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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.

1 Introduction

The first distance-based topological index was the Wiener index introduced in 1947 by H. Wiener [11]. Later, in 1988 H. Hosoya [6] 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 [9]. 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 [1], the edge-Wiener index [7], and the edge-hyper-Wiener index [8]. In this paper we study the relationships between the vertex-versions and the edge-versions of the Hosoya polynomial, the Wiener index, and the hyper-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 usual shortest-path distance between vertices $x, y \in V(G)$. 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:

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

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

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

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 [3] 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. ■

The following theorem is the main result of this paper.

Theorem 3.2 *Let T be a tree. Then*

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

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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 $F : V_k \to E_{k-1}$. 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 it true and the proof is complete. ■

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. Note that Equation 4 was first proved in [2].

Corollary 3.3 *Let T be a tree. Then*

$$W_e(T) = W(T) - \binom{|V(T)|}{2} \tag{4}$$

and

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

Proof. First we notice that if G is a graph, then

$$H(G,1) = \sum_{k\geq 0} d(G,k) = \binom{|V(G)|}{2} + |V(G)|. \tag{5}$$

After differentiating Equation 3 we obtain

$$H_e'(T,x) = \frac{H'(T,x)x - H(T,x) + |V(T)|}{x^2} \tag{6}$$

and

$$H_e''(T,x) = \frac{H''(T,x)x^3 - 2H'(T,x)x^2 + 2H(T,x)x - 2x|V(T)|}{x^4}. \tag{7}$$

Using Equation 6 and Equation 5 it follows,

$$W_e(T) = H_e'(T,1) = H'(T,1) - H(T,1) + |V(T)| = W(T) - \binom{|V(T)|}{2}.$$

Finally, Theorem 3.1, Equation 6, Equation 7, and Equation 2 imply

$$\begin{aligned} WW_e(T) &= H_e'(T,1) + \frac{1}{2}H_e''(T,1) = H'(T,1) - H(T,1) + |V(T)| \\ &+ \frac{1}{2}H''(T,1) - H'(T,1) + H(T,1) - |V(T)| = WW(T) - W(T). \end{aligned}$$

■

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" [5].

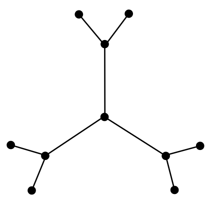

Figure 1. Regular dendrimer $T_{2,3}$.

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

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

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

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

and

$$\begin{aligned} WW_e(T_{k,d}) &= d\frac{2(d-1)+(d-1)^k\,(4-5d^2)}{2(d-2)^4} \\ &+ d\frac{(d-1)^{2k}\Big(-2-8k+d\,(-2+5d+16k-d(d+4)k+2(d-2)^2k^2)\Big)}{2(d-2)^4}. \end{aligned}$$

Since the Wiener index and the hyper-Wiener index of regular dendrimers are already known (see [4, 5, 10]), the edge-Wiener index and the edge-hyper-Wiener index could also be computed in terms of Corollary 3.3.

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