Relationship Between the Hosoya Polynomial and the Edge-Hosoya Polynomial of Trees

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Abstract

We prove the relationship between the Hosoya polynomial and the edge-Hosoya polynomial of trees. The connection between the edge-hyper-Wiener index and the edge-Hosoya polynomial is established. With these results we also prove formulas for the computation of the edge-Wiener index and the edge-hyper-Wiener index of trees using the Wiener index and the hyper-Wiener index. Moreover, the closed formulas are derived for a family of chemical trees called regular dendrimers.

Keywords: Hosoya polynomial, edge-Hosoya polynomial, tree, dendrimer, edge-hyper-Wiener index

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1. Introduction

The first distance-based topological index was the Wiener index introduced in 1947 by H. Wiener \cite{1}. Later, in 1988 H. Hosoya \cite{2} introduced some counting polynomials in chemistry, among them the Wiener polynomial, which is strongly connected to the Wiener index. Nowadays, it is known as the Hosoya polynomial. Another distance-based topological index, the hyper-Wiener index, was introduced in 1993 by M. Randić \cite{3}. All these concepts found many applications in different fields, such as chemistry, biology, networks.

The Hosoya polynomial, the Wiener index, and the hyper-Wiener index are based on the distances between pairs of vertices in a graph, and similar concepts have been introduced for distances between pairs of edges under the names the edge-Hosoya polynomial \cite{4}, the edge-Wiener index \cite{5}, and the edge-hyper-Wiener index \cite{6}. In this paper we study the relationships between the vertex-versions and the edge-versions of the Hosoya polynomial, the Wiener index, and the edge-Wiener index of trees.

2. Preliminaries

Unless stated otherwise, the graphs considered in this paper are connected. We define \(d(x, y)\) to be the distance between vertices \(u, v \in V(G)\). The distance \(d(e, f)\) between edges \(e\) and \(f\) of graph \(G\) is defined as the distance between vertices \(e\) and \(f\) in the line graph \(L(G)\).
If $G$ is a connected graph with $n$ vertices, and if $d(G, k)$ is the number of (unordered) pairs of its vertices that are at distance $k$, then the Hosoya polynomial of $G$ is defined as

$$H(G, x) = \sum_{k \geq 0} d(G, k) x^k.$$ 

Note that $d(G, 0) = n$. Similarly, if $d_e(G, k)$ is the number of (unordered) pairs of edges that are at distance $k$, then the edge-Hosoya polynomial of $G$ is defined as

$$H_e(G, x) = \sum_{k \geq 0} d_e(G, k) x^k.$$ 

Obviously, for any connected graph $G$ it holds $H_e(G, x) = H(L(G), x)$.

The Wiener index and the edge-Wiener index of a connected graph $G$ are defined in the following way:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v), \quad W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e, f).$$ 

It is easy to see that $W_e(G) = W(L(G))$. The main property of the Hosoya polynomial and the edge-Hosoya polynomial, that makes them interesting in chemistry, follows directly from the definitions (see also [7]):

$$W(G) = H'(G, 1), \quad W_e(G) = H'_e(G, 1). \tag{1}$$

The hyper-Wiener index and the edge-hyper-Wiener index of a connected graph $G$ are defined as:

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

$$WW_e(G) = \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d(e, f) + \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d^2(e, f).$$

Again, it holds $WW_e(G) = WW(L(G))$. Moreover, the following relationship was proved in [8] for any connected graph $G$:

$$WW(G) = H'(G, 1) + \frac{1}{2} H''(G, 1). \tag{2}$$

3. The edge-Hosoya polynomial of trees

In this section we first show how the edge-hyper-Wiener index of an arbitrary connected graph can be calculated from the edge-Hosoya polynomial.

**Theorem 3.1.** Let $G$ be a connected graph. Then

$$WW_e(G) = H'_e(G, 1) + \frac{1}{2} H''_e(G, 1).$$

**Proof.** Using Equation 2, we obtain

$$WW_e(G) = WW(L(G)) = H'(L(G), 1) + \frac{1}{2} H''(L(G), 1) = H'_e(G, 1) + \frac{1}{2} H''_e(G, 1)$$

and the proof is complete. \[\square\]

The following theorem is the main result of this paper.
Theorem 3.2. Let $T$ be a tree. Then

$$H_e(T, x) = \frac{1}{x} H(T, x) - \frac{|V(T)|}{x}. \tag{3}$$

\textbf{Proof.} It suffices to prove that

$$H(T, x) = xH_e(T, x) + |V(T)|.$$ 

Let $V_k$ be the set of all (unordered) pairs of vertices of $T$ that are at distance $k$ and let $E_k$ be the set of all (unordered) pairs of edges of $T$ that are at distance $k$, where $k \geq 0$. That means

$$V_k = \{ \{x, y\} \mid x, y \in V(T), \; d(x, y) = k \},$$

$$E_k = \{ \{e, f\} \mid e, f \in E(T), \; d(e, f) = k \}.$$ 

We first show that for any $k \geq 1$ there exists a bijective function $F : V_k \rightarrow E_{k-1}$. To define $F$, let $k \geq 1$ and let $x, y \in V(T)$ such that $d(x, y) = k$. Furthermore, let $P$ be the unique path in $T$ connecting $x$ and $y$. Obviously, $d(x, y) = |E(P)| = k$. We define $e_x$ to be the edge of $P$ which has $x$ for one end-vertex. Similarly, $e_y$ is the edge of $P$ which has $y$ for one end-vertex. It is easy to see that $d(e_x, e_y) = k - 1$. With this notation we can define

$$F(\{x, y\}) = \{e_x, e_y\}$$

for every $\{x, y\} \in V_k$. Obviously, $F$ is a well-defined function.

To show that $F$ is injective, let $\{x, y\}, \{a, b\} \in V_k, \; k \geq 1$, and suppose $F(\{x, y\}) = F(\{a, b\})$. It follows that $\{e_x, e_y\} = \{e_a, e_b\}$ and without loss of generality we can assume $e_x = e_a$ and $e_y = e_b$. If $x = a$, we also get $y = b$, since otherwise $e_y \neq e_b$. Therefore, $\{x, y\} = \{a, b\}$. If $x \neq a$, it follows that $x = b$ and $y = a$. Again, $\{x, y\} = \{a, b\}$ and we are done.

To show that $F$ is surjective, we take $\{e, f\} \in E_{k-1}$. Let $x$ be the end-vertex of $e$ and $y$ the end-vertex of $f$ such that $d(x, y) = d(e, f) + 1 = k$. Obviously, $x$ and $y$ are uniquely defined. It is easy to see that

$$F(\{x, y\}) = \{e, f\}.$$ 

We have shown that for every $k \geq 1$ it holds $d(T, k) = |V_k| = |E_{k-1}| = d_e(T, k-1)$. It is also obvious that $d(T, 0) = |V(T)|$. Hence, polynomials $H(T, x)$ and $xH_e(T, x) + |V(T)|$ have the same coefficients. Therefore, Equation (3) is true and the proof is complete. \hfill \square

As a corollary we can now express the edge-Wiener index and the edge-hyper-Wiener index of trees with the Wiener index and the hyper-Wiener index.

\textbf{Corollary 3.3.} Let $T$ be a tree. Then

$$W_e(T) = W(T) - \left(\frac{|V(T)|}{2}\right)$$

and

$$WW_e(T) = WW(T) - W(T).$$
Proof. First we notice that if $G$ is a graph, then

$$H(G, 1) = \sum_{k \geq 0} d(G, k) = \left(\frac{|V(G)|}{2}\right) + |V(G)|. \quad (4)$$

After differentiating Equation 3 we obtain

$$H'_e(T, x) = H'(T, x) - H(T, 1) + |V(T)|$$

and

$$H''_e(T, x) = \frac{H''(T, x)x^3 - 2H'(T, x)x^2 + 2H(T, x)x - 2x|V(T)|}{x^4}. \quad (6)$$

Using Equation 5 and Equation 4 it follows,

$$W_e(T) = H'_e(T, 1)$$

$$= H'(T, 1) - H(T, 1) + |V(T)|$$

$$= W(T) - \left(\frac{|V(T)|}{2}\right).$$

Finally, Theorem 3.1, Equation 5, Equation 6 and Equation 2 imply

$$WW_e(T) = H'_e(T, 1) + \frac{1}{2}H''_e(T, 1)$$

$$= H'(T, 1) - H(T, 1) + |V(T)|$$

$$+ \frac{1}{2}H''(T, 1) - H'(T, 1) + H(T, 1) - |V(T)|$$

$$= WW(T) - W(T).$$

\[\square\]

4. The edge-Hosoya polynomial of dendrimers

Dendrimers are highly regular trees, which are of interest to chemists, since they represent repetitively branched molecules. In this section we compute the edge-Hosoya polynomial, the edge-Wiener index and the edge-hyper-Wiener index of regular dendrimers.

In particular, $T_{k, d}$ stands for the $k$-th regular dendrimer of degree $d$. For any $d \geq 3$, $T_{0, d}$ is the one-vertex graph and $T_{1, d}$ is the star with $d + 1$ vertices. Then for any $k \geq 2$ and $d \geq 3$, the tree $T_{k, d}$ is obtained by attaching $d - 1$ new vertices of degree one to the vertices of degree one of $T_{k-1, d}$. For an example see Figure 1. The parameter $k$ corresponds to what in dendrimer chemistry is called “number of generations” [9].

In [10] the Wiener polynomial $W(G, x)$ of a graph $G$ was considered and the definition of this polynomial is slightly different from the definition of the Hosoya polynomial, such that $H(G, x) = W(G, x) + |V(G)|$. Hence, from Equation 3 it follows

$$H_e(G, x) = \frac{1}{x}W(G, x).$$
Therefore, to compute the edge-Hosoya polynomial we can use this formula and the result regarding the Wiener polynomial of a regular dendrimer in [10]. After changing some labels we obtain

$$H_e(T_{k,d}, x) = \sum_{i=0}^{k-1} \frac{(d-1)^{2i} d^i}{d-2} \left( \frac{d}{2} \right)^i \left( \frac{(d-1)^{k-1} - 1}{d-2} + 1 \right) x^{2i+1}.$$ 

It follows from Equation 1 and Theorem 3.1 that the edge-Wiener index and the edge-hyper-Wiener index can be easily computed from the derivatives of the edge-Hosoya polynomial. Therefore, we obtain

$$W_e(T_{k,d}) = \frac{d \left( 2 - 2d + (d-1)^k (d^2 + 4d - 4) + (d-1)^{2k} (2 - d(d+2) + 2(d-2)dk) \right)}{2(d-2)^3}$$

and

$$WW_e(T_{k,d}) = \frac{d^2 (d-1) + (d-1)^k (4 - 5d^2)}{2(d-2)^4} + \frac{(d-1)^{2k} \left( -2 - 8k + d \left( -2 + 5d + 16k - d(d+4)k + 2(d-2)^2 k^2 \right) \right)}{2(d-2)^4}.$$ 

Since the Wiener index and the hyper-Wiener index of regular dendrimers are already known (see [9, 10, 11]), the edge-Wiener index and the edge-hyper-Wiener index could also be computed in terms of Corollary 3.3.

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