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Research Article

A note on polyomino chains with extremum general sum-connectivity index

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Abstract: The general sum-connectivity index of a graph G is defined as $\chi_\alpha(G) = \sum_{uv\in E(G)}(d_u + d_v)^\alpha$ where d_u is degree of the vertex $u \in V(G)$, α is a real number different from 0 and uv is the edge connecting the vertices u, v. In this note, the problem of characterizing the graphs having extremum χ_α values from a certain collection of polyomino chain graphs is solved for $\alpha < 0$. The obtained results together with already known results (concerning extremum χ_α values of polyomino chain graphs) give the complete solution of the aforementioned problem.

Keywords: chemical graph theory, topological index, Randić index, general sum-connectivity index; polyomino chain

AMS Subject classification: 05C50

1. Introduction

All graphs considered in this note are simple, finite and connected. Those notations and terminologies from graph theory which are not defined here can be found in the books [19, 28].

The connectivity index (also known as Randić index and branching index) is one of the most studied graph invariants, which was introduced in 1975 within the study of molecular branching [44]. The connectivity index for a graph G is defined as

$$R(G) = \sum_{uv\in E(G)} (d_u d_v)^{-\frac{1}{2}},$$

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where d_u represents the degree of the vertex $u \in V(G)$ and uv is the edge connecting the vertices u, v of G. Detail about the mathematical properties of this index can be found in the survey [34], recent papers [9, 15, 22, 25, 30, 32, 38] and related references contained therein.

Several modified versions of the connectivity index were appeared in literature. One of such versions is the sum-connectivity index [50], which is defined as

$$\chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-\frac{1}{2}}.$$

Soon after the appearance of sum-connectivity index, its generalized version was proposed [51], whose definition is given as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha,$$

where α is a non-zero real number. In this note, we are concerned with the general sum-connectivity index χ_α. Details about χ_α can be found in the survey [14], recent papers [1–4, 7, 8, 10, 12, 17, 21, 31, 39, 41–43, 45, 46, 49] and related references listed therein. We recall that $2\chi_{-1}(G) = H(G)$, where H is the harmonic index [24], and χ_1 coincides with the first Zagreb index [27], whose mathematical properties can be found in the recent surveys [11, 20] and related references cited therein. It needs to be mentioned here that χ_2 is same as the hyper-Zagreb index, which is a member of the well-studied Zagreb indices; see for example the recent papers [18, 33, 35, 36, 40] about this index.

A polyomino system is a connected geometric figure obtained by concatenating congruent squares side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and a number of finite (internal) regions, and all internal regions must be congruent squares. For possible applications of polyomino systems, see, for example, [26, 29, 37, 48] and related references mentioned therein. Two squares in a polyomino system are adjacent if they share a side. A polyomino chain is a polyomino system in which every square is adjacent to at most two other squares. Every polyomino chain can be represented by a graph known as polyomino chain graph. For the sake of simplicity, in the rest of this note, by the term *polyomino chain* we always mean *polyomino chain graph*.

The problem of characterizing graphs having extremum χ_α values over the collection of certain polyomino chains, with fixed number of squares, was solved in [5, 6, 47] for $\alpha = 1$. The results established in [23] give a solution of the aforementioned problem for $\alpha = -1$. An and Xiong [16] solved this problem for $\alpha > 1$. While, the same problem was also addressed in [13] and its solution for the case $0 < \alpha < 1$ was reported there. The main purpose of the present note is to give the solution of the problem under consideration for all remaining values of α, that is, for $\alpha < -1$ and $-1 < \alpha < 0$.

2. Main Results

Before proving the main results, we recall some definitions concerning polyomino chains. In a polyomino chain, a square adjacent with only one (respectively two) other square(s) is called terminal (respectively non-terminal) square. A kink is a non-terminal square having a vertex of degree 2. A polyomino chain, with n squares, without kinks is called *linear chain* and it is denoted by L_n. A polyomino chain, with n squares, consisting of only kinks and terminal squares is known as zigzag chain and it is denoted by Z_n. A segment is a maximal linear chain in a polyomino chain, including the kinks and/or terminal squares at its ends. The number of squares in a segment S_r is called its length and is denoted by $l(S_r)$ (or simply by l_r). If a polyomino chain B_n has segments $S_1, S_2, ..., S_s$ then the vector $(l_1, l_2, ..., l_s)$ is called length vector of B_n. A segment S_r is said to be external (internal, respectively) segment if S_r contains (does not contain, respectively) terminal square.

Definition 1. [47] For $2 \leq i \leq s-1$ and $1 \leq j \leq s$,

$$\alpha_i = \begin{cases} 1 & \text{if } l_i = 2 \\ 0 & \text{if } l_i \geq 3 \end{cases}$$

$$\beta_j = \begin{cases} 1 & \text{if } l_j = 2 \\ 0 & \text{if } l_j \geq 3 \end{cases}$$

and $\alpha_1 = \alpha_s = 0$.

Let Ω_n be the collection of all those polyomino chains, having n squares, in which no internal segment of length 3 has edge connecting the vertices of degree 3.

Theorem 1. [13] Let $B_n \in \Omega_n$ be a polyomino chain having s segment(s) $S_1, S_2, S_3, ..., S_s$ with the length vector $(l_1, l_2, ..., l_s)$. Then,

$$\begin{aligned} \chi_\alpha(B_n) &= 3 \cdot 6^\alpha n + (2 \cdot 5^\alpha - 6^{\alpha+1} + 4 \cdot 7^\alpha)s + (2 \cdot 4^\alpha + 2 \cdot 5^\alpha + 6^\alpha - 4 \cdot 7^\alpha) \\ &+ (2 \cdot 6^\alpha - 5^\alpha - 7^\alpha)[\beta_1 + \beta_s] + (5 \cdot 6^\alpha - 2 \cdot 5^\alpha - 4 \cdot 7^\alpha + 8^\alpha) \sum_{i=1}^{s} \alpha_i. \end{aligned}$$

Let

$$f(\alpha) = 2 \cdot 5^\alpha - 6^{\alpha+1} + 4 \cdot 7^\alpha, \ g(\alpha) = 2 \cdot 6^\alpha - 5^\alpha - 7^\alpha,$$

$$h(\alpha) = 5 \cdot 6^\alpha - 2 \cdot 5^\alpha - 4 \cdot 7^\alpha + 8^\alpha.$$

Furthermore, let $\Psi_{\chi_\alpha}(S_1) = f(\alpha) + g(\alpha)\beta_1$, $\Psi_{\chi_\alpha}(S_s) = f(\alpha) + g(\alpha)\beta_s$ and for $s \geq 3$, assume that $\Psi_{\chi_\alpha}(S_i) = f(\alpha) + h(\alpha)\alpha_i$ where $2 \leq i \leq s-1$. Then

$$\Psi_{\chi_\alpha}(B_n) = \sum_{i=1}^{s} \Psi_{\chi_\alpha}(S_i) = f(\alpha)s + g(\alpha)(\beta_1 + \beta_s) + h(\alpha) \sum_{i=1}^{s} \alpha_i \ . \quad (1)$$

Hence, the formula given in Theorem 1 can be rewritten as

$$\chi_\alpha(B_n) = 3 \cdot 6^\alpha n + (2 \cdot 4^\alpha + 2 \cdot 5^\alpha + 6^\alpha - 4 \cdot 7^\alpha) + \Psi_{\chi_\alpha}(B_n). \tag{2}$$

The next lemma is a direct consequence of the relation (2).

Lemma 1. [13] For any polyomino chain B_n having $n \geq 3$ squares, $\chi_\alpha(B_n)$ is maximum (respectively minimum) if and only if $\Psi_{\chi_\alpha}(B_n)$ is maximum (respectively minimum).

Lemma 1 will play a vital role in proving the main results of the present note.

Lemma 2. [13] Let $B_n \in \Omega_n$ be a polyomino with $n \geq 3$ squares. If $f(\alpha)$, $f(\alpha) + 2g(\alpha)$ and $f(\alpha) + 2h(\alpha)$ are all negative, then

$$\chi_\alpha(Z_n) \leq \chi_\alpha(B_n) \leq \chi_\alpha(L_n).$$

Right (respectively left) equality holds if and only if $B_n \cong L_n$ (respectively $B_n \cong Z_n$).

Proposition 1. Let $B_n \in \Omega_n$ be a polyomino chain having $n \geq 3$ squares. Let $x_0 \approx -3.09997$ be a root of the equation $f(\alpha) = 0$. Then, for $x_0 < \alpha < 0$, it holds that

$$\chi_\alpha(Z_n) \leq \chi_\alpha(B_n) \leq \chi_\alpha(L_n),$$

with right (respectively left) equality if and only if $B_n \cong L_n$ (respectively $B_n \cong Z_n$).

Proof. It can be easily checked that $f(\alpha)$, $f(\alpha)+2g(\alpha)$ and $f(\alpha)+2h(\alpha)$ are negative for $x_0 < \alpha < 0$, and hence, from Lemma 2, the required result follows. □

Proposition 2. Let $B_n \in \Omega_n$ be a polyomino with $n \geq 3$ squares. Let $x_0 \approx -3.09997$ be a root of the equation $f(\alpha) = 0$. Then, for $\alpha \leq x_0$, the following inequality holds

$$\chi_\alpha(B_n) \geq \chi_\alpha(Z_n),$$

with equality if and only if $B_n \cong Z_n$.

Proof. We note that $f(\alpha)$ is non-negative and both $g(\alpha)$, $h(\alpha)$ are negative for $\alpha \leq x_0 \approx -3.09997$. Suppose that the polyomino chain $B_n^* \in \Omega_n$ has the minimum Ψ_{χ_α} value for $\alpha \leq x_0$. Further suppose that $S_1, S_2, ..., S_s$ be the segments of B_n^* with the length vector $(l_1, l_2, ..., l_s)$. It holds that

$$\Psi_{\chi_\alpha}(Z_n) = 2f(\alpha) + 2g(\alpha) + (n-3)(f(\alpha) + h(\alpha)) \leq 2f(\alpha) + 2g(\alpha) < f(\alpha) = \Psi_{\chi_\alpha}(L_n),$$

which implies that $s \geq 2$.

If at least one of external segments of B_n^* has length greater than 2. Without loss of generality, assume that $l_1 \geq 3$. Then, there exist a polyomino chain $B_n^{(1)} \in \Omega_n$ having length vector $(\underbrace{2, 2, \cdots, 2}_{(l_1-1)-times}, l_2, ..., l_s)$ and

$$\Psi_{\chi_\alpha}(B_n^{(1)}) - \Psi_{\chi_\alpha}(B_n^*) = g(\alpha) + (l_1 - 2)\left(f(\alpha) + h(\alpha)\right) \leq f(\alpha) + g(\alpha) + h(\alpha) < 0,$$

for $\alpha \leq x_0 \approx -3.09997$, which is a contradiction to the definition of B_n^*. Hence both external segments of B_n^* must have length 2.
If some internal segment of B_n^* has length greater than 2, say $l_j \geq 3$ where $2 \leq j \leq s-1$ and $s \geq 3$. Then, there exists a polyomino chain $B_n^{(2)} \in \Omega_n$ having length vector $(l_1, l_2, ..., l_{j-1}, 2, l_j - 1, ..., l_s)$ and

$$\Psi_{\chi_\alpha}(B_n^{(2)}) - \Psi_{\chi_\alpha}(B_n^*) = f(\alpha) + (1 + y)h(\alpha) < 0, \quad \text{(where } y = 0 \text{ or } 1)$$

for $\alpha \leq x_0 \approx -3.09997$, which is again a contradiction. Hence, every internal segment of B_n^* has length 2.
Therefore, $B_n^* \cong Z_n$ and from Lemma 1, the desired result follows. □

Proposition 3. Let $B_n \in \Omega_n$ be a polyomino with $n \geq 3$ squares. Let $\alpha \approx -3.09997$ be a root of the equation $f(\alpha) = 0$. Then, the following inequality holds

$$\chi_\alpha(B_n) \leq 3 \cdot 6^\alpha n + (2 \cdot 4^\alpha + 2 \cdot 5^\alpha + 6^\alpha - 4 \cdot 7^\alpha),$$

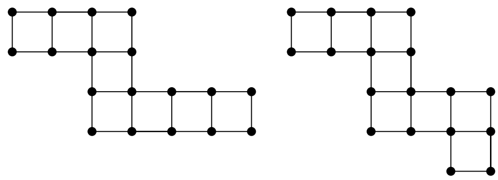
with equality if and only if B_n does not contain any segment of length 2.

Proof. From Equation (1), it follows that

$$\Psi_{\chi_\alpha}(B_n) = g(\alpha)(\beta_1 + \beta_s) + h(\alpha) \sum_{i=1}^{s} \alpha_i \leq 0.$$

Clearly, the equality $\Psi_{\chi_\alpha}(B_n) = 0$ holds if and only if B_n does not contain any segment of length 2. Hence, by using Lemma 1, we have the required result. □

Let $\mathcal{Z}_n^*$ be a subclass of Ω_n consisting of those polyomino chains which do not contain any segment of length equal to 2 or greater than 4, and contain at most one segment of length 4 (for example, see Figure 1(a)). Let $\mathcal{Z}_n$ be a subclass of Ω_n consisting of those polyomino chains in which every internal segment (if exists) has length 3 or 4, every external segment has length at most 4, at most one external segment has length 2, at most one segment has length 4 and if some internal segment has length 4 then both the external segments have length 3 (for example, see Figure 1). An arbitrary member of $\mathcal{Z}_n$ is denoted by $Z_n^{\maltese}$. Let $Z_n^\dagger \in \mathcal{Z}_n$ be the polyomino chain in which every internal segment (if exists) has length 3, every external segment has length at most 3 and at most one external segment has length 2 (for example, see Figure 1(b)).



(a) (b)

Figure 1. **(a) a member of the collections $\mathcal{Z}_8^*$ and $\mathcal{Z}_8$ (b) the polyomino chain $Z_8^\dagger$.**

Proposition 4. Let $B_n \in \Omega_n$ be a polyomino with $n \geq 3$ squares. Let $x_0 \approx -3.09997$ and $x_1 \approx -5.46343$ be the roots of the equations $f(\alpha) = 0$ and $f(\alpha) + g(\alpha) = 0$, respectively. Then, for $x_1 < \alpha < x_0$, the following inequality holds

$$\chi_\alpha(B_n) \leq \chi_\alpha\left(Z_n^*\right), \tag{3}$$

with equality if and only if $B_n \cong Z_n^* \in \mathcal{Z}_n^*$. Also, for $\alpha = x_1$, the following inequality holds

$$\chi_\alpha(B_n) \leq \chi_\alpha\left(Z_n^{\maltese}\right), \tag{4}$$

with equality if and only if $B_n \cong Z_n^{\maltese} \in \mathcal{Z}_n$. Furthermore, for $\alpha < x_1$, the following inequality holds

$$\chi_\alpha(B_n) \leq \chi_\alpha\left(Z_n^\dagger\right), \tag{5}$$

with equality if and only if $B_n \cong Z_n^\dagger$.

Proof. For $n = 3$, the result is obvious. We assume that $n \geq 4$. It can be easily checked that $f(\alpha)$ is positive and both $g(\alpha)$, $h(\alpha)$ are negative for $x_1 < \alpha < x_0$. Suppose that for the polyomino chain $B_n^* \in \Omega_n$, $\Psi_{\chi_\alpha}(B_n^*)$ is maximum for $\alpha < x_0$. Let B_n^* has s segments $S_1, S_2, ..., S_s$ with the length vector $(l_1, l_2, ..., l_s)$.
If $s \geq 3$ and at least one of internal segments of B_n^* has length 2, say $l_i = 2$ for $2 \leq i \leq s-1$, then there exists a polyomino chain $B_n^{(1)} \in \Omega_n$ having length vector

$$\begin{cases} (l_1, l_2, ..., l_{s-1} + l_s - 1) & \text{if } i = s-1, \\ (l_1, l_2, ..., l_{i-1}, l_i + l_{i+1} - 1, l_{i+2}, ..., l_s) & \text{otherwise,} \end{cases}$$

and

$$\Psi_{\chi_\alpha}(B_n^*) - \Psi_{\chi_\alpha}(B_n^{(1)}) = \begin{cases} f(\alpha) + x \cdot g(\alpha) + h(\alpha) < 0 & \text{if } i = s-1, \\ f(\alpha) + (1+y)h(\alpha) < 0 & \text{otherwise,} \end{cases}$$

for $\alpha < x_0$, where $x, y \in \{0, 1\}$. This is a contradiction. Hence, every internal segment (if exists) of B_n^* has length greater than 2.

If at least one of segments of B_n^* has length greater than 4, say $l_i \geq 5$ for $1 \leq i \leq s$, then there exists a polyomino chain $B_n^{(2)} \in \Omega_n$ having length vector

$$\begin{cases} (3, l_1 - 2, l_2, l_3, ..., l_s) & \text{if } i = 1, \\ (l_1, l_2, ..., l_{i-1}, 3, l_i - 2, l_{i+1}, l_{i+2}, ..., l_s) & \text{if } 2 \leq i \leq s-1, \\ (l_1, l_2, ..., l_{s-1}, 3, l_s - 2) & \text{if } i = s, \end{cases}$$

and

$$\Psi_{\chi_\alpha}(B_n^*) - \Psi_{\chi_\alpha}(B_n^{(2)}) = -f(\alpha) < 0,$$

a contradiction. Hence, every segment of B_n^* has length less than than 5.
If at least two segments of B_n^* have length 4, say $l_i = l_j = 4$ for $1 \leq i, j \leq s$, then there exists a polyomino chain $B_n^{(3)} \in \Omega_n$ having length vector $(3, l_1, l_2, ..., l_{i-1}, l_i - 1, l_{i+1}, ..., l_{j-1}, l_j - 1, l_{j+1}, ..., l_s)$ and

$$\Psi_{\chi_\alpha}(B_n^*) - \Psi_{\chi_\alpha}(B_n^{(3)}) = -f(\alpha) < 0,$$

a contradiction. Hence, B_n^* contains at most one segment of length 4.
If both the external segments of B_n^* have length 2, then ($s \geq 3$ because $n \geq 4$) there exists a polyomino chain $B_n^{(4)} \in \Omega_n$ having length vector $(l_1 + 1, l_2, l_3, ..., l_{s-1})$ and

$$\Psi_{\chi_\alpha}(B_n^*) - \Psi_{\chi_\alpha}(B_n^{(4)}) = f(\alpha) + 2g(\alpha) < 0,$$

which is again a contradiction. Hence, at most one external segment has length 2. In what follows, without loss of generality, we assume that $l_s = 2$ whenever some external segment has length 2.
If some external segment of B_n^* has length greater 2, say $l_1 = 2$, then there exists a polyomino chain $B_n^{(5)} \in \Omega_n$ having length vector $(l_2 + 1, l_3, l_4, ..., l_s)$ and

$$\Psi_{\chi_\alpha}(B_n^*) - \Psi_{\chi_\alpha}(B_n^{(5)}) = f(\alpha) + g(\alpha) < 0, \quad (\text{because } l_2 \geq 3)$$

for $x_1 < \alpha < x_0$, which is again a contradiction. Hence, if $\Psi_{\chi_\alpha}(B_n^*)$ is maximum for $x_1 < \alpha < x_0$ then every external segment of B_n^* has length greater than 2. Therefore, if $\Psi_{\chi_\alpha}(B_n^*)$ is maximum for $x_1 < \alpha < x_0$ then $B_n^* \cong Z_n^*$ and thence from Lemma 1, inequality (3) follows.
In the remaining proof, we assume $\alpha \leq x_1$.
If B_n^* contains a segment of length 4, say $l_i = 4$ for $1 \leq i \leq s$, then there exists a polyomino chain $B_n^{(6)} \in \Omega_n$ having length vector

$$\begin{cases} (2, l_1 - 1, l_2, l_3, ..., l_s) & \text{if } i = 1, \\ (l_1, l_2, ..., l_{i-1}, l_i - 1, l_{i+1}, l_{i+2}, ..., l_s + 1) & \text{if } 2 \leq i \leq s-1 \text{ and } l_s = 2, \\ (l_1, l_2, ..., l_{i-1}, l_i - 1, l_{i+1}, l_{i+2}, ..., l_s, 2) & \text{if } 2 \leq i \leq s-1 \text{ and } l_s = 3, \\ (l_1, l_2, ..., l_{s-1}, l_s - 1, 2) & \text{if } i = s, \end{cases}$$

and

$$\Psi_{\chi_\alpha}(B_n^*) - \Psi_{\chi_\alpha}(B_n^{(6)}) = \begin{cases} g(\alpha) & \text{if } 2 \le i \le s-1 \text{ and } l_s = 2, \\ -f(\alpha) - g(\alpha) & \text{otherwise.} \end{cases}$$

This last equation together with the fact that for $\alpha < x_1$, both $g(\alpha)$ and $-f(\alpha)-g(\alpha)$ are negative, gives a contradiction. The same equation together with the fact that for $\alpha = x_1$, only $g(\alpha)$ is negative, arises also a contradiction if $2 \le i \le s-1$ and $l_s = 2$. Therefore, if $\Psi_{\chi_\alpha}(B_n^*)$ is maximum for $\alpha < x_1$ then $B_n^* \cong Z_n^\dagger$ and if $\Psi_{\chi_\alpha}(B_n^*)$ is maximum for $\alpha = x_1$ then $B_n^* \in \mathcal{Z}_n$, and thence from Lemma 1, inequalities (4) and (5) follow. □

Propositions 1, 2, 3 and 4, together with the already reported results in [5, 6, 13, 16, 23, 47], yield Table 1 which gives information about the polyomino chains having extremum χ_α values in the collection Ω_n for $n \ge 3$.

	Polyomino Chain(s) with Maximal χ_α Value	Polyomino Chain(s) with Minimal χ_α Value
$\alpha > 0$	Z_n	L_n
$x_0 < \alpha < 0$	L_n	Z_n
$\alpha = x_0$	chains having no segment of length 2	Z_n
$x_1 < \alpha < x_0$	members of $\mathcal{Z}_n^*$	Z_n
$\alpha = x_1$	members of $\mathcal{Z}_n$	Z_n
$\alpha < x_1$	$Z_n^\dagger$	Z_n

Table 1. Polyomino chains having extremum χ_α values in the collection Ω_n for $n \ge 3$.

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