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TEMO-TYPE REGULARITY FOR TOPOLOGICAL INDICES

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Abstract. TEMO (topological effect on molecular orbitals) problem is an interesting topic in chemical graph theory. In 2022, Gutman studied TEMO-type regularity for the degree-based topological indices. In this paper, we show that the general TEMO-type regularity holds for the (a, b)-KA index, the A_α-spectral radius and the third leap Zagreb index.

1. Introduction

Let G be a simple graph with the vertex set $V(G)$ and edge set $E(G)$. For any two vertex-disjoint graphs F and H, we assume that u and v are two distinct vertices of F, and p and q are two distinct vertices of H. Then G_1 is the graph obtained from F and H by connecting u with p and v with q. The graph G_2 is obtained analogously, by connecting u with q and v with p, see Figure 1.

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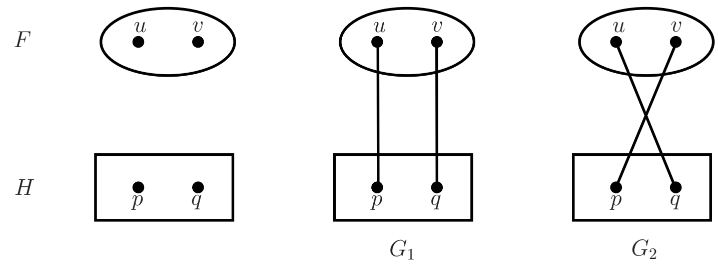

Figure 1. The structure of the graphs G_1 and G_2 and the labeling of their vertices.

In 1982, Polansky and Zander [**9**] studied the property of the graphs G_1 and G_2, and compared the characteristic polynomials of adjacency matrix of G_1 and G_2 in the special case $F \cong H$, that is $\phi(G_2, \lambda) \geqslant \phi(G_1, \lambda)$. Meanwhile, they called this a "topological effect on molecular orbitals" and used the acronym TEMO. After that, Gutman, Graovac and Polansky [**1, 3, 4, 8**] made the research express that the inequality $\phi(G_2, \lambda) \geqslant \phi(G_1, \lambda)$ implies certain regularities for the distribution of the eigenvalues of G_1 and G_2 and have appropriate (experimentally verifiable) consequences on the distribution of the molecular orbital energy levels. Eventually, TEMO regularity problem was extensively studied, see the references in [**2**].

In 2022, Gutman [**2**] studied TEMO-type regularity for the degree based topological index. Let d_u be the degree of the vertex u in G. He showed that a TEMO-type regularity holds for the Sombor index, the second Zagreb index, the Randić index, the reciprocal Randić index, and the Nirmala index under $d_u > d_v$ and $d_p > d_q$ conditions, as indicated in Figure 1. More generally, Wang et al. [**10**] study TEMO-type regularity for the (a, b)-KA index of a graph G, which is defined as

$$KA_{a,b}(G) = \sum_{uv \in E(G)} (d_u^a + d_v^a)^b.$$

For any real $\alpha \in [0, 1]$, Nikiforov [**7**] defined a new matrix $A_\alpha(G)$ as

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G),$$

where $A(G)$ is the adjacency matrix of G and $D(G)$ is the diagonal matrix of the degrees of G. The largest eigenvalue of $A_\alpha(G)$, denoted by $\lambda(A_\alpha(G))$, is called the A_α-spectral radius of G. Since the A_α matrix unifies the adjacency matrix $A_0(G)$ and the signless Laplacian matrix $2A_{1/2}(G)$, the A_α-spectral radius is the generalization of $\lambda(A_0(G))$ and $2\lambda(A_{1/2}(G))$. The second degree of a vertex v in a graph G, denoted by τ_v, is the number of vertices of G whose distance to v is equal to 2. In 2017, Naji et al. [**6**] introduced the concept of the third leap Zagreb index based on the second degrees of vertices, that is,

$$LM_3(G) = \sum_{v \in V(G)} d_v \tau_v = \sum_{uv \in E(G)} (\tau_u + \tau_v).$$

In this paper, we prove that the general TEMO-type regularity holds for the (a, b)-KA index, the A_α-spectral radius and the third leap Zagreb index.

2. Main results

Suppose $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ are two non-increasing sequences of real numbers, we say (x) is majorized by (y), denoted by $(x) \trianglelefteq (y)$, if and only if $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i = \sum_{i=1}^{j} y_i$ for all $1 \leqslant j \leqslant n$. Furthermore, by $(x) \triangleleft (y)$ we mean that $(x) \trianglelefteq (y)$ and (x) is not the rearrangement of (y).

Lemma 2.1. (**[5]**) *Suppose $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ are non-increasing sequences of real numbers. If $(x) \triangleleft (y)$ and f is a strictly convex function, then $\sum_{i=1}^{n} f(x_i) < \sum_{i=1}^{n} f(y_i)$.*

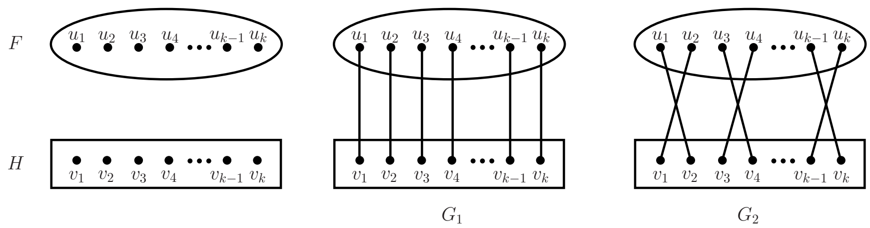

Figure 2. The structure of the graphs G_1 and G_2 and the labeling of their vertices.

Theorem 2.1. *Let F and H be arbitrary vertex-disjoint connected graphs with $V(F) = \{u_1, u_2, \ldots, u_n\}$ and $V(H) = \{v_1, v_2, \ldots, v_n\}$, shown in Figure 2. If $d_{u_1} > d_{u_2} > \cdots > d_{u_k}$ and $d_{v_1} > d_{v_2} > \cdots > d_{v_k}$ for even k, then*
(i) *$KA_{a,b}(G_1) > KA_{a,b}(G_2)$ for $a \neq 0$ and $b \in (-\infty, 0) \cup (1, +\infty)$;*
(ii) *$KA_{a,b}(G_1) < KA_{a,b}(G_2)$ for $a \neq 0$ and $b \in (0, 1)$.*

Proof. (i) Note that $d_{u_1} > d_{u_2} > \cdots > d_{u_k}$ and $d_{v_1} > d_{v_2} > \cdots > d_{v_k}$ for even k. For $a > 0$, we assume that $(x) = (d_{u_1}^a + d_{v_1}^a, d_{u_2}^a + d_{v_2}^a, \ldots, d_{u_k}^a + d_{v_k}^a)$ and $(y) = (d_{u_1}^a + d_{v_2}^a, d_{u_2}^a + d_{v_1}^a, \ldots, d_{u_k}^a + d_{v_{k-1}}^a)$, where the terms in y allow for interchangeability between term 1 and term 2, term 3 and term 4, term 5 and term 6, and so on. For $a < 0$, we assume that $(x) = (d_{u_k}^a + d_{v_k}^a, d_{u_{k-1}}^a + d_{v_{k-1}}^a, \ldots, d_{u_1}^a + d_{v_1}^a)$ and $(y) = (d_{u_k}^a + d_{v_{k-1}}^a, d_{u_{k-1}}^a + d_{v_k}^a, \ldots, d_{u_2}^a + d_{v_1}^a)$, where the terms in y allow for interchangeability between term 1 and term 2, term 3 and term 4, term 5 and term 6, and so on. It is not difficult to find that $(y) \triangleleft (x)$ for $a \neq 0$. Moreover, $f(x) = x^b$ is a strictly convex function for $x > 0$ and $b \in (-\infty, 0) \cup (1, +\infty)$. By Lemma 2.1, we have

$$
\begin{aligned}
& KA_{a,b}(G_1) - KA_{a,b}(G_2) \\
= & (d_{u_1}^a + d_{v_1}^a)^b + (d_{u_2}^a + d_{v_2}^a)^b + \cdots + (d_{u_k}^a + d_{v_k}^a)^b \\
& - (d_{u_1}^a + d_{v_2}^a)^b - (d_{u_2}^a + d_{v_1}^a)^b - \cdots - (d_{u_k}^a + d_{v_{k-1}}^a)^b \\
> & 0.
\end{aligned}
$$

for $b \in (-\infty, 0) \cup (1, +\infty)$.

(ii) Observe that for $x > 0$, and $g(x) = -x^b$ is a strictly convex function if $b \in (0,1)$. Using similar arguments as in the proof of (i), we may prove (ii).

This completes the proof. □

THEOREM 2.2. *Let F and H be arbitrary vertex-disjoint connected graphs and u, v, p, q their vertices, shown in Figure 1. Suppose $|V(F)| + |V(H)| = n$, and $X = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $A_\alpha(G_2)$, where x_i corresponds to the vertex i $(1 \leqslant i \leqslant n)$. If $x_u > x_v$ and $x_p > x_q$, then $\lambda(A_\alpha(G_1)) > \lambda(A_\alpha(G_2))$ for $\alpha \in [0,1)$.*

PROOF. Let $X = (x_1, x_2, \ldots, x_n)^T$ be a unit eigenvector (Perron vector) of $A_\alpha(G_2)$ corresponding to $\lambda(A_\alpha(G_2))$. By the Rayleigh's principle, we have

$$\begin{aligned}
\lambda(A_\alpha(G_2)) &= X^T A_\alpha(G_2) X \\
&= \max_{Y^T Y = 1} Y^T A_\alpha(G_2) Y \\
&= \alpha \sum_{i \in V(G_2)} d_i x_i^2 + 2(1-\alpha) \sum_{ij \in E(G_2)} x_i x_j.
\end{aligned}$$

Thus,

$$\begin{aligned}
\lambda_\alpha(G_1) - \lambda_\alpha(G_2) &\geqslant X^T A(G_1) X - X^T A(G_2) X \\
&= \alpha \sum_{i \in V(G_1)} d_i x_i^2 + 2(1-\alpha) \sum_{ij \in E(G_1)} x_i x_j \\
&\quad -\alpha \sum_{i \in V(G_2)} d_i x_i^2 + 2(1-\alpha) \sum_{ij \in E(G_2)} x_i x_j \\
&= 2(1-\alpha)(x_1 x_p + x_2 x_q - x_1 x_q - x_2 x_p) \\
&= 2(1-\alpha)(x_1 - x_2)(x_p - x_q) \\
&> 0
\end{aligned}$$

for $x_u > x_v$ and $x_p > x_q$. This completes the proof. □

THEOREM 2.3. *Let G_1 and G_2 be arbitrary vertex-disjoint graphs and u, v, p, q their vertices as indicated in Figure 1. If $d_u > d_v$ and $d_p > d_q$, then*

$$LM_3(G_1) > LM_3(G_2).$$

PROOF. Observe first that

$$\begin{aligned}
LM_3(G_1) &= (\tau_u + d_p) + (\tau_p + d_u) + d_u(\tau_u + d_p) + d_p(\tau_p + d_u) \\
&\quad +(\tau_v + d_q) + (\tau_q + d_v) + d_v(\tau_v + d_q) + d_q(\tau_q + d_v) + LM_3^\star, \\
LM_3(G_2) &= (\tau_u + d_q) + (\tau_q + d_u) + d_u(\tau_u + d_q) + d_q(\tau_q + d_u) \\
&\quad +(\tau_v + d_p) + (\tau_p + d_v) + d_v(\tau_v + d_p) + d_p(\tau_p + d_v) + LM_3^\star,
\end{aligned}$$

where $LM_3^\star$ is the sum of the terms $\tau_u + \tau_v$ over other edges of G_1 or G_2. Thus,

$$\begin{aligned} & LM_3(G_1) - LM_3(G_2) \\ &= (d_u+1)[(\tau_u+d_p)-(\tau_u+d_q)] - (d_v+1)[(\tau_v+d_p)-(\tau_v+d_q)] \\ &\quad + (d_p+1)[(\tau_p+d_u)-(\tau_p+d_v)] - (d_q+1)[(\tau_q+d_u)-(\tau_q+d_v)] \\ &= 2(d_u-d_v)(d_p-d_q) \\ &> 0. \end{aligned}$$

Thus, we have $LM_3(G_1) > LM_3(G_2)$. This completes the proof. □

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