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The Edge Szeged Index of Polyomino Chains of 4*k*-Cycles

Jafar Asadpour
Department of Mathematics, South Tehran Branch,
Islamic Azad University, Tehran, Iran
jafar_asadpour@yahoo.com

Rasoul Mojarad
Department of science, Bushehr Branch,
Islamic Azad University, Bushehr, Iran,
mojarad.rasoul@gmail.com

ABSTRACT

The edge Szeged index is a new molecular structure descriptor equal to the sum of products $n_{eu}(e \mid G)n_{ev}(e \mid G)$ over all edges $e = uv$ of the molecular graph G, where $n_{eu}(e \mid G)$ is the number of edges which its distance to vertex u is smaller than the distance to vertex v, and $n_{ev}(e \mid G)$ is defined analogously. In this paper we compute the edge Szeged index of polyomino chains of 4k-cycles and establish bounds for it.

KEYWORDS: Graph invariant, Edge Szeged index, Polyomino chain.

1 INTRODUCTION

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, we denote the distance between two arbitrary vertices x and y of G by $d(x, y)$ and it is defined as the number of edges in the minimal path connecting the vertices x and y. Given an edge $e = uv$ of G, we define the distance of e to a vertex $w \in V(G)$ as the minimum of the distances of its edges to w, i.e.,

$$d(w,e) := \min\{d(w,u), d(w,v)\}.$$

Let us denote the number of edges lying closer to the vertex u than the vertex v of e by $n_{eu}(e|G)$ and the number of edges lying closer to the vertex v than the vertex u by $n_{ev}(e|G)$. Thus, $n_{eu}(e|G) := |\{f \in E(G) \mid d(u,f) < d(v,f)\}|$ and similarly for $n_{ev}(e|G)$. The edge Szeged index of a graph G is defined as

$$Sz_e(G) = \sum_{e=uv\in E(G)} n_{eu}(e|G) n_{ev}(e|G),$$

see [5, 6]. Note that in this definitions the edges equidistant from the two ends of the edge $e = uv$ (i.e., edges f with $d(u,f) = d(v,f)$ are not counted. We call such edges parallel to e, and is denoted by $M(e)$.

A k-polyomino system is a finite 2-connected plane graph such that each interior face (also called *cell*) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells. For the origin of polyominoes see, for example, Golomb [2, 3]. At the present time they are widely known by mathematicians, physicists and chemists and have been considered in many different applications [1]. All notations is taken from [7].

For calculating the edge Szeged index of a k-polyomino chain, we introduce some concepts for a k-polyomino chain. A kink of a k-polyomino chain is any branched or angularly connected $4k$-cycle. A segment of a k-polyomino chain is a maximal linear chain in the polyomino chain, including the kinks and/or terminal $4k$-cycles at its end. The number of $4k$-cycles in a segment S is called its length and is denoted by $\ell(S)$. For any segment S of a polyomino chain with $n \geq 2$ $4k$-cycles one has $2 \leq \ell(S) \leq n$. In particular, a k-polyomino chain is a linear chain if and only if it contains exactly one segment, and is denoted by $L_{n,k}$, see Fig. 1.

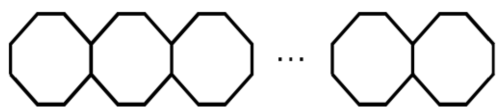

Fig. 1. The linear chain of 8-cycles

A k-polyomino chain is a zig-zag chain if and only if the length of each segment is 2, and is denoted by $Z_{n,k}$, see Fig. 2.

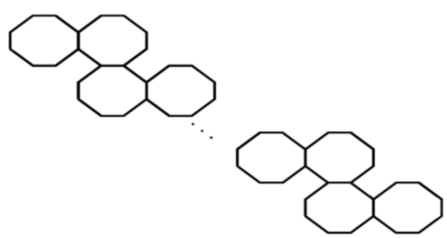

Fig. 2. The zig-zag chain of 8-cycles

A k-polyomino chain consists of a sequence of segments $S_1, S_2, \ldots, S_s$, $s \geq 1$, with Lengths

$\ell(S_i) \equiv \ell_i$, $i = 1,2,\ldots,s$, where $\sum_{i=1}^{s} \ell_i = n + s - 1$

(n denotes the number of $4k$-cycles of the polyomino chain) since two neighboring segments have always one $4k$-cycle in common. In the following we will abbreviate the vector of lengths by ℓ, i.e., $\ell = (\ell_1, \ldots, \ell_s)$.

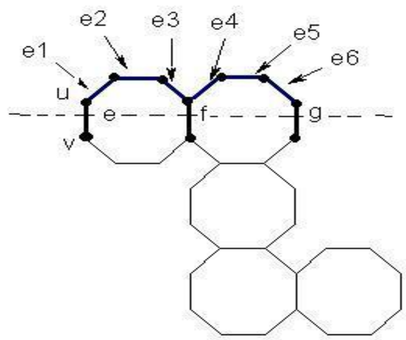

Fig. 3. The graph $B_{5,2}$

For example, let k = 2 and consider the polyomino with lengths $\ell_1 = 2$, $\ell_2 = 3$ and $\ell_3 = 2$, see Fig. 3. Thus, s = 3 and n = 5. We denote it by $B_{5,2}$. We consider the edge $e = uv$ in segment S_1. The edges parallel to e are f and g, thus $M(e) = 3$. On other hand the edges that its distance to vertex u is smaller than the distance to vertex v are the edges $e_1, e_2, \ldots, e_6$, see Fig. 3. Thus $n_{eu}(e \mid G) = 6$ and $n_{ev}(e \mid G) = |E(G)| - n_{eu}(e \mid G) - M(e) = 27$.

We apply this way for all edges of segments S_i, $i \geq 1$, and using this method we compute the edge Szeged index of k-polyomino chains for arbitrary k.

2 MAINE RESULTS

In this section we compute the edge Szeged index of k-polyomino chain for arbitrary k and derive bounds for it.

Theorem 2.1. Let $B_{n,k|\ell}$ be a k-polyomino chain with n $4k$-cycles consisting of $s \geq 1$ segments $S_1, S_2, \ldots, S_s$ with lengths $\ell_1, \ell_2, \ldots, \ell_s$. Then

$$\begin{aligned} Sz_e(B_{n,k|\ell}) &= \left(-2kx - \tfrac{2}{3}xy^2\right)\sum_{i=1}^{s}\ell_i^{\,3} + \left(2xy^2 - 2kx + 4knxy\right)\sum_{i=1}^{s}\ell_i^{\,2} - y^2\sum_{i=2}^{s-1}\ell_i^{\,2}\alpha_{i+1} \\ &- \left(4kx^2 + \tfrac{4}{3}xy^2 + 2nxy^2\right)\sum_{i=1}^{s}\ell_i + \left(y(4x-1) + ny^2\right)\sum_{i=2}^{s-1}\ell_i\alpha_{i+1} - y\sum_{i=2}^{s-1}\ell_i\alpha_{i+1}^2 \\ &- \left(2y(k-1) + 3nxy\right)\sum_{i=2}^{s-1}\alpha_{i+1} + 3x\sum_{i=2}^{s-1}\alpha_{i+1}^2 - 2y^2(k-1)\ell_1^{\,2} + 2y^2(k-1)(n+1)\ell_1 \\ &+ \left(8k^2x + 2nx^2y\right)s + 2ny(3k-1) - 8kx^2, \end{aligned}$$

where $x = (2k-1)$, $y = (4k-1)$ and $\alpha_{i+1} = \sum_{r=i+1}^{s}\left|E'(S_r)\right|$.

Proof**.** Let us first observe that the edges of $B_{n,k|\ell}$ fall into two distinct classes, namely the ones which are cut across by the straight line passing through the centers of the $4k$-cycles of S_i and those which are not. We denote the edges of the first type contained in S_i by $E_c(S_i)$ and those of the second type by $E_{nc}(S_i)$. Thus, for each segment S_i one has $E(S_i) = E_c(S_i) \cup E_{nc}(S_i)$. However, the set of edges $E(B_{n,k|\ell})$ is not the disjoint union of the $E(S_i)$ since two neighboring segments have one 4*k*-cycle in common. We can, therefore, write

$$E(B_{n,k|\ell}) = E(S_1) \cup \bigcup_{i=2}^{s} \{E(S_i) \setminus (E(S_i) \cap E(S_{i-1}))\}$$

which now is a disjoint union.

Let us introduce the sets $E'(S_i) := \{E(S_i) \setminus (E(S_i) \cap E(S_{i-1}))\}$ whose elements are those edges in S_i which are not contained in the previous segment S_{i-1}. Thus $E(B_{n,k|\ell}) = E(S_1) \cup \bigcup_{i=2}^{s} E'(S_i)$. It is easy to see that $|E(S_1)| = (4k-1)\ell_1 + 1$ and $|E'(S_i)| = (4k-1)(\ell_i - 1)$, $2 \le i \le s$.

Since $\sum_{i=1}^{s} \ell_i = n + s - 1$, so $|E(B_{n,k|\ell})| = (4k-1)n + 1$.

By the definition, we have:

$$Sz_e(B_{n,k|\ell}) = \sum_{e=uv \in E(B_{n,k|\ell})} n_{eu}(e|G) n_{ev}(e|G) = \sum_{e=uv \in E(S_1)} n_{eu}(e|G) n_{ev}(e|G)$$

$$+ \sum_{i=2}^{s-1} \sum_{e=uv \in E'(S_i)} n_{eu}(e|G) n_{ev}(e|G) + \sum_{e=uv \in E'(S_s)} n_{eu}(e|G) n_{ev}(e|G).$$

We now compute the contributions for S_1, S_i with $2 \le i \le s-1$ and S_s separately.

The Contribution for S_1: We first observe that $E(S_1) = E_c(S_1) \cup E_{nc}(S_1)$. Let us begin with $e = uv \in E_c(S_1)$. For such an edge only the other edges in S_1 are equidistant which are also in $E_c(S_1)$. Thus, $M(e) = \ell_1 + 1$, $n_{eu}(e|G) = (2k-1)\ell_1$ and $n_{ev}(e|G) = |E(G)| - n_{eu}(e|G) - (\ell_1 + 1)$. So,

$$n_{eu}(e|G) n_{ev}(e|G) = (|E(G)| - 1)(2k-1)\ell_1 - 2k(2k-1)\ell_1^2.$$

Using $|E_c(S_1)| = \ell_1 + 1$, we find that

$$\sum_{e=uv \in E_c(S_1)} n_{eu}(e|G) n_{ev}(e|G) = (\ell_1 + 1)\left((|E(G)| - 1)(2k-1)\ell_1 - 2k(2k-1)\ell_1^2\right).$$

Now, let us consider the edges in $E_{nc}(S_1)$. Here we have to be careful because there are two types of them: the first type consists of those edges which are cut across by the straight line for S_2 while the other edges are not. Denoting the edges of the first type by $\hat{E}_{nc}(S_1)$ and those of the second type by $\tilde{E}_{nc}(S_1)$, we thus have the disjoint union $E_{nc}(S_1) = \hat{E}_{nc}(S_1) + \tilde{E}_{nc}(S_1)$. Clearly, there are exactly two edges in $\hat{E}_{nc}(S_1)$. For those two edges *e* only the other edges in S_2 are equidistant which are also in $E_c(S_2)$. Thus, $M(e) = \ell_2 + 1$,

$$n_{eu}(e|G) = (2k-1)\ell_2 + \sum_{r=3}^{s} |E'(S_r)|, \; n_{ev}(e|G) = |E(G)| - n_{eu}(e|G) - (\ell_2 + 1).$$

Using $|\hat{E}_{nc}(S_1)|=2$, we find that

$$\sum_{e=uv\in\hat{E}_{nc}(S_1)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=2(|E(G)|-1)(2k-1)\ell_2-4k(2k-1)\ell_2{}^2$$

$$-2(4k-1)\ell_2\sum_{r=3}^{s}|E'(S_r)|+2(|E(G)|-1)\sum_{r=3}^{s}|E'(S_r)|-2(\sum_{r=3}^{s}|E'(S_r)|)^2.$$

Now, consider $e=uv\in\tilde{E}_{nc}(S_1)$. For each such edge there exists exactly one edge which is equidistant to it, namely the edge which lies in the same $4k$-cycle and is opposite to e, thus $M(e)=2$. Let C_{1j}, $1\le j\le\ell_1$, be j^{th} $4k$-cycle in segment S_1. We consider two cases:

a) If $e=uv\in C_{1j}$, $1\le j\le\ell_1-1$, then

$n_{eu}(e\,|\,G)=(2k-1)+(j-1)(4k-1)=(4k-1)j-2k$, $n_{ev}(e\,|\,G)=|E(G)|-n_{eu}(e\,|\,G)-2.$

So

$$n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=$$
$$(|E(G)|+2(2k-1))(4k-1)j-4k(4k-1)^2j^2-2k(|E(G)|+2(k-1)).$$

Using $|E(C_{1j})\setminus\{E_c(S_1)\cup\hat{E}_{nc}(S_1)\}|=2(2k-1)$, we find that

$$\sum_{j=1}^{\ell_1-1}\sum_{e=uv\in C_{1j}} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=(2k-1)(4k-1)(|E(G)|+2(4k-1)-1)\ell_1{}^2$$

$$-\frac{2}{3}(2k-1)(4k-1)^2\ell_1{}^3-\{(2k-1)(4k-1)(|E(G)|+2(4k-1)-1)+$$
$$4k(2k-1)(|E(G)|+2(k-1)\}\ell_1+4k(2k-1)(|E(G)|+2(k-1)).$$

b) if $e=uv\in C_{1j}$ for $j=\ell_1$, then

$n_{eu}(e\,|\,G)=(2k-1)$ or $n_{eu}(e\,|\,G)=(4k-1)\ell_1-2k$ and in both cases

$$n_{ev}(e\,|\,G)=|E(G)|-n_{eu}(e\,|\,G)-2.$$

Using $|E(C_{1\ell_1})\setminus\{E_c(S_1)\cup\hat{E}_{nc}(S_1)\}|=2(2k-1)$, we find that

$$\sum_{e=uv\in E(C_{1\ell_1})} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=2(k-1)(4k-1)(|E(G)|-2k-1)\ell_1-2(k-1)(4k-1)^2\ell_1{}^2$$

$$+2(k-1)(2k-1)(|E(G)|-2k-1))-4k(k-1)(|E(G)|+2(k-1)).$$

Now by the cases (a) and (b) we have:

$$\sum_{e=uv\in \tilde{E}_{nc}(S_1)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G) =$$

$$\{(2k-1)(4k-1)(|E(G)|+2(4k-1)-1)-2(k-1)(4k-1)^2\}\ell_1{}^2-\tfrac{2}{3}(2k-1)(4k-1)^2\ell_1{}^3$$
$$-\{(2k-1)(4k-1)(|E(G)|+2(4k-1)-1)+4k(2k-1)(|E(G)|+2(k-1))$$
$$+2(k-1)(4k-1)(|E(G)|-2k-1)\}\ell_1+4k(2k-1)(|E(G)|+2(k-1))$$
$$+2(k-1)(2k-1)(|E(G)|-2k-1))-4k(k-1)(|E(G)|+2(k-1)).$$

For simplicity, we set

$$x:=(2k-1),\;\; y:=(4k-1)\text{ and }\alpha_i := \sum_{r=i}^{s}\left|E'(S_r)\right|.$$

Collecting the above results, the contribution for S_1 with some calculations is given by

$$\sum_{e=uv\in E(S_1)} n_{eu}(e|G)n_{ev}(e|G)=(-2kx-\tfrac{2}{3}xy^2)\ell_1{}^3+(4knxy+2ky^2-2kx))\ell_1{}^2$$
$$-(2ky^2(n+1)+2y^2+4kx^2+\tfrac{4}{3}xy^2)\ell_1+4kx+4nx^2y-2ny^2(k-1)+2nxy\ell_2$$
$$-4kx\ell_2^2-2y(\ell_2-n)\alpha_3-2\alpha_3{}^2. \qquad (1)$$

The Contribution for S_i, ($2\le i\le s-1$): The procedure is analogous to the case of S_1. Observe that $E'(S_i)=E'_c(S_i)\bigcup E'_{nc}(S_i)$. Let us begin with $e=uv\in E'_c(S_i)$. The same argument as above yields that $M(e)=\ell_i+1$,

$$n_{eu}(e\,|\,G)=(2k-1)\ell_i+\sum_{r=i+1}^{s}|E'(S_r)|,\;\; n_{ev}(e\,|\,G)=\left|E(G)\right|-n_{eu}(e\,|\,G)-(\ell_i+1).$$

Using $|E'_c(S_i)|=|E_c(S_i)|-2=\ell_i-1$, one has

$$\sum_{e=uv\in E'_c(S_1)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=(\ell_i-1)\{nxy\ell_i-2kx\ell_i{}^2-y\alpha\ell_i+ny\alpha-\alpha^2\}.$$

As above we have the disjoint union $E'_{nc}(S_i)=\hat{E}'_{nc}(S_i)\bigcup \tilde{E}'_{nc}(S_i)$. For the two edges $e=uv\in \hat{E}'_{nc}(S_i)$ the contribution is given by

$$n_{eu}(e\,|\,G)=(2k-1)\ell_{i+1}+\sum_{r=i+2}^{s}\left|E'(S_r)\right|=x\ell_{i+1}+\alpha_{i+2}\;\;\text{and}$$
$$n_{ev}(e\,|\,G)=|E(G)|-n_{eu}(e\,|\,G)-(\ell_{i+1}+1).$$

Thus ,

$$\sum_{e=uv\in \hat{E}'_{nc}(S_1)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=$$
$$2\{nxy\ell_{i+1}-2kx\ell_{i+1}{}^2-y\alpha_{i+2}\ell_{i+1}+ny\alpha_{i+2}-(\alpha_{i+2})^2\}.$$

For $e=uv\in \tilde{E}'_{nc}(S_i)$, we have $M(e)=2$.

I. If $e\in C_{ij}$, $2\le j\le \ell_i-1$, then

$$n_{eu}(e|G)=(2k-1)+(4k-1)(\ell_i-j)+\sum_{r=i+1}^{s}|E'(S_r)|=x+y(\ell_i-j)+\alpha_{i+1},$$

$$n_{ev}(e|G)=|E(G)|-n_{eu}(e|G)-2.$$

Using $|E(C_{ij})\setminus\{E_c(S_i)\cup\hat{E}_{nc}(S_i)\}|=2(2k-1)$, we find that

$$\sum_{j=2}^{\ell_i-1}\sum_{e=uv\in C_{ij}}n_{eu}(e|G)n_{ev}(e|G)=(-\tfrac{2}{3}xy^2)\ell_i{}^3+(xy^2(n+2))\ell_i{}^2$$
$$-(2nx^2y-4kx^2-3nxy^2-\tfrac{4}{3}xy^2)\ell_i-2xy\alpha_{i+1}\ell_i{}^2+(2xy(n+2))\alpha_{i+1}\ell_i$$
$$-2x(\ell_i-2)(\alpha_{i+1})^2-4nxy\alpha_{i+1}+2nxy+8kx^2.$$

II. If $e=uv\in C_{ij}$ for $j=\ell_i$, then $n_{eu}(e|G)=(2k-1)$ or

$n_{eu}(e|G)=(2k-1)+\sum_{r=i+1}^{s}|E'(S_r)|=x+\alpha_{i+1}$, and in both cases we have

$$n_{ev}(e|G)=|E(G)|-n_{eu}(e|G)-2.$$

Using $|E(C_{ij})\setminus\{E_c(S_i)\cup\hat{E}_{nc}(S_i)\}|=2(2k-1)$, we find that

$$\sum_{e=uv\in E(C_{i\ell_i})}n_{eu}(e|G)n_{ev}(e|G)=$$
$$2y(k-1)(n-1)\alpha_{i+1}-2(k-1)(\alpha_{i+1})^2+4x(k-1)(ny-2k).$$

Now by (I) and (II) we have:

$$\sum_{e=uv\in\tilde{E}'_{nc}(S_i)}n_{eu}(e|G)n_{ev}(e|G)=(-\tfrac{2}{3}xy^2)\ell_i{}^3+(xy^2(n+2))\ell_i{}^2-(2nx^2y-4kx^2$$
$$-3nxy^2-\tfrac{4}{3}xy^2)\ell_i-2xy\alpha_{i+1}\ell_i{}^2+(2xy(n+2))\alpha_{i+1}\ell_i-\{2x(\ell_i-2)+$$
$$2(k-1)\}(\alpha_{i+1})^2+\{2y(k-1)(n-1)-4nxy\}\alpha_{i+1}+2nxy+8kx^2+4x(k-1)(ny-2k).$$

Collecting the results yields for S_i that

$$\sum_{i=2}^{s-1}\sum_{e=uv\in E'(S_i)}n_{eu}(e|G)n_{ev}(e|G)=(-2kx-\tfrac{2}{3}xy^2)\sum_{i=2}^{s-1}\ell_i^3+(4knxy+2xy^2-2kx)\sum_{i=2}^{s-1}\ell_i^2$$
$$-(2nxy^2+4kx^2+\tfrac{4}{3}xy^2)\sum_{i=2}^{s-1}\ell_i+(ny^2+4xy-y)\sum_{i=2}^{s-1}\ell_i\alpha_{i+1}-y^2\sum_{i=2}^{s-1}\ell_i^2\alpha_{i+1}$$
$$-y\sum_{i=2}^{s-1}\ell_i\alpha_{i+1}^2+3x\sum_{i=2}^{s-1}\alpha_{i+1}^2-(3nxy+2y(k-1))\sum_{i=2}^{s-1}\alpha_{i+1}+(2nx^2y+8k^2x)(s-2)$$
$$+2nxy\ell_s-4kx\ell_s^2-2nxy\ell_2+4kx\ell_2^2+2y(\ell_2-n)\alpha_3+2\alpha_3{}^2. \qquad (2)$$

The Contribution for S_s: The procedure is analogous to the case of S_1. Let us begin with $e=uv\in E'_c(S_i)$. The same argument as above yields that $M(e)=\ell_s+1$, $n_{eu}(e\,|\,G)=(2k-1)\ell_s$ and

$$n_{ev}(e\,|\,G)=\left|E(G)\right|-n_{eu}(e\,|\,G)-(\ell_s+1).$$

Using $|E'_c(S_s)|=|E_c(S_s)|-2=\ell_s-1$, one has

$$\sum_{e=uv\in E'_c(S_1)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=(\ell_s-1)\{nxy\ell_s-2kx\ell_s^2\}.$$

In contrast to above we have $E'_{nc}(S_s)=\tilde{E}'_{nc}(S_s)$ since S_s has no successor (hence, $\hat{E}'_{nc}(S_s)$ is empty). For each edge $e=uv\in\tilde{E}'_{nc}(S_s)$, $M(e)=2$.

If $e=uv\in C_{sj}$, $2\le j\le \ell_s-1$, then $n_{eu}(e\,|\,G)=(4k-1)j-2k$ and

$$n_{ev}(e\,|\,G)=|E(G)|-n_{eu}(e\,|\,G)-2.$$

Thus,

$$n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=\\(\left|E(G)\right|+2(2k-1))(4k-1)j-4k(4k-1)^2j^2-2k(|E(G)|+2(k-1)).$$

Using $|E(C_{sj})\setminus E_c(S_s)|=2(2k-1)$, we find that

$$\sum_{j=2}^{\ell_s-1}\sum_{e=uv\in C_{sj}} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=(-\tfrac{2}{3}xy^2)\ell_s^3+(xy^2(n+2))\ell_s^2\\-(nxy(y+4k)-4kx^2-\tfrac{4}{3}xy^2)\ell_s+2nxy+8kx^2$$

If $e=uv\in C_{sj}$ for $j=\ell_s$, then $n_{eu}(e\,|\,G)=(2k-1)$ and

$$n_{ev}(e\,|\,G)=|E(G)|-n_{eu}(e\,|\,G)-2.$$

Using $|E(C_{sj})\setminus E_c(S_s)|=2(2k-1)$, we find that

$$\sum_{e=uv\in E(C_{s\ell_s})} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=2nx^2y$$

Thus,

$$\sum_{e=uv\in\tilde{E}'_{nc}(S_s)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=(-\tfrac{2}{3}xy^2)\ell_s^3+(xy^2(n+2))\ell_s^2\\-(nxy(y+4k)-4kx^2-\tfrac{4}{3}xy^2)\ell_s+2nx^2y.$$

Collecting the results yields for S_s that

$$\sum_{e=uv\in E'(S_s)} n_{eu}(e\,|\,G)n_{ev}(e\,|\,G)=(-2kx-\tfrac{2}{3}xy^2)\ell_s^3+(4knxy+2kx+2xy^2))\ell_s^2\\-(8knxy+4kx^2+\tfrac{4}{3}xy^2)\ell_s+4knxy+4kx^2. \qquad (3)$$

Having done these computations all the necessary informations to determine the edge Szeged index of $B_{n,k|\ell}$ are at hand. By sum of the equations (1), (2) and (3) the proof is completed. □

By Theorem 2.1, we get the following corollaries.

Corollary 2.2. The edge Szeged index of the linear chain $L_{n,k}$ is given by

$$Sz_e(L_{n,k}) = \{\tfrac{2}{3}xy(x+2) - 2kx\}n^3 - 2kxn^2 + \{8kx^2 - \tfrac{2}{3}xy(x+2)\}n.$$

Proof. Since in the linear chain $s = 1$ and $\ell_1 = n$, thus by Theorem 2.1 and some calculations the result now follows. □

Corollary 2.3. The edge Szeged index of the zig-zag chain $Z_{n,k}$ is

$$Sz_e(Z_{n,k}) = \tfrac{1}{6}y^2(14k-11)n^3 + \{2xy(x+2) - y^2(11k-8)\}n^2$$
$$+\{\tfrac{1}{6}y^2(y+30) - 2xy - 8kx(k+2)\}n + 16kx - 3y^2.$$

Proof. In the zig-zag chain $\ell_i = 2\ (1 \le i \le s)$, and $s = n-1$. On other hand $|E'(S_i)| = (4k-1)(\ell_i - 1) = 4k-1$, so

$$\sum_{i=2}^{s-1}\alpha_{i+1} = (4k-1)\sum_{i=2}^{s-1}(s-i) = \tfrac{1}{2}(4k-1)(s^2 - 3s + 2),$$
$$\sum_{i=2}^{s-1}\alpha_{i+1}^2 = (4k-1)^2\sum_{i=2}^{s-1}(s-i)^2 = \tfrac{1}{6}(4k-1)^2(2s^3 - 9s^2 + 13s - 6).$$

Thus by Theorem 2.1 and some calculations the proof is completed. □

For instance in the case $k = 1$, the edge Szeged index of 1-polyomino chain with *n* square is given by

$$Sz_e(B_{n,1}) = -8\sum_{i=1}^{s}\ell_i^3 + (12n+16)\sum_{i=1}^{s}\ell_i^2 - (18n+16)\sum_{i=1}^{s}\ell_i - 3\sum_{i=2}^{s-1}\ell_i\alpha_{i+1}^2 - 9\sum_{i=2}^{s-1}\ell_i^2\alpha_{i+1}$$
$$+(9n+9)\sum_{i=2}^{s-1}\ell_i\alpha_{i+1} - (9n)\sum_{i=2}^{s-1}\alpha_{i+1} + 3x\sum_{i=2}^{s-1}\alpha_{i+1}^2 + (6n+8)s + 12n - 8.$$

Moreover, by Corollaries 2.2 and 2.3, the edge Szeged index of linear chain and zig-zag chain with *n* square are

$$Sz_e(L_{n,1}) = 4n^3 - 2n^2 + 2n.$$
$$Sz_e(Z_{n,1}) = \frac{9}{2}n^3 - 9n^2 + \frac{39}{2}n - 11.$$

In [7] proved that $PI(L_{n,k}) \le PI(B_{n,k}) \le PI(Z_{n,k})$. Here we state the obvious following result that these results are contrary.

Corollary 2.4. In the set of all k-polyominoes with n $4k$-cycles the zig-zag chain $Z_{n,k}$ has the smallest edge Szeged index whereas the linear chain $L_{n,k}$ has the largest edge Szeged index, i.e., for any k-polyomino $B_{n,k}$ with n $4k$-cycles one has

$$Sz_e(Z_{n,k}) \le Sz_e(B_{n,k}) \le Sz_e(L_{n,k}).$$

Example 2.5. Consider the graph $B_{5,2}$ as in Fig. 3. Clearly, $B_{5,2}$ has $7 \cdot 5 + 1 = 36$ edges. Let us proceed as in the proof of Theorem 2.1 to determine $Sz_e(B_{n,k})$ explicitly. Since there are 3 edges in $E_c(S_1)$ each counting $n_{eu}(e \mid B_{5,2}) n_{ev}(e \mid B_{5,2}) = 6 \cdot 27$, we find (with the obvious abbreviation) $Sz_e(E_c(S_1) = 3(6 \cdot 27) = 486$.

Similarly, one finds that $Sz_e(\hat{E}_{nc}(S_1) = 2(16 \cdot 16) = 512$, as well as

$$Sz_e(\tilde{E}_{nc}(S_1) = 8(3 \cdot 31) + 2(10 \cdot 24) = 1224.$$

Thus, S_1 contributes $Sz_e(S_1) = 2222$.

The segment S_2 contributes in a similar manner

$$Sz_e(S_2) = Sz_e(E'_c(S_2) + Sz_e(\hat{E}'_{nc}(S_2) + Sz_e(\tilde{E}'_{nc}(S_2) = 2(16 \cdot 16) + 2(6 \cdot 27)$$
$$+ 6(17 \cdot 17) + 2(3 \cdot 31) + 2(10 \cdot 24) = 3236.$$

The segment S_3 contributes in a similar fashion

$$Sz_e(S_3) = Sz_e(E'_c(S_3) + Sz_e(\tilde{E}'_{nc}(S_3) = (6 \cdot 27) + 6(3 \cdot 31) = 720.$$

Thus, one obtains $Sz_e(B_{5,2}) = Sz_e(S_1) + Sz_e(S_2) + Sz_e(S_3) = 6178$, which coincides with the result from Theorem 2.1.

3 CONCLUSION

In this paper we have calculated the edge Szeged index of a polyomino chain of $4k$-cycles with arbitrary k. The following generalizations of the situation considered here seem to deserve further study. At first one should allow regular $2k$-cycles instead of $4k$-cycles (thus including, e.g., configurations of hexagons). Then one should allow "heterogeneous" segments where $2k$-cycles with different k are allowed. Finally, one should allow more general configurations where the segments do not necessarily meet at the endpoints (and with an angle of 90 degree).

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