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

1. Introduction

All graphs considered in this paper are simple, undirected, and connected. Let G be a graph with vertex set \( V(G) = \{v_1, \ldots , v_n\} \) and edge set \( E(G) = \{e_1, \ldots , e_m\} \). 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 \( (H) \), 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 \( D(G) = \text{diag}(d_1, d_2, \ldots , d_n) \) 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 \( \mu_1, \ldots , \mu_n \), 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 \( U_1, \ldots , U_k \). 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 \( K_{s_1, \ldots , s_k} \), is a \( k \)-partite graph with \( k \) different independent sets \( |U_1| = s_1, \ldots , |U_k| = s_k \), 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
Then, there exists \( k \) positive integers such that the modified-Wiener index, the signless Laplacian spectral radius, the Kirchhoff index, the spectral radius, the eccentricity-based topological indices of graphs. Let \( G + uv \) be the graph obtained from \( G \) by adding an edge \( uv \in E(G) \). Let \( I(G) \) be a graph invariant, if \( I(G + uv) > I(G) \) (or \( I(G + uv) < I(G) \), respectively) for any edge \( uv \in E(G) \), then we call \( I(G) \) a monotonic increasing (or decreasing, respectively) graph invariant with the addition of edges [5]. Let \( \mathcal{G}_{n,m,k} \) 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 \( \mathcal{G}_{n,m,k} \), such as the Kirchhoff index, the spectral radius, the signless Laplacian spectral radius, the modified-Wiener index, the eccentricity-based topological indices of chemical networks and their applications. Let \( G \) be an arbitrary graph in \( \mathcal{G}_{n,m,k} \), such as the \( k \)-partite graph with \( k \)-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 \( \mathcal{G}_{n,m,k} \).

### 2. Preliminaries

The join of two-vertex-disjoint graphs \( G_1, G_2 \), denoted by \( G = G_1 \cup G_2 \), 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 \( V(G) = \bigcup_{j=1}^{k} V(G_j) \) and:

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

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 \( \mathcal{G}_{n,m,k} \) and \( I(G) \) be a monotonic increasing graph invariant. Then, there exists \( k \) positive integers \( s_1, \cdots, s_k \) satisfying \( \sum_{i=1}^{k} s_i = n - m \), such that \( I(G) \leq I(\hat{G}) \) holds for all graphs \( G \in \mathcal{G}_{n,m,k} \), where \( \hat{G} = K_m \cup (K_k [O_{s_1}, \cdots, O_{s_k}]) \in \mathcal{G}_{n,m,k} \), with equality holds if and only if \( G \cong \hat{G} \).

**Proof.** Choose \( \tilde{G} \in \mathcal{G}_{n,m,k} \) with the maximum value of a monotonic increasing graph invariant such that \( I(G) \leq I(\tilde{G}) \) for all \( G \in \mathcal{G}_{n,m,k} \). Assume that the \( k \)-partiteness of graph \( \tilde{G} \) is \( m' \), then there exists a vertex set \( U \) of graph \( \tilde{G} \) with order \( m' \) such that \( \tilde{G} - U \) 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, \( n = \sum_{i=1}^{k} s_i + m' \).

Firstly, we claim that \( \tilde{G} - U = K_k [O_{s_1}, \cdots, O_{s_k}] \). Otherwise, there exists at least two vertices \( u \in U_i \) and \( v \in U_j \), for some \( i \neq j \), which are not adjacent in \( \tilde{G} \). By joining the vertices \( u \) and \( v \), we get a new graph \( \tilde{G} + uv \), obviously, \( \tilde{G} + uv \in \mathcal{G}_{n,m,k} \). Then, \( I(\tilde{G}) < I(\tilde{G} + uv) \), 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 \( \tilde{G} + uv \), obviously, \( \tilde{G} + uv \in \mathcal{G}_{n,m,k} \). Then, we have \( I(\tilde{G}) < I(\tilde{G} + uv) \), a contradiction again.
Using a similar method, we can get $\tilde{G} = K_{m'} \vee (K_k[O_{s_1}, \ldots, O_{s_k}])$.

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 $\tilde{G} = K_{m'+1} \vee (K_k[O_{s_1}, O_{s_2}, \ldots, O_{s_k}])$. It is easy to check that $\tilde{G} \in \mathcal{G}_{n,m,k}$ has $s_1 - 1$ edges more than the graph $\hat{G}$. By the definition of the monotonic increasing graph invariant, we get $I(\tilde{G}) < I(\hat{G})$, which is obviously another contradiction.

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

The proof of the lemma is completed. \(\square\)

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

### 3. Main Results

In this section, we will characterize the graphs with an extremal monotonic increasing (or decreasing, respectively) graph invariant in $\mathcal{G}_{n,m,k}$. 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 $\pi$-electron energy on the molecular orbitals, introduced by Gutman and Trinajstić [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 $d_G(e) = d_G(u) + d_G(v) - 2$. Milčević et al. [10] introduced the reformulated first Zagreb index, defined as:

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

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 $\mathcal{M}_1(G) < \mathcal{M}_1(G + uv)$.

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

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

Theorem 1. Let $\hat{G}$ 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., $\hat{G} = K_m \vee (K_k | O_{s_1}, \cdots, O_{s_k})$. By moving one vertex from the part of $O_{s_1}$ to the part of $O_{s_2}$, we get a new graph $\tilde{G} = K_m \vee (K_k | O_{s_1-1}, O_{s_2+1}, \cdots, O_{s_k})$. If $s_1 - 1 \geq s_2 + 1$, then $\mathcal{M}_1(\tilde{G}) > \mathcal{M}_1(\hat{G})$.

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

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

Therefore,

$$\mathcal{M}_1(\tilde{G}) - \mathcal{M}_1(\hat{G}) = m(s_1 - 1)(2n - s_1 - 2)^2 + m(s_2 + 1)(2n - s_2 - 4)^2$$  

$$+(s_1 - 1)(s_2 + 1)(2n - s_1 - s_2 - 2)^2 - ms_1(2n - s_1 - 3)^2$$  

$$+ ms_2(2n - s_2 - 3)^2 - s_1s_2(2n - s_1 - s_2 - 2)^2$$  

$$+ \sum_{i=3}^k (s_1 - 1)s_i(2n - s_1 - s_i - 1)^2 + \sum_{i=5}^k (s_2 + 1)s_i(2n - s_2 - s_i - 3)^2$$  

$$- \sum_{i=3}^k s_1s_i(2n - s_1 - s_i - 2)^2 - \sum_{i=3}^k s_2s_i(2n - s_2 - s_i - 2)^2$$  

$$= (s_1 - s_2 - 1)(5n + 3p - 12)p + (n + p - 2)^2$$  

$$+(7n + 8m - 12) \sum_{i=3}^k s_i + \sum_{i=3}^k s_i^2 + \sum_{i=3}^k s_i(3 \sum_{i=3}^k s_i - 4s_i)$$  

$$= (s_1 - s_2 - 1)(n - 2)^2 + (7n - 16)m + 4m^2$$  

$$+(7n + 8m - 12) \sum_{i=3}^k s_i + 4(\sum_{i=3}^k s_i^2 - \sum_{i=3}^k s_i^3)$$  

$$> (s_1 - s_2 - 1)(n - 2)^2 + (4n - 8)m + 4m^2$$  

$$= (s_1 - s_2 - 1)(n - 2 + 2m)^2 > 0. \quad \Box$$

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 $K_m \vee (K_k | (k - t)O_{s} \{s\}O_{s+1}) = K_m \vee (K_k | O_{s}, \cdots, O_{s}, O_{s+1}, \cdots, O_{s+1})$. Then, the extremal value and the corresponding graph of the reformulated first Zagreb index $\mathcal{M}_1(G)$ can be shown as follows.

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

$$\mathcal{M}_1(G) \leq \frac{m(m-1)}{2}(2n-4)^2 + m(n-m)(6n-3s-11)$$  

$$+ 2(n-m)(n-m-s)(n-s-1)^2$$  

$$+ t(s+1)(-6(n-s-1)^2 + n + 2m(5 - 2n + s) + (t-2)(s+1),$$  

$$where$$

$$s_1, \cdots, s_k$$

are positive integers with $\sum_{i=1}^k s_i = n - m$.
Then, \[ \Pi_{G} = \text{max} \] 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 \( \mathcal{G}_{n,m,k} \) is the graph \( K_{m} \vee (K_{k}\{k-t\}O_{s}, \{s\}O_{s+1}) \).

Let \( \tilde{G} = K_{m} \vee (K_{k}\{k-t\}O_{s}, \{s\}O_{s+1}) \).

Then, we obtain that:

\[
\tilde{M}_{1}(\tilde{G}) = \frac{m(m-1)}{2} (2n-2)^{2} + (k-t)ms(2n-s-3)^{2}
+ tm(s+1)(2n-s-4)^{2} + \frac{t(t-1)}{2} (s+1)^{2}(2n-2s-4)^{2}
+ \frac{(k-t)(k-t-1)}{2} s^{2}(2n-2s-2)^{2} + t(k-t)s(s+1)(2n-2s-3)^{2}
= \frac{m(m-1)}{2} (2n-2)^{2} + m(n-m)(6n-3s-11)
+ 2(n-m)(n-m-s)(n-s-1)^{2}
+ t(s+1)[-6(n-s-1)^{2} + n + 2m(5-2n+s) + (t-2)(s+1)]. \]

**Theorem 3.** Let \( \tilde{G} \) 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., \( \tilde{G} = K_{m} \vee (K_{k}\{O_{s_{1}}, \ldots, O_{s_{k}}\}) \). 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 \( \tilde{G} = K_{m} \vee (K_{k}\{O_{s_{1}-1}, O_{s_{2}+1}, \ldots, O_{s_{k}}\}) \).

Then, \( \Pi_{1}(\tilde{G}) > \Pi_{1}(\tilde{G}) \).

**Proof.** By the definition of the multiplicative-sum Zagreb index \( \Pi_{1}(G) \), it is easy to see that:

\[
\Pi_{1}(\tilde{G}) = (2n-2)^{\frac{m(m-1)}{2}} \Pi_{i=1}^{k}(2n-s_{i} - 1)^{m_{i}} \Pi_{1<i<j<k}(2n-s_{i} - s_{j})^{s_{i}s_{j}}.
\]

Hence,

\[
\frac{\Pi_{1}(\tilde{G})}{\Pi_{1}(\tilde{G})} = (2n-s_{1} - s_{2})^{(s_{1}-s_{2} - 1)} \frac{2n-s_{2} - 2}{2n-s_{1} - 1} a^{m(s_{1}-1)} b^{m_{2}}
\Pi_{i=3}^{k}(s_{i} - s_{1})^{s_{i}} \Pi_{i=3}^{k}(s_{i} - s_{2})^{s_{i}}
\Pi_{i=3}^{k}(s_{i} - s_{1})^{s_{i}} \Pi_{i=3}^{k}(s_{i} - s_{2})^{s_{i}}
\geq (ab)^{m_{2}} \Pi_{i=3}^{k}(cd)^{s_{i}}.
\]

where \( a = \frac{2n-s_{1} - 1}{2n-s_{2} - 1}, b = \frac{2n-s_{2} - 2}{2n-s_{2} - 1}, c = \frac{2n-s_{1} - s_{2} + 1}{2n-s_{1} - 1}, d = \frac{2n-s_{2} - s_{1} - 1}{2n-s_{2} - 1} \).

By a simple calculation, we have:

\[
(2n-s_{1})(2n-s_{2} - 2) - (2n-s_{1} - 1)(2n-s_{2} - 1) = s_{1} - s_{2} - 1 > 0,
(2n-s_{1} - s_{2} + 1)(2n-s_{2} - s_{1} - 1) - (2n-s_{1} - s_{2})(2n-s_{2} - s_{1}) = s_{1} - s_{2} - 1 > 0.
\]

Therefore, \( \frac{\Pi_{1}(\tilde{G})}{\Pi_{1}(\tilde{G})} > 1 \).

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

\[
\Pi_{1}(G) \leq (2n-2)^{\frac{m(m-1)}{2}} (2n-s-1)^{m(s-k)} (2n-s-2)^{m(s+1)}
(2n-2)^{\frac{2(k-t)(k-t-1)}{2}} (2n-2)^{\frac{(s_{1}-1)^{2}(t-1)}{2}} (2n-2)^{\frac{(s_{2}+1)^{2}(t-1)}{2}} (2n-2)^{\frac{(s_{3}+1)^{2}(t-1)}{2}} (2n-2)^{\frac{(s_{k}+1)^{2}(t-1)}{2}}
\]

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 \( \mathfrak{G}_{n,m,k} \) should be the graph \( K_m \cup (K_k \cup \{k-1\}O_s, \{s\}O_{s+1}) \).

Let \( \hat{G} = K_m \cup (K_k \cup \{k-1\}O_s, \{s\}O_{s+1}) \). We get that,

\[
\Pi^*_k(\hat{G}) = (2n-2)\frac{n(n-1)}{2} (2n-s-1)^{ms(k-1)} (2n-s-2)^{m(s+1)t} \\
(2n-2s)^{\frac{(k-1)(s-1)}{2} - 1} (2n-2s-2)^{s(s+1)t(k-1)}.
\]

\( \square \)

### 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:

\[
S_n(G) = \sum_{\lambda \geq 0} \lambda^n,
\]

where \( \lambda \) is an arbitrary real number.

\( S_n(G) \) 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 \( S_{\alpha}(G) > S_{\alpha}(G + vu) \) for \( \alpha < 0 \), and \( S_{\alpha}(G) < S_{\alpha}(G + u\overline{G}) \) 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 \( G \cup G' \) 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 \( K_{s_1, s_2} = O_{s_1} \cup O_{s_2} \) are \( s_1 + s_2, s_2, \cdots, s_2, s_1, 1 \), where the multiplicity of \( s_2 \) is \( s_1 - 1 \) and the multiplicity of \( s_1 \) is \( s_2 - 1 \). The Laplacian eigenvalues of \( K_{s_1, s_2, s_3} = K_{s_1, s_2} \cup O_{s_3} \) 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 \( \sum_{i=1}^{k} s_i \), \( \cdots \), \( \sum_{i=1}^{k} s_i \), \( \cdots \), \( \sum_{i=1}^{k} s_i - s_1, \cdots, \sum_{i=1}^{k} s_i - s_{k-1}, \cdots, \sum_{i=1}^{k} s_i - s_k, 0 \), 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 \( \hat{G} \) 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., \( \hat{G} = K_m \cup (K_k \cup \{k-1\}O_s, \{s\}O_{s+1}) \). Then, the Laplacian eigenvalues of \( \hat{G} \) 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 \( \hat{G} \) 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 \( \mathfrak{G}_{n,m,k} \) i.e., \( \hat{G} = K_m \cup (K_k \cup \{k-1\}O_s, \{s\}O_{s+1}) \). 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 $\tilde{G} = K_m \lor (K_k[O_{s_1-1}, O_{s_2+1}, \ldots, O_{s_1}])$. Then, $S_\alpha(\tilde{G}) < S_\alpha(\tilde{G})$ for $\alpha < 0$, and $S_\alpha(\tilde{G}) > S_\alpha(\tilde{G})$ for $0 < \alpha < 1$.

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

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

Therefore:

$$S_\alpha(\tilde{G}) - S_\alpha(\tilde{G}) = (s_1 - 2)(n - s_1 + 1)^a + s_2(n - s_2 - 1)^a$$

$$- (s_1 - 1)(n - s_1)^a - (s_2 - 1)(n - s_2)^a$$

$$= (s_1 - 2)(n - s_1)^a - (n - s_1)^a$$

$$+ (s_2 - 1)(n - s_2 - 1)^a - (n - s_2 - 1)^a + (n - s_2 - 1)^a - (n - s_1)^a.$$ 

For $\alpha < 0$, we have:

$$S_\alpha(\tilde{G}) - S_\alpha(\tilde{G}) < (s_1 - 2)[(n - s_1 + 1)^a - (n - s_1)^a] + (s_2 - 1)[(n - s_2 - 1)^a - (n - s_2)^a]$$

$$= (s_1 - 2)[f(n - s_1) - f(n - s_2 - 1)],$$

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

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

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

$$S_\alpha(\tilde{G}) - S_\alpha(\tilde{G}) > (s_1 - 2)[(n - s_1 + 1)^a - (n - s_1)^a] + (s_2 - 1)[(n - s_2 - 1)^a - (n - s_2)^a]$$

$$> (s_2 - 1)[(n - s_2 - 1)^a - (n - s_2 - 1)^a + (n - s_2 - 1)^a - (n - s_2)^a]$$

$$= (s_2 - 1)[f(n - s_1) - f(n - s_2 - 1)],$$

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

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

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

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

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

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

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

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

where $a$ is a non-zero real number.
0Rα(G) is the inverse degree [28], the zeroth-Randić index [29], the first Zagreb index [30], and the forgotten index [31] when α = −1, α = −1/2, α = 2, and α = 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 ∈ V(G). If uv ∈ E(Ḡ), then 0Rα(G) > 0Rα(G + uv) for α < 0, and 0Rα(G) < 0Rα(G + uv) for α > 0.

**Theorem 7.** Let Ġ 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 G κ,m,k, i.e., Ġ = K m ∨ (K k[O s1, . . . , O s k]). If s1 − 1 ≥ s2 + 1, by moving one vertex from the part of O s k to the part of O s1, we get a new graph Ġ = K m ∨ (K k[O s1−1, O s2+1, . . . , O s k]). Then, 0Rα(Ḡ) < 0Rα(Ḡ) for α < 0, and 0Rα(Ḡ) > 0Rα(Ḡ) for 0 < α < 1.

**Proof.** By the definition of the general zeroth-order Randić index 0Rα(G), we have:

\[ 0Rα(Ḡ) = m(n - 1)^α + \sum_{i=1}^{k} s_i(n - s_i)^α \]

Then,

\[ 0Rα(Ḡ) - 0Rα(Ḡ) = (s1 - 1)(n - s1 + 1)^α - s1(n - s1)^α + (s2 + 1)(n - s2 - 1)^α - s2(n - s2)^α = (n - s2 - 1)^α - (n - s1)^α + (s1 - 1)(n - s1 + 1)^α - (n - s1 - 1)^α + s2[(n - s2 - 1)^α - (n - s2)^α]. \]

For α < 0, we have:

\[ 0Rα(Ḡ) - 0Rα(Ḡ) < (s1 - 1)[(n - s1 + 1)^α - (n - s1)^α + (n - s2 - 1)^α - (n - s2)^α] = (s1 - 1)[f(n - s1) - f(n - s2 - 1)], \]

where \( f(x) = (x + 1)^α - x^α \), \( f'(x) = α(x + 1)^{α-1} - αx^{α-1} > 0 \). Then, \( f(n - s1) < f(n - s2 - 1) \), \( 0Rα(Ḡ) < 0Rα(Ḡ). \)

For 0 < α < 1, we have:

\[ 0Rα(Ḡ) - 0Rα(Ḡ) > s2[(n - s1 + 1)^α - (n - s1)^α + (n - s2 - 1)^α - (n - s2)^α] = s2[f(n - s1) - f(n - s2 - 1)], \]

where \( f(x) = (x + 1)^α - x^α \), \( f'(x) = α(x + 1)^{α-1} - αx^{α-1} < 0 \). Then, \( f(n - s1) > f(n - s2 - 1) \), \( Rα(Ḡ) > Rα(Ḡ). \)

**Theorem 8.** Let G be an arbitrary graph in G κ,m,k. Then,

for α < 0, \( 0Rα(G) ≥ m(n - 1)^α + (k - t)s(n - s)^α + t(s + 1)(n - s - 1)^α \),

for 0 < α < 1, \( 0Rα(G) ≤ m(n - 1)^α + (k - t)s(n - s)^α + t(s + 1)(n - s - 1)^α \),

with the equality holding if and only if G ≌ Kn ∨ (K t[O s1, {s}O s1+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 G κ,m,k should be the graph Kn ∨ (K t[O s1, {s}O s1+1]).

Let Ġ = Km ∨ (K t[O s1, {s}O s1+1]). By a simple calculation, we have

\[ 0Rα(Ḡ) = m(n - 1)^α + (k - t)s(n - s)^α + t(s + 1)(n - s - 1)^α. \]
3.4. The Modified-Wiener Index and k-Partiteness

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

\[ W_\lambda(G) = \sum_{u,v \in V(G)} d^\lambda_G(u,v), \]

where \( \lambda \) 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 \( \overline{G} \) 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., \( \overline{G} = K_m \vee (K_k[O_{s_1}, \cdots, O_{s_k}]) \). 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 \( \overline{G}' = K_m \vee (K_k[O_{s_1 - 1}, O_{s_2 + 1}, \cdots, O_{s_k}]) \). Then, \( W_\lambda(\overline{G}) > W_\lambda(\overline{G}') \) for \( \lambda < 0 \), and \( W_\lambda(\overline{G}) < W_\lambda(\overline{G}') \) for \( \lambda > 0 \).

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

\[ W_\lambda(\overline{G}) = \frac{m(m - 1)}{2} + \sum_{i=1}^{k} s_i(s_i - 1)2^\lambda + \sum_{i=1}^{k} ms_i + \sum_{1 \leq i < j \leq k} s_is_j. \]

Then,

\[ W_\lambda(\overline{G}) - W_\lambda(\overline{G}') = \frac{(s_1 - 1)(s_1 - 2)2^\lambda}{2} + \frac{(s_2 + 1)s_22^\lambda}{2} + m(s_1 - 1) \]
\[ + m(s_2 + 1) + (s_1 - 1)(s_2 + 1) + \sum_{i=1}^{k} (s_i - 1)s_i + \sum_{i=3}^{k} (s_i + 1)s_i \]
\[ - \frac{s_1(s_1 - 1)2^\lambda}{2} - \frac{s_2(s_2 - 1)2^\lambda}{2} - ms_1 - ms_2 - s_1s_2 - \sum_{i=3}^{k} s_is_i \]
\[ = (s_1 - s_2 - 1)(1 - 2^\lambda). \]

For \( \lambda > 0 \), we have \( W_\lambda(\overline{G}) < W_\lambda(\overline{G}') \). For \( \lambda < 0 \), we have \( W_\lambda(\overline{G}) > W_\lambda(\overline{G}') \). \( \square \)

**Theorem 10.** Let \( G \) be an arbitrary graph in \( \mathcal{G}_{n,m,k} \). Then,
for \( \lambda < 0 \), \( W_\lambda(G) \leq \frac{1}{2}[m(m - 1) + (n - m)(n + m - s) - (s + 1)t + s(n - m + t - k)2^\lambda] \),
for \( \lambda > 0 \), \( W_\lambda(G) \geq \frac{1}{2}[m(m - 1) + (n - m)(n + m - s) - (s + 1)t + s(n - m + t - k)2^\lambda] \),
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 \( \mathcal{G}_{n,m,k} \) should be the graph \( K_m \vee (K_k[\{k - t\}O_s, \{s\}O_{s+1}]) \). Consequently, we have that:

\[ W_\lambda(\overline{G}) = \frac{m(m - 1)}{2} + (k - t)\frac{s(s - 1)2^\lambda}{2} + \frac{s(s + 1)2^\lambda}{2} + tm(s + 1) + (k - t)ms \]
\[ = \frac{1}{2}[m(m - 1) + (n - m)(n + m - s) - (s + 1)t + s(n - m + t - k)2^\lambda]. \] \( \square \)

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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