

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

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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, \dots, S_s then the vector (l_1, l_2, \dots, 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) $S_1, S_2, S_3, \dots, S_s$ with the length vector (l_1, l_2, \dots, l_s) . Then,

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

Let

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

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

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

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

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. \square

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, \dots, S_s be the segments of B_n^* with the length vector (l_1, l_2, \dots, 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 $(\underbrace{2, 2, \dots, 2}_{(l_1-1)\text{-times}}, l_2, \dots, l_s)$ and

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

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 $(l_1, l_2, \dots, l_{j-1}, 2, l_j - 1, \dots, l_s)$ 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^* . 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)).

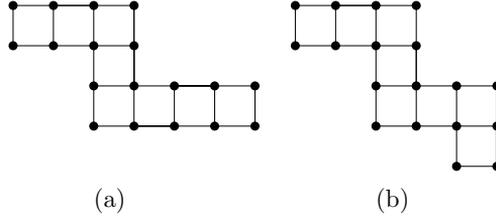


Figure 1. (a) a member of the collections \mathcal{Z}_s^* and \mathcal{Z}_s (b) the polyomino chain Z_s^\dagger .

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

$$\chi_\alpha(B_n) \leq \chi_\alpha(Z_n^*), \quad (3)$$

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

$$\chi_\alpha(B_n) \leq \chi_\alpha(Z_n^{\boxtimes}), \quad (4)$$

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

$$\chi_\alpha(B_n) \leq \chi_\alpha(Z_n^\dagger), \quad (5)$$

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, \dots, S_s with the length vector (l_1, l_2, \dots, 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

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

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

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

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 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 $(3, l_1, l_2, \dots, l_{i-1}, l_i - 1, l_{i+1}, \dots, l_{j-1}, l_j - 1, l_{j+1}, \dots, l_s)$ 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 $(l_1 + 1, l_2, l_3, \dots, l_{s-1})$ 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 $(l_2 + 1, l_3, l_4, \dots, l_s)$ 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

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

and

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

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 $2 \leq i \leq s-1$ 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. \square

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 $n \geq 3$.

	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 $n \geq 3$.

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