Iran University of Science &Technology
3TH INTERNATIONAL CONFERENCE ON COMBINATORICS, CRYPTOGRAPHY AND COMPUTATION

Computing the Wiener Index of Polyomino Chain by Cutting Method

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

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

ABSTRACT

Let G be a molecular graph with vertex set V. The Wiener index of G which is denoted by $W(G)$ is defined by $W(G)=\sum_{\{u,v\}\subseteq V\times V} d(u,v)$ where $d(u,v)$, denotes the distance between the vertices u and v. In this paper we will find the Wiener index of polyomino chain of $4k$-cycles.

KEYWORDS: Wiener Index, Polyomino Chain, Cycles

1 INTRODUCTION

Let G be a simple connected graph with vertex set V and edge set E. The distance between two vertices u and v of V is the length of the shortest path between u and v and is denoted by $d(u,v)$. The Wiener index of G is defined by $W(G)=\sum_{\{u,v\}\in V\times V} d(u,v)$, see Dobrynin et al. (2002), Gutman, and Klavzar (1998), Hosoya (1971).

The first mathematical definition of the Wiener index, based on the concept of graphtheoretical distance is due to Hosoya (Hosoya, 1971) which was already used by Wiener for chemical graphs. Its importance is on the fact that it is related to the boiling point of a molecule.

The research on Wiener number of polycyclic hydrocarbons has a long history. There are a great deal of results on hexagonal systems. XIE and ZHANG (2010) established relations between Wiener numbers of quasi-hexagonal chains and quasi-polyomino chains by means of the method of elementary cuts.

In this paper, we will compute the Wiener number of the polyomino chains based on the method of elementary cuts.

A *k-polyomino system* is a finite 2-connected plane graph such that each interior face (also called *cell*) is surrounded by a regular 4*k*-cycle of length one. In other words, it is an edge-connected union of cells. For the origin of polyominoes see, for example, Klarner (1997) and Golomb (1954 and 1965). At the present time they are widely known by mathematicians, physicists and chemists and have been considered in many different applications, (Alonso and Cerf ,1996).

For calculating the Wiener 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 4*k*-cycle. A *segment* of a *k*-polyomino chain is a maximal linear chain in the polyomino chain, including the kinks and/or terminal 4*k*-cycles at its end. The number of 4*k*-cycles in a segment *S* is called its *length* and is denoted by $\ell(S)$. For any segment *S* of a polyomino chain with $n \geq 2$ 4*k*-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.

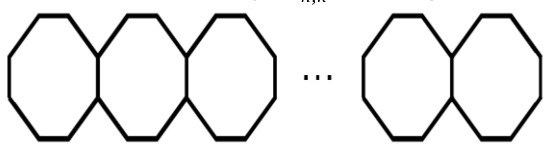

Fig. 1 The linear chain of 8-cycles

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.

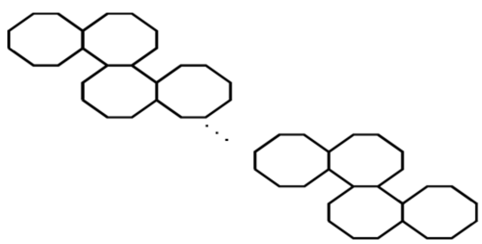

Fig. 2. The zig-zag chain of 8-cycles

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 4*k*-cycles of the polyomino chain) since two neighboring segments have always one 4*k*-cycle in common.

A subgraph *H* of a graph *G* is said to be convex if it is connected and if any shortest path in the graph *G* between two vertices of *H* lies entirely in *H*. For an edge *e=uv* of a graph *G*, let $N_u(e \mid G)$ be the set of vertices in *G* which are closer to *u* than to *v*, i.e.,

$$N_u(e \mid G) = \{w \in V(G) \mid d(u,w) < d(v,w)\}.$$

A graph G is a binary Hamming graph if and only if G is bipartite and for every edge $e=uv$ of G, $N_u(e|G)$ and $N_v(e|G)$ induce convex subgraphs of G. It was shown in [2] that a quasi-hexagonal chain is a binary Hamming graph. By the same method, it is easy to show that a k-polyomino chain is also a binary Hamming graph.

A straight line $\boldsymbol{C}$ in the plane is said to be a cut line of a binary Hamming graph if $\boldsymbol{C}$ is orthogonal to one of the edge directions [10] and go through the centers of the edges that intersect with $\boldsymbol{C}$. An elementary cut C is a set of edges intersected by a cut line $\boldsymbol{C}$ such that $G-C$ has exactly two connected components. And it is obvious that for any elementary cut C of G, $|V(G)|=|V(G'(C)|+|V(G''(C)|$, where $|V(G'(C)|$ and $|V(G''(C)|$ are the number of vertices in the two connected components G' and G'' of $G-C$, respectively.

The Wiener number of the molecular graph G is defined as

$$W(G)=\sum_{\{u,v\}\subseteq V\times V} d(u,v)$$

which is the sum of distances between all pairs of vertices in G. Thus, the Wiener number of a binary Hamming graph G can be calculated by the method of elementary cuts

$$W(G)=\sum_i |V(G'(C_i))||V(G''(C_i))| \qquad (1)$$

with the summation going over all elementary cuts of G, XIE and ZHANG (2010).

For the case $k=1$, XIE and ZHANG (2010), showed that the Wiener index of the linear chain and the zig-zag chain of 1-polyomino chain with n squares are given by

$$W(L_{n,1})=\frac{2}{3}n^3+3n^2+\frac{10}{3}n+1 \qquad (2)$$

$$W(Z_{n,1})=\frac{2}{3}n^3+2n^2+\frac{19}{3}n-1 \qquad (3)$$

In this paper we extend these results to the case of k-polyomino chains for arbitrary k.

2 MAINE RESULTS

Theorem 1. Let $B_{n,k}$ 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

$$\begin{aligned}W(B_{n,k})=&(-\tfrac{4}{3}x^3)\sum_{i=1}^{s}\ell_i^3+\left(8x^3n+x^2(8k-5)\right)\sum_{i=1}^{s}\ell_i^2-\left(\tfrac{8}{3}x^3+4x(k-1)(2xn+k)\right)\sum_{i=1}^{s}\ell_i+\\&\left(8x^3n+4x^2(4k-3)\right)\sum_{i=1}^{s}\ell_i\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)-\left(4x^2n(3k-2)+4x^2(k-1)\right)\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)\\&-4x^3\sum_{i=1}^{s}\ell_i^2\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)-4x^3\sum_{i=1}^{s}\ell_i\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)^2+4x^2(3k-2)\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r-1))\right)^2+\\&\left([6x+8kx(k-2)]n+8k^2(k-1)+1\right)s+8k^2xn-8k^2(k-1).\end{aligned}$$

Where $x=2k-1$.

Proof. The cut lines of $B_{n,k}$ are divided into three classes: i) they intersect the centers of the 4*k*-cycles in every segment; ii) they intersect every kink and they are orthogonal to the same edge direction; iii) and they intersect only one 4*k*-cycles and they are orthogonal to the same edge direction, which are denoted by C_i, K_i and F_i, respectively,. It is easy to prove that $B_{n,k}$ has *s* elementary cuts of type i) and 2(*s*-1) elementary cuts of type ii) and (2k-1)(*n*-*s*+1) elementary cuts of type iii).

By the formula (1) we have

$$W(B_{n,k}) = \sum_i |V(B'_{n,k}(C_i))||V(B''_{n,k}(C_i))| + \sum_i |V(B'_{n,k}(K_i))||V(B''_{n,k}(K_i))| + \sum_i |V(B'_{n,k}(F_i))||V(B''_{n,k}(F_i))|.$$

We now compute the contributions for the elementary cuts C_i, K_i and F_i, separately. For simplicity, we set $x := (2k-1)$. Since the number of vertices of this graph is 2(2*k*-1)*n*+2=2*xn*+2, we can write for the elementary cuts C_i:

$$\sum_i |V(B'_{n,k}(C_i))||V(B''_{n,k}(C_i))| = \sum_{i=1}^{s}\left(1 + x\ell_i + 2x\sum_{r=1}^{i-1}(\ell_r - 1)\right)\left(|V(G)| - (1 + x\ell_i + 2x\sum_{r=1}^{i-1}(\ell_r - 1))\right)$$
$$= 2x^2 n\sum_{i=1}^{s}\ell_i - x^2\sum_{i=1}^{s}\ell_i^2 - 4x^2\sum_{i=1}^{s}\ell_i\left(\sum_{r=1}^{i-1}(\ell_r - 1)\right) + 4x^2 n\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r - 1)\right)$$
$$- 4x^2\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r - 1)\right)^2 + (2xn+1)s. \qquad (4)$$

Also for the elementary cuts K_i we obtain:

$$\sum_i |V(B'_{n,k}(K_i))||V(B''_{n,k}(K_i))| = (k-1)\sum_{i=1}^{s-1} 2k(|V(G)| - 2k)$$
$$+ (k-1)\sum_{i=1}^{s-1}\left((2k + 2x\sum_{r=1}^{i}(\ell_r - 1)\right)\left(|V(G)| - (2k + 2x\sum_{r=1}^{i}(\ell_r - 1))\right)$$
$$= \left[4x^2(n-1)\sum_{i=1}^{s-1}\left(\sum_{r=1}^{i}(\ell_r - 1)\right) - 4x^2\sum_{i=2}^{s-1}\left(\sum_{r=1}^{i}(\ell_r - 1)\right)^2 + \left(8kxn - 4k(2x-1)\right)(s-1)\right](k-1)$$
$$= \left[4x^2(n-1)\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r - 1)\right) - 4x^2\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r - 1)\right)^2 + \left(8kxn - 4k(2x-1)\right)(s-1)\right](k-1). \qquad (5)$$

Finally for the elementary cuts F_i we have:

$$\sum_i |V(B'_{n,k}(F_i))||V(B''_{n,k}(F_i))| = 2k(|V(G)|-2k)2x$$

$$+x\sum_{i=1}^{s}\sum_{j=2}^{\ell_i-1}\left(2k+2x(\ell_i-j)+2x\sum_{r=1}^{i-1}(\ell_r-1)\right)\left(|V(G)|-(2k+2x(\ell_i-j)+2x\sum_{r=1}^{i-1}(\ell_r-1))\right)$$

$$=(-\tfrac{4}{3}x^3)\sum_{i=1}^{s}\ell_i^3+2x^3(n+2)\sum_{i=1}^{s}\ell_i^2+(2x^2n(2k-3x)-4kx(1-k)-\tfrac{8}{3}x^3)\sum_{i=1}^{s}\ell_i$$

$$+4x^3(n+2)\sum_{i=1}^{s}\ell_i\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)-4x^3\sum_{i=1}^{s}\ell_i^2\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)-4x^3\sum_{i=1}^{s}\ell_i\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)^2$$

$$-8x^3n\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)+8x^3\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}(\ell_r-1)\right)^2+(8kx(k-1)-4x^2n)s+8kx^2n-8kx(k-1). \qquad (6)$$

Now by sum of the equations (4), (5) and (6) the proof is completed. ■

By Theorem 1, we get the following corollaries.

Corollary 2. The Wiener index of the linear chain $L_{n,k}$ is given by

$$W(L_{n,k})=\tfrac{2}{3}x^3n^3+3x^2n^2+\left(12k^2x-\tfrac{2}{3}x^2(8k+5)\right)n+1 \qquad (7)$$

Where $x=2k-1$.

Proof. Since in the linear chain $s=1$ and $\ell_1=n$, thus by Theorem 1 and some calculation the result is follows. ■

Corollary 3. The Wiener index of the zig-zag chain $Z_{n,k}$ is

$$W(Z_{n,k})=\tfrac{2}{3}kx^2n^3+\left(8k^2x-2x^2(k-1)-2x(4k-1)\right)n^2+$$
$$\left(\tfrac{4}{3}x^2(7k-3)+4x(k-1)+4k(k-1)-20kx(k-1)+1\right)n$$
$$-8k(k-1)-1, \qquad (8)$$

Where $x=2k-1$.

Proof. In the zig-zag chain $\ell_i=2$ $(1\le i\le s)$, and $s=n-1$, thus by Theorem 1 we obtain

$$W(Z_{n,k})=(-\tfrac{4}{3}x^3)\sum_{i=1}^{n-1}8+\left(8x^3n+x^2(8k-5)\right)\sum_{i=1}^{n-1}4-\left(\tfrac{8}{3}x^3+4x(k-1)(2xn+k)\right)\sum_{i=1}^{n-1}2$$

$$+\left(16x^3n+8x^2(4k-3)\right)\sum_{i=1}^{n-1}\left(\sum_{r=1}^{i-1}1\right)-\left(4x^2n(3k-2)+4x^2(k-1)\right)\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}1\right)-16x^3\sum_{i=1}^{n-1}\left(\sum_{r=1}^{i-1}1\right)$$

$$-8x^3\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}1\right)^2+4x^2(3k-2)\sum_{i=1}^{s}\left(\sum_{r=1}^{i-1}1\right)^2+\left([6x+8kx(k-2)]n+8k^2(k-1)+1\right)(n-1)$$

$$+8k^2xn-8k^2(k-1).$$

On other hand $\sum_{i=1}^{n-1}\sum_{r=1}^{i-1}1=\sum_{i=1}^{n-1}(i-1)=\frac{1}{2}(n^2-3n+2)$ and $\sum_{i=1}^{n-1}\left(\sum_{r=1}^{i-1}1\right)^2=\sum_{i=1}^{n-1}(i-1)^2=\frac{1}{6}(2n^3-9n^2+13n-6)$. Thus with some calculations the proof is completed. ■

Note that choosing k = 1 in (7) and (8) yields indeed (2) and (3) respectively.
By Theorem 1 and corollaries 2 and 3 we can determine the Wiener index of k-polyomino chains and its Linear and zig-zag chains for cases k=1,2, in Tables 1 and 2, respectively.

Table 1. The Wiener index of 1-polyomino chain with n squares

$W(B_{n,1})$	$-\frac{4}{3}\sum_{i=1}^{s}\ell_i^3+(2n+3)\sum_{i=1}^{s}\ell_i^2-\frac{8}{3}\sum_{i=1}^{s}\ell_i+4(n+1)\sum_{i=1}^{s}\ell_i\sum_{k=1}^{i-1}(\ell_k-1)-4n\sum_{i=1}^{s}\sum_{k=1}^{i-1}(\ell_k-1)$ $-4\sum_{i=1}^{s}\ell_i^2\sum_{k=1}^{i-1}(\ell_k-1)-4\sum_{i=1}^{s}\ell_i(\sum_{k=1}^{i-1}(\ell_k-1))^2+4\sum_{i=1}^{s}(\sum_{k=1}^{i-1}(\ell_k-1))^2-(2n-1)s+8n$
$W(L_{n,1})$	$\frac{n}{3}\left(2n^2+9n+10\right)+1$
$W(Z_{n,1})$	$\frac{n}{3}\left(2n^2+6n+19\right)-1$

Table 2. The Wiener index of 2-polyomino chain with n octagonals

$W(B_{n,2})$	$-36\sum_{i=1}^{s}\ell_i^3+9(6n+11)\sum_{i=1}^{s}\ell_i^2-12(6n+8)\sum_{i=1}^{s}\ell_i+18(6n+10)\sum_{i=1}^{s}\ell_i\sum_{k=1}^{i-1}(\ell_k-1)$ $-12(12n+3)\sum_{i=1}^{s}\sum_{k=1}^{i-1}(\ell_k-1)-108\sum_{i=1}^{s}\ell_i(\sum_{k=1}^{i-1}(\ell_k-1))^2-108\sum_{i=1}^{s}\ell_i^2\sum_{k=1}^{i-1}(\ell_k-1)$ $+144\sum_{i=1}^{s}(\sum_{k=1}^{i-1}(\ell_k-1))^2+3(6n+11)s+16(6n-2)$
$W(L_{n,2})$	$18n^3+27n^2+18n+1$
$W(Z_{n,2})$	$12n^3+36n^2+33n-17$

4 CONCLUSION

In this paper we have calculated the Wiener index of a polyomino chain of $4k$-cycles with arbitrary k, thereby generalizing the result of XIE and ZHANG (2010) for $k = 1$ to the case of 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 "heterogenous" 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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