Hosoya polynomial of some cactus chains

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Abstract: Let $G = (V, E)$ be a simple graph. Hosoya polynomial of $G$ is $H(G, x) = \sum_{(u, v) \subseteq V(G)} x^{d(u, v)}$, where $d(u, v)$ denotes the distance between vertices $u$ and $v$. A cactus graph is a connected graph in which no edge lies in more than one cycle. In this paper we compute the Hosoya polynomial of some cactus chains. As a consequence, Wiener and hyper-Wiener indices of these kind of chains are also obtained.

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1. Introduction

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of $G$ called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The Hosoya polynomial of a graph is a generating function about distance distributing, introduced by Hosoya (1988) and for a connected graph $G$ is defined as:

$$H(G, x) = \sum_{(u, v) \subseteq V(G)} x^{d(u, v)},$$

where $d(u, v)$ denotes the distance between vertices $u$ and $v$. This polynomial has computed for some nano-structures (e.g. Alikhani & Iranmanesh, 2014; Xu & Zhang, 2009). The Hosoya polynomial

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PUBLIC INTEREST STATEMENT

A simple graph $G = (V, E)$ is a finite nonempty set $V$ of objects called vertices together with a (possibly empty) set $E$ of unordered pairs of distinct vertices of $G$ called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. A graphical invariant is a number related to a graph which is structural invariant, that is to say it is fixed under graph automorphisms. In chemistry and for chemical graphs, these invariant numbers are known as the topological indices. One of the most important topological indices is the Wiener index of a connected graph $G$ is denoted by $W(G)$, is the sum of distances between all pairs of vertices in $G$. It found numerous applications. The first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index. In this paper we computed the Hosoya polynomial of some cactus chains that are of importance in chemistry.
has many chemical applications (Deutsch & Klavžar, 2013; Estrada, Ivanciuc, Gutman, Gutierrez, & Rodriguez, 1998; Gutman, Klavžar, Petkovsek, & Zigert, 2001; Gutman et al., 2012). Especially, the two well-known topological indices, i.e. Wiener index and hyper-Wiener index, can be directly obtained from the Hosoya polynomial. The Wiener index of a connected graph $G$ is denoted by $W(G)$, is defined as the sum of distances between all pairs of vertices in $G$ (Hosoya, 1971), i.e. 

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

The hyper-Wiener index is denoted by $WW(G)$ and defined as follows:

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d^2(u,v).$$

Note that the first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index:

$$W(G) = (H(G,x))'_{x=1}. $$

Also we have the following relation:

$$WW(G) = \frac{1}{2} (xH(G,x))''_{x=1}. $$

In this paper we consider a class of simple linear polymers called cactus chains. Cactus graphs were first known as Husimi tree, they appeared in the scientific literature sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics (Harary & Uhlenbeck, 1953; Husimi, 1950; Riddell, 1951). We refer the reader to papers (Chellali, 2006; Majstorović, Došlić, & Klobučar, 2012) for some aspects of parameters of cactus graphs. A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus $G$ are cycles of the same size $i$, the cactus is $i$-uniform. The cactus graphs whose are $i$-uniform for $i = 3, 4, 6$ are of importance in chemistry and so we consider them in this paper. A triangular cactus is a graph whose blocks are triangles, i.e. a 3-uniform cactus. A vertex shared by two or more triangles is called a cut-vertex. If each triangle of a triangular cactus $G$ has at most two cut-vertices, and each cut-vertex is shared by exactly two triangles, we say that $G$ is a chain triangular cactus. By replacing triangles in these definitions by cycles of length 4 we obtain cacti whose every block is $C_4$. We call such cacti square cacti. Note that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square (Alikhani, Jahari, Mehryar, & Hasni, 2014).

In the next section, we compute the Hosoya polynomial of triangular and square cacti chains. In Section 3, we compute this polynomial for two kind of chain hexagonal cactus. As a consequence, the Wiener and the hyper-Wiener indices of these kind of chains are also obtained.

2. Hosoya polynomial of triangular and square cactus chains

In this section we compute the Hosoya polynomial of triangular and square cactus chains. First we consider a chain triangular. An example of a chain triangular cactus is shown in Figure 1. We call the number of triangles in $G$, the length of the chain. Obviously, all chain triangular cacti of the same length are isomorphic. Hence, we denote the chain triangular cactus of length $n$ by $T_n$. Here we compute the Hosoya polynomial of $T_n$.

![Figure 1. Chain triangular cactus $T_n$.](image-url)
Theorem 2.1 The Hosoya polynomial of the chain triangular cactus $T_n$ ($n \geq 2$) is

$$H(T_n, x) = 3nx + \sum_{k=2}^{n-1} (4n - 4k + 4)x^k + 4x^n.$$ 

Proof Let $u$ and $v$ be two arbitrary vertices of $T_n$. Suppose that $d(u, v) = k$. For $k = 1$, there are two such pair of vertices with $\deg(u) = \deg(v) = 2$, there are $2n$ pair of vertices with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - 2$ such pair of vertices with $\deg(u) = \deg(v) = 4$. Therefore the coefficient of $x$ in $H(T_n, x)$ is $3n$. For $2 \leq k \leq n - 1$, there are $n - k + 3$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, and $2(n - k + 1)$ pair of vertices $u, v \in V(G)$ with $\deg(u) = 2$ and $\deg(v) = 4$, and $n - k - 1$ pair of vertices such as $u, v \in V(G)$ with $\deg(u) = \deg(v) = 4$. So the coefficient of $x^k$ for $2 \leq k \leq n - 1$ is $4n - 4k + 4$. Finally for $k = n$, there are four pair of vertices $u, v \in V(G)$ with $\deg(u) = \deg(v) = 2$, and so the coefficient of $x^n$ is 4. Therefore by definition of Hosoya polynomial we have the result. 

The following corollary gives the Wiener index and hyper-Wiener index of $I_n$:

Corollary 2.2

(i) The Wiener index of triangular cactus $T_n$ ($n \geq 2$) is

$$W(T_n) = 7n + 4 \sum_{k=2}^{n-1} k(n - k + 1).$$

(ii) The hyper-Wiener index of $T_n$ ($n \geq 2$) is

$$WW(T_n) = n(2n + 5) + 2 \sum_{k=2}^{n-1} k(k + 1)(n - k + 1).$$

Proof

(i) It follows from Theorem 2.1 and the identity $W(G) = (H(G, x))'|_{x=1}$.

(ii) It follows from Theorem 2.1 and the identity

$$WW(G) = \frac{1}{2}(xH(G, x))'|_{x=1}.$$ 

By replacing triangles in the definitions of triangular cactus $T_n$ by cycles of length 4 we obtain cacti whose every block is $C_4$. We call such cacti, square cacti. An example of a square cactus chain is shown in Figure 2. We see that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square. We consider a para-chain of length $n$,
which is denoted by $Q_n$ as shown in Figure 2. The following theorem gives the Hosoya polynomial of $Q_n$.

**Theorem 2.3** The Hosoya polynomial of the para-chain square cactus graph $Q_n$ $(n \geq 2)$ is

$$H(Q_n, x) = (6n - 4)x^2 + \sum_{s=0}^{n-2} (4n - 4s)x^{2s+1} + \sum_{s=2}^{n-1} (5n - 5s + 1)x^{2s} + 4x^{2n-1} + x^n.$$  

**Proof** Suppose that $u$ and $v$ are two arbitrary vertices of $Q_n$, and let $d(u, v) = k$. For $k = 2s + 1$ $(0 \leq s \leq n - 2)$, there are four pair of vertices $u$, $v$ with $\deg(u) = \deg(v) = 2$, there are $4(n - s - 1)$ pair of vertices $u$, $v$ with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x^{2s+1}$ is $4n - 4s$. For $k = 2$, there are $5(n - 1) + 1$ pair of vertices $u$, $v$ with $\deg(u) = \deg(v) = 2$, there are two pair of vertices $u$, $v$ with $\deg(u) = 2$ and $\deg(v) = 4$ and there are $n - 2$ pair of vertices such as $u$, $v$ with $\deg(u) = \deg(v) = 4$. So the degree of $x^2$ is $6n - 4$. For $k = 2s$ $(2 \leq s \leq n - 1)$, there are $4(n - s)$ pair of vertices $u$, $v$ with $\deg(u) = \deg(v) = 2$, there are two pair of vertices $u$, $v$ with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - s - 1$ pair of vertices $u$, $v$ with $\deg(u) = \deg(v) = 4$. So the coefficient of $x^{2s}$ $(2 \leq s \leq n - 1)$ is $5n - 5s + 1$. For $k = 2n - 1$, there are four pair of vertices $u$, $v$ with $\deg(u) = \deg(v) = 2$ and for $k = 2n$, there is one pair of vertices $u$, $v$ with $\deg(u) = \deg(v) = 2$. Therefore by the definition of Hosoya polynomial, we have the result. \[\Box\]

The following corollary gives the Wiener index and hyper-Wiener index of $Q_n$ Figure 5:

**Corollary 2.4**

(i) The Wiener index of the para-chain square cactus $Q_n$ $(n \geq 2)$ is

$$W(Q_n) = 22n - 12 + 4 \sum_{s=0}^{n-2} (2s + 1)(n - s) + \sum_{s=2}^{n-1} 2s(5n - 5s + 1).$$

(ii) The hyper-Wiener index of $Q_n$ $(n \geq 2)$ is

$$WW(Q_n) = 10n^2 + 15n - 12 + 6 \sum_{s=0}^{n-2} (s + 1)(2s + 1)(n - s) + \sum_{s=2}^{n-1} s(2s + 1)(5n - 5s + 1).$$

Now we consider another kind of square cactus chain and compute its Hosoya polynomial (Figure 3).

**Theorem 2.5** The Hosoya polynomial of the ortho-chain square cactus graph $O_n$ $(n \geq 5)$ is

$$H(O_n, x) = x^{n^2} + 6x^{n+1} + 15x^n + \sum_{k=4}^{n-1} (9n - 9k + 15)x^k + (8n - 12)x^3 + (6n - 4)x^2 + 4nx.$$  

**Proof** Suppose that $u$ and $v$ are two vertices of $O_n$, and let $d(u, v) = k$. For $k = 1$, there are $n + 2$ of vertices $u$, $v$ with $\deg(u) = \deg(v) = 2$, there are $2n$ pair of vertices $u$, $v$ with $\deg(u) = 2$ and $\deg(v) = 4$, and there are $n - 2$ pair of vertices such as $u$, $v$ with $\deg(u) = \deg(v) = 4$. So the coefficient of $x$ in $H(O_n, x)$ is
4n. For \( k = 2 \), there are \( n + 3 \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), there are \( 4(n - 1) \) pair of vertices \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \), and there are \( n - 3 \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 4 \). So the coefficient of \( x^k \) in \( H(O_n, x) \) is \( 6n - 4 \). For \( k = 3 \) there are \( 3n \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), there are \( 4(n - 3) + 4 \) pair of vertices \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \), and there are \( n - 4 \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 4 \). So the coefficient of \( x^k \) in \( H(O_n, x) \) is \( 8n - 14 \).

For \( 4 \leq k \leq n - 1 \), there are \( 4(n - k + 3) \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), there are \( 4(n - k + 1) \) pair of vertices \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \) and \( n - k + 1 \) pair of vertices such as \( u, v \) with \( \deg(u) = \deg(v) = 4 \). So the coefficient of \( x^k \) (\( 4 \leq k \leq n - 1 \)) in \( H(O_n, x) \) is \((9n - 9k + 13)\). For \( k = n \) there are \( 13 \) pairs of vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), there are \( 2 \) pairs of vertices \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \). So the coefficient of \( x^k \) in \( H(O_n, x) \) is \( 15 \). Finally observe that there are \( 6 \) pairs of vertices \( u, v \) with \( \deg(u) = \deg(v) = 4 \) and one pair of vertices such as \( u, v \) with \( \deg(u) = \deg(v) = n + 2 \). Therefore we have the result.

The following corollary gives the Wiener index and the hyper-Wiener index of \( O_n \).

**Corollary 2.6**

(i) The Wiener index of the ortho-chain square cactus graph \( O_n \) (\( n \geq 5 \)) is

\[
W(O_n) = 62n - 36 + 2 \sum_{k=4}^{n-1} k(9n - 9k + 15).
\]

(ii) The hyper-Wiener index of \( O_n \) (\( n \geq 5 \)) is

\[
WW(O_n) = 11n^2 + 55n - 51 + \frac{1}{2} \sum_{k=4}^{n-1} k(9n - 9k + 15).
\]

**3. Hosoya polynomial of chain hexagonal cactus**

In this section we shall compute the Hosoya polynomial of some hexagonal cactus chains. By replacing triangles in the definitions of triangular cactus, by cycles of length 6 we obtain cacti whose every block is \( C_6 \). We call such cacti, hexagonal cacti. An example of a hexagonal cactus chain is shown in Figure 4. We see that the internal hexagonal may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-hexagonal; if the cut-vertices are not adjacent, we call the square a para-hexagonal. We consider a para-chain of length \( n \), which is denoted by \( L_n \) as shown in Figure 4. The following theorem gives the Hosoya polynomial of \( L_n \). In this section, we shall compute the Hosoya polynomial of two kinds of para-chain hexagonal cactus. The following theorem gives the Hosoya polynomial of \( L_n \).

**Theorem 3.1** The Hosoya polynomial of the para-chain hexagonal cactus graph \( L_n \) (\( n \geq 3 \)) is

\[
H(L_n, x) = x^{3n} + 4x^{3n-1} + 8x^{3n-2} + \sum_{i=2}^{n-1} (9n - 9s + 1)x^{3s} + \sum_{i=2}^{n-2} (8n - 8s - 4)x^{3s+2} + \sum_{i=1}^{n-2} 8(n - s)x^{3s+1} + (11n - 8)x^3 + (10n - 4)x^2 + 6nx.
\]

**Proof** Suppose that \( u \) and \( v \) are two vertices of \( L_n \) and let \( d(u, v) = k \). For \( k = 1 \), there are \( 2n + 4 \) vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), there are \( 4(n - 1) \) pair of vertices \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \). So the coefficient of \( x \) is \( 6n \). For \( k = 2 \), there are \( 6n \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), and there are \( 4(n - 1) \) pair of vertices such as \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \). So the coefficient of \( x^3 \) is \( 10n - 4 \). For \( k = 3 \), there are \( 10(n - 1) + 2 \) pair of vertices \( u, v \) with \( \deg(u) = \deg(v) = 2 \), there are two pair of vertices \( u, v \) with \( \deg(u) = 2 \) and \( \deg(v) = 4 \) and \( n - 2 \) pair of vertices such as \( u, v \) with \( \deg(u) = \deg(v) = 4 \). So the coefficient of \( x^3 \) is \( 11n - 8 \).
For $k = 3s + 1$ ($1 \leq s \leq n - 2$) there are $4(n - s + 1)$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, there are $4(n - s - 1)$ pair of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x^{3n+1}$ ($1 \leq s \leq n - 2$) is $8(n - s)$.

For $k = 3s + 2$ ($1 \leq s \leq n - 2$), there are $4(n - s)$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, there are $4(n - s - 1)$ pair of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x^{3n+2}$ is $(8n - 8s - 4)$. For $k = 3s$ ($2 \leq s \leq n - 1$) there are $8(n - s)$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, there are two pairs of vertices such as $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$, and $n - s - 1$ pair of vertices such as $u, v$ with $\deg(u) = \deg(v) = 4$. So the coefficient of $x^{3n}$ ($2 \leq s \leq n - 1$) is $9n - 9s + 1$.

For $k = 3n - 2$, there are eight pairs of vertices $u, v$ with $\deg(u) = \deg(v) = 2$. For $k = 3n - 1$ and $k = 3n$, there are four and one pair of vertices, respectively. Therefore we have the result. $lacksquare$

The following corollary gives the Wiener index of $L_n$.

**Corollary 3.2** The Wiener index of the para-chain hexagonal cactus graph $L_n$ ($n \geq 3$) is equal to

$$98n - 52 + \sum_{s=1}^{n-2} [(24s + 8)(n - s) + (3s + 2)(8n - 8s - 4)] + \sum_{s=2}^{n-1} 3s(9n - 9s + 1).$$

**Theorem 3.3** The Hosoya polynomial of the para-chain hexagonal cactus graph $M_n$ ($n \geq 4$) is

$$H(M_n, x) = x^{2n+1} + 4x^{2n+1} + 10x^{2n} + 16x^{2n-1} + \sum_{s=3}^{n-1} (13n - 13s + 10)x^{2s} + \sum_{s=2}^{n-2} (12n - 12s + 4)x^{2s+1} + (12n - 16)x^4 + (11n - 8)x^3 + (8n - 2)x^2 + 6nx.$$

**Proof** Suppose that $u$ and $v$ are two vertices of $Q_6$, and let $d(u, v) = k$. For $k = 1$ there are $2n + 4$ vertices $u, v$ with $\deg(u) = \deg(v) = 2$ and $4(n - 1)$ pair of vertices with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x$ is $6n$. For $k = 2$ there are $5n$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, there are $2n$ pair of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$, and $n - 2$ pair of vertices such as $u, v$ with $\deg(u) = \deg(v) = 4$. So the coefficient of $x^2$ is $8n - 2$. For $k = 3$ there are $5n + 2$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$ and $n - 10$ pair of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x^3$ is $11n - 8$. For $k = 4$, there are $9(n - 1) - 2$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, there are $2(n - 1)$ pair of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$ and $n - 3$ pair of vertices such as $u, v$ with $\deg(u) = \deg(v) = 4$. So the coefficient of $x^4$ is $12n - 16$.

For $k = 2s + 1$ ($2 \leq s \leq n - 2$) there are $6(n - s + 1) + 2$ pairs of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, and $6(n - s - 1) + 2$ pairs of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x^{2s+1}$ ($2 \leq s \leq n - 2$) is $(12n - 12s + 4)$.

For $k = 2s$ ($3 \leq s \leq n - 1$) there are $10(n - s + 1) - 1$ pair of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, there are $2(n - s + 1)$ pair of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$ and $n - s - 1$ pair of vertices such as $u, v$ with $\deg(u) = \deg(v) = 4$. The coefficient of $x^{2s}$ ($3 \leq s \leq n - 1$) is $(13n - 13s + 10)$.

For $k = 2n - 1$ there are $14$ pairs of vertices $u, v$ with $\deg(u) = \deg(v) = 2$, and two pairs of vertices $u, v$ with $\deg(u) = 2$ and $\deg(v) = 4$. So the coefficient of $x^{2n-1}$ is $16$. For $k = 2n, k = 2n + 1$ and $k = 2n + 2$, there are ten, four, and one pair of vertices. Therefore we have the result. $lacksquare$

The following corollary gives the Wiener index of $M_n$.

**Corollary 3.4** The Wiener index of the Para-chain hexagonal cactus graph $M_n$ ($n \geq 4$) is equal to

$$165n - 102 + \sum_{s=2}^{n-2} (2s + 1)(12n - 12s + 4) + \sum_{s=3}^{n-1} 2s(13n - 13s + 10).$$
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