Applied Mathematical Sciences, Vol. 6, 2012, no. 58, 2891 - 2897

The Wiener Polynomial of Polyomino Chains

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Abstract

The Wiener index is a graphical invariant and is the sum of distances between all pairs vertices in a connected graph G. We define a generating function, which we call the Wiener polynomial, whose derivative is a x-analog of the Wiener index. The Wiener polynomial of G which is denoted by $W(G;x)$ and is defined by $W(G;x) = \sum_{\{u,v\}\subseteq V} x^{d(u,v)}$ where $d(u,v)$, denotes the distance between the vertices u and v. In this paper we will find the Wiener polynomial of polyomino chains.

Keywords: Wiener Polynomial, Polyomino Chain, Linear Chain

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 $W(G) = \sum_{\{u,v\}\subseteq V} d(u,v)$, see [2-4]. We wish to define and study a related generating function. If x is a parameter, then the Wiener polynomial of G is $W(G;x) = \sum_{\{u,v\}\subseteq V} x^{d(u,v)}$. It is easy to see that the derivative of is a x-analog of $W(G)$, i.e., $W'(G;1) = W(G)$.

The Wiener Polynomial is initially defined by Haruo Hosoya [9], and so termed in honour of Harold Wiener who coined the earlier index. It is often called the Hosoya Polynomial and appears in slightly different forms in the literature. The readers interested in the continuing saga of Wiener Indices and Polynomials will have to refer to a dedicated survey (see, for example, [3, 9,11]).

A polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular square of length one. In other words, it is an edge-connected union of cells. For the origin of polyominoes see, for example, Klarner [10] and Golomb [4,5]. At the present time they are widely known by mathematicians, physicists and chemists and have been considered in many different applications [1]. A polyomino chain is a polyomino system, in which the joining of the centres of its adjacent regular forms a path $c_1, c_2, ..., c_n$, where c_i is the centre of the $i-$th square and denoted by B_n.

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

A polyomino chain is a zig-zag chain if and only if the length of each segment is 2, and denoted by Z_n, see Fig. 2. A polyomino chain consists

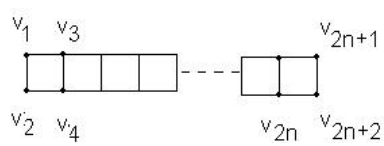

Figure 1: The Linear chain.

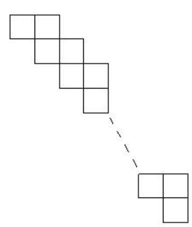

Figure 2: The Zig-Zag chain.

of a sequence of segments $S_1, ..., S_s, s \geq 1$, with Lengths $\ell(S_i) \equiv \ell_i$ where $\sum_{i=1}^{s} \ell_i = n + s - 1$ (n denotes the number of squares of the polyomino chain) since two neighboring segments have always one squares in common. In this paper, we calculate the Wiener polynomial of polyomino chains.

2 Main Results

The Wiener polynomial of G is defined by $W(G,x) = \sum_{\{u,v\}\subseteq V} x^{d(u,v)}$, and also we define $W(S_1,S_2;x) = \sum_{u\in S_1, v\in S_2} x^{d(u,v)}$, for the subsets S_1 and S_2 of vertices of G , see [8,9,12].

Now we suppose that the set be the all vertices of G. Then by the definition of Wiener polynomial we obtain

$$W(G;x) = \sum_{\{u,v\}\subseteq V} x^{d(u,v)} = \sum_{i=2}^{n} x^{d(v_1,v_i)} + \sum_{i=3}^{n} x^{d(v_2,v_i)} + \ldots + \sum_{i=n-1}^{n} x^{d(v_{n-2},v_i)} + x^{d(v_{n-1},v_n)} = \sum_{j=1}^{n-1}\sum_{i=j+1}^{n} x^{d(v_j,v_i)}.$$

Let $S_1 = \{u_1, u_2, \ldots, u_m\}$ and $S_2 = \{w_1, w_2, \ldots, w_r\}$ be the subsets of V. Then the set of distances the vertex u of S_1 from the vertices of S_2 we show by $D_u^{S_2} = \{d(u,w_1), d(u,w_2), \ldots, d(u,w_r)\}$. Moreover, the set distances the vertices of S_1 with themselves and with the vertices of S_2 we show by

$$D_{S_1}^{S_1} = \{D_{u_1}^{S_1\setminus\{u_1\}}, D_{u_2}^{S_1\setminus\{u_1,u_2\}}, \ldots, D_{u_{m-1}}^{S_1\setminus\{u_1,u_2,\ldots,u_{m-1}\}}\}$$

and

$$D_{S_1}^{S_2} = \{D_{u_1}^{S_2}, D_{u_2}^{S_2}, \ldots, D_{u_m}^{S_2}\},$$

respectively.
Therefore by the above notations the Wiener polynomial of G is given by

$$W(G;x) = \sum_{k\in D_V^V} N(k)x^k, \tag{1}$$

where $N(k)$ is the number of k in the set D_V^V . Also the Wiener polynomial of the subsets and of vertices of G is obtained by

$$W(S_1,S_2;x) = \sum_{k\in D_{S_1}^{S_2}} N(k)x^k, \tag{2}$$

where $N(k)$ is the number of k in the set $D_{S_1}^{S_2}$.

Now we suppose that L_n be the linear chain with n square. The number of vertices of L_n is $2n+2$, which we show by $V = \{v_1, v_2, \ldots, v_{2n+2}\}$, see Fig 1. It is easy to see that for $1 \le k \le n$ we have

$$D_{v_{2k-1}}^{V\setminus\{v_1,v_2,\ldots,v_{2k-1}\}} = \{1, 1, 2, 2, 3, 3, \ldots, n+1-k, n+1-k, n+2-k\},$$

$$D_{v_{2k}}^{V\setminus\{v_1,v_2,\ldots,v_{2k}\}} = \{1, 2, 2, 3, 3, \ldots, n+1-k, n+1-k, n+2-k\},$$

Table 1:

k	1	2	3	...	n	n+1
N(k)	3n+1	4n-2	4n-6	...	6	2

and $D_{v_{2n+1}}^{V\setminus\{v_1,v_2,\ldots,v_{2n+1}\}} = \{1\}$. Now by the formula (1), to calculate the Wiener polynomial of L_n, it is enough to count $N(1), N(2), \ldots, N(n+1)$, which we showed them in following table 1.

Therefore we have proved the following theorem.

Theorem 2.1 *The Wiener polynomial of the linear chain L_n is given by*

$$W(L_n; x) = (3n+1)x + \sum_{i=2}^{n+1} (4(n-i)+6)x^i. \qquad (3)$$

The following table show the Wiener polynomial of L_n for some n.

Table 2:

$n = 1$	$4x + 2x^2$
$n = 2$	$7x + 6x^2 + 2x^3$
$n = 3$	$10x + 10x^2 + 6x^3 + 2x^4$
$n = 4$	$13x + 14x^2 + 10x^3 + 6x^4 + 2x^5$

For computing Wiener polynomial of B_n we introduce some concepts for a polyomino chain. The common kink in segments S_i and S_{i+1} we denote by $K_{i(i+1)}$, and also the vertex of $K_{i(i+1)}$ which makes right angles between segments S_i and S_{i+1} , we denote by $a_{i(i+1)}$, see Fig. 3.

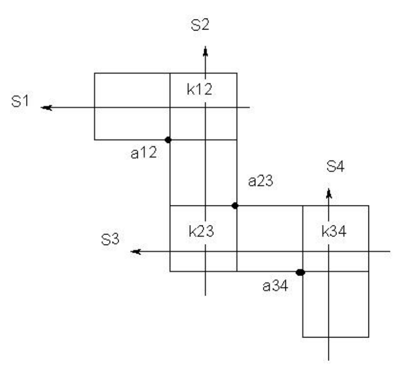

Figure 3: The graph B_7 and its segments.

By formulas (1) and (2), we must compute $D_{S_i}^{S_i}$ for $1 \leq i \leq s$ and $D_{S_j \setminus K_{j(j+1)}}^{S_i \setminus K_{(i-1)i}}$ for $1 \leq j \leq s-1$ and $j+1 \leq i \leq s$.
Since every kink is common in two segments, thus the Wiener polynomial of B_n is obtained by

$$W(B_n;x) = \sum_{i=1}^{s} W(S_i;x) - \sum_{i=1}^{s-1} W(K_{i(i+1)};x)$$
$$+\sum_{j=1}^{s-1}\sum_{i=j+1}^{s} W(\{S_j \setminus K_{j(j+1)}\}, \{S_i \setminus K_{i,(i+1)}\}; x). \quad (4)$$

By Theorem 1, we have $W(S_i;x) = (3\ell_i + 1)x + \sum_{k=2}^{\ell_i+1} (4(n-k)+6)x^k$ and $W(K_{i(i+1)};x) = 4x + 2x^2$.

Now we suppose that the vertices u and v be the vertices of $S_j \setminus K_{j(j+1)}$ and $S_i \setminus K_{i,(i+1)}$, respectively. Then

$$d(u,v) = d(u, a_{j(j+1)}) + d(a_{j(j+1)}, a_{(i-1)i}) + d(a_{(i-1)i}, v).$$

Thus $D_{S_j \setminus K_{j(j+1)}}^{S_i \setminus K_{(i-1)i}} = D_{a_{j(j+1)}}^{S_j \setminus K_{j(j+1)}} + D_{a_{j(j+1)}}^{a_{(i-1)i}} + D_{a_{(i-1)i}}^{S_i \setminus K_{(i-1)i}}$. But

$$d(a_{j(j+1)}, a_{(i-1)i}) = \sum_{k=j+1}^{i-1} (\ell_k - 1).$$

On other hand, we have

$$D_{a_{j(j+1)}}^{S_j \setminus K_{j(j+1)}} = \{1, 2, 2, 3, 3, \ldots, \ell_j - 1, \ell_j - 1, \ell_j\},$$

$$D_{a_{(i-1)i}}^{S_i \setminus K_{(i-1)i}} = \{1, 2, 2, 3, 3, \ldots, \ell_i - 1, \ell_i - 1, \ell_i\}.$$

Computing $D_{S_j \setminus K_{j(j+1)}}^{S_i \setminus K_{(i-1)i}}$ for segments of different length is complicated, so in this paper we compute its in the case that $\ell_i = 2$ for all i, i.e., the zig-zag chain.

Theorem 2.2 *The Wiener polynomial of the zig-zag chain is given by*

$$W(Z_n;x) = (3n+1)x + (5n-4)x^2 + (5n-9)x^3 + 4\sum_{i=4}^{n}(n+1-i)x^i + x^{n+1}. \quad (5)$$

Proof . Using Table 2, we have $W(S_i;x) = 7x + 6x^2 + 2x^3$ and $W(K_{i(i+1)};x) = 4x + 2x^2$ for all i. Since $\ell_i = 2$, so $S_j \setminus K_{j(j+1)}$ and $S_i \setminus K_{(i-1)i}$ have exactly two vertices. Thus $d(u, a_{j(j+1)})$ and $d(a_{(i-1)i}, v)$ are equal to 1 or 2.
On other hand, $d(a_{j(j+1)}, a_{(i-1)i}) = \sum_{k=j+1}^{i+1} (\ell_k - 1) = i - j + 1$. Thus

$$D_{S_j \backslash K_{j(j+1)}}^{S_i \backslash K_{(i-1)i}} = \{1+i-j, 2+i-j, 2+i-j, 3+i-j\}.$$

Therefore

$$\sum_{j=1}^{s-1} \sum_{i=j+1}^{s} W(\{S_j \setminus K_{j(j+1)}\}, \{S_i \setminus K_{i,(i+1)}\}; x) =$$

$$\sum_{j=1}^{s-1} \sum_{i=j+1}^{s} (x^{1+i-j} + 2x^{2+i-j} + x^{3+i-j}) =$$

$$\sum_{i=2}^{s} (s+1-i)x^i + 2\sum_{i=3}^{s+1} (s+2-i)x^i + \sum_{i=4}^{s+2} (s+3-i)x^i =$$

$$(s-1)x^2 + (3s-4)x^3 + 4\sum_{i=4}^{s+1} (s+2-i)x^i + x^{s+2}.$$

Now using the formula (4), we obtain

$$W(Z_{n,k}; x) = (3s+4)x + (5s+1)x^2 + (5s-4)x^3 + 4\sum_{i=4}^{s+1} (s+2-i)x^i + x^{s+2}.$$

Since in zig-zag chain $s = n-1$, so the proof is completed. ■

Derivative of the formulas (3) and (5), we get

$$W'(L_n; 1) = \frac{2}{3}n^3 + 3n^2 + \frac{10}{3}n + 1. \quad (6)$$

$$W'(Z_n; 1) = \frac{2}{3}n^3 + 2n^2 + \frac{19}{3}n - 1. \quad (7)$$

Formulas (6) and (7) are the Wiener index of L_n and Z_n, respectively, which is obtained by XIE and ZHANG in [13].

ACKNOWLEDGEMENTS. This research is supported by the research council of the Islamic Azad University of Bushehr.

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Received: October, 2011