s_1)^\alpha + (n-s_2-1)^\alpha - (n-s_2)^\alpha] \\ &= s_2[f(n-s_1) - f(n-s_2-1)], \end{aligned} $$

where $f(x) = (x+1)^\alpha - x^\alpha$, $f'(x) = \alpha(x+1)^{\alpha-1} - \alpha x^{\alpha-1} < 0$.

Then, $f(n-s_1) > f(n-s_2-1)$, $R_\alpha(\widetilde{G}) > R_\alpha(\widehat{G})$. □

Theorem 8. *Let G be an arbitrary graph in $\mathcal{G}_{n,m,k}$. Then,*
for $\alpha < 0$, ${}^0R_\alpha(G) \geq m(n-1)^\alpha + (k-t)s(n-s)^\alpha + t(s+1)(n-s-1)^\alpha$,
for $0 < \alpha < 1$, ${}^0R_\alpha(G) \leq m(n-1)^\alpha + (k-t)s(n-s)^\alpha + t(s+1)(n-s-1)^\alpha$,
with the equality holding if and only if $G \cong K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Proof. By Lemma 8 and Theorem 7, in view of Lemmas 1 and 2, the extremal graph having the extremal value of the general zeroth-order Randić index in $\mathcal{G}_{n,m,k}$ should be the graph $K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Let $\widehat{G} = K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$. By a simple calculation, we have ${}^0R_\alpha(\widehat{G}) = m(n-1)^\alpha + (k-t)s(n-s)^\alpha + t(s+1)(n-s-1)^\alpha$. □

3.4. The Modified-Wiener Index and k-Partiteness

The modified-Wiener index is defined by Gutman [35] as:

$$W_\lambda(G) = \sum_{u,v \in V(G)} d_G^\lambda(u,v),$$

where λ is a non-zero real number.

Lemma 9. *Let G be a graph with $u, v \in V(G)$. If $uv \in E(\overline{G})$, then $W_\lambda(G) < W_\lambda(G+uv)$ for $\lambda < 0$, and $W_\lambda(G) > W_\lambda(G+uv)$ for $\lambda > 0$.*

Theorem 9. *Let $\widehat{G}$ be a graph of order $n > 2$, and the join of a complete graph with order m and a complete k-partite graph with order $n-m$ in $\mathscr{G}_{n,m,k}$, i.e., $\widehat{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}])$. If $s_1 - 1 \geq s_2 + 1$, by moving one vertex from the part of O_{s_1} to the part of O_{s_2}, we get a new graph $\widetilde{G} = K_m \vee (K_k[O_{s_1-1}, O_{s_2+1}, \cdots, O_{s_k}])$. Then, $W_\lambda(\widetilde{G}) > W_\lambda(\widehat{G})$ for $\lambda < 0$, and $W_\lambda(\widetilde{G}) < W_\lambda(\widehat{G})$ for $\lambda > 0$.*

Proof. By the definition of the modified-Wiener index $W_\lambda(G)$, we have the following result.

$$W_\lambda(\widehat{G}) = \frac{m(m-1)}{2} + \sum_{i=1}^{k} \frac{s_i(s_i-1)}{2} 2^\lambda + \sum_{i=1}^{k} ms_i + \sum_{1 \leq i < j \leq k} s_i s_j$$

Then,

$$\begin{aligned}
W_\lambda(\widetilde{G}) - W_\lambda(\widehat{G}) &= \frac{(s_1-1)(s_1-2)}{2} 2^\lambda + \frac{(s_2+1)s_2}{2} 2^\lambda + m(s_1-1) \\
&\quad + m(s_2+1) + (s_1-1)(s_2+1) + \sum_{i=3}^{k} (s_1-1)s_i + \sum_{i=3}^{k} (s_2+1)s_i \\
&\quad - \frac{s_1(s_1-1)}{2} 2^\lambda - \frac{s_2(s_2-1)}{2} 2^\lambda - ms_1 - ms_2 - s_1 s_2 - \sum_{i=3}^{k} s_1 s_i - \sum_{i=3}^{k} s_2 s_i \\
&= (s_1 - s_2 - 1)(1 - 2^\lambda).
\end{aligned}$$

For $\lambda > 0$, we have $W_\lambda(\widetilde{G}) < W_\lambda(\widehat{G})$. For $\lambda < 0$, we have $W_\lambda(\widetilde{G}) > W_\lambda(\widehat{G})$. □

Theorem 10. *Let G be an arbitrary graph in $\mathscr{G}_{n,m,k}$. Then,*
for $\alpha < 0$, $W_\lambda(G) \leq \frac{1}{2}[m(m-1) + (n-m)(n+m-s) - (s+1)t + s(n-m+t-k)2^\lambda]$,
for $\alpha > 0$, $W_\lambda(G) \geq \frac{1}{2}[m(m-1) + (n-m)(n+m-s) - (s+1)t + s(n-m+t-k)2^\lambda]$,
with the equality holding if and only if $G \cong K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Proof. By Lemma 9 and Theorem 9, in view of Lemmas 1 and 2, the extremal graph having the extremal value of the modified-Wiener index in $\mathscr{G}_{n,m,k}$ should be the graph $K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$.

Let $\widehat{G} = K_m \vee (K_k[\{k-t\}O_s, \{s\}O_{s+1}])$. Consequently, we have that:

$$\begin{aligned}
W_\lambda(\widehat{G}) &= \frac{m(m-1)}{2} + (k-t)\frac{s(s-1)}{2} 2^\lambda + t\frac{s(s+1)}{2} 2^\lambda + tm(s+1) + (k-t)ms \\
&= \frac{1}{2}[m(m-1) + (n-m)(n+m-s) - (s+1)t + s(n-m+t-k)2^\lambda]. \quad \square
\end{aligned}$$

4. Conclusions

In this paper, we consider connected graphs of order n with vertex k-partiteness not more than m and characterize some extremal monotonic graph invariants such as the reformulated first Zagreb index, the multiplicative-sum Zagreb index, the general Laplacian-energy-like invariant, the general zeroth-order Randić index, and the modified-Wiener index among these graphs, and we investigate the corresponding extremal graphs of these invariants.

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