MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **55** (2006) 359-362

ISSN 0340 - 6253

On generalization of the Hosoya-Wiener polynomial

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(Received October 10, 2005)

Abstract

It is shown that some of the well-known relations of the Hosoya-Wiener polynomial to the Wiener number and the hyper-Wiener index generalize naturally to weighted graphs.

Weighted graphs can be used in chemical graph theory to model molecules with heteroatoms. While vertex weighted graphs have been considered frequently [5, 2, 14, 11, 9], the edge weighted case seems to be less studied [16]. A *weighted graph* $G = (V, E, w, \lambda)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of *vertices*, a set $E = E(G)$ of unordered pairs $\{x, y\} = xy$ of distinct vertices of G called *edges*, and two *weighting functions*, w and λ. $w : V(G) \mapsto \mathbb{R}^+$ assigns positive real numbers (weights) to vertices and $\lambda : E(G) \mapsto \mathbb{R}^+$ assigns positive real numbers (lengths) to edges. A *simple path* from u to v is a finite sequence of distinct vertices $P = x_0, x_1, \ldots, x_\ell$ such that each pair x_{i-1}, x_i is connected by an edge and $x_0 = u$ and $x_\ell = v$. The *length* of the path is the sum of the lengths of its edges, $l(P) = \sum_{i=1}^{\ell} \lambda(x_{i-1}x_i)$. For any pair of vertices u, v we define the *distance* $d(u, v)$ to be the minimum of lengths over all paths between u and v. If there is no such path, we write $d(u, v) = \infty$.

The Hosoya-Wiener polynomial of a graph G is defined as

$$H(\lambda; x) = H(G, \lambda; x) = \sum_{u,v \in V(G)} x^{d(u,v)}.$$

This definition, which is used for example in [6], slightly differs from the definition used by Hosoya [7] (see also [13]):

$$\hat{H}(\lambda; x) = \hat{H}(G, \lambda; x) = \sum_{u,v \in V(G); u \neq v} x^{d(u,v)}. \tag{1}$$

Obviously, $H(\lambda; x) = \hat{H}(\lambda; x) + |V(G)|$. We explicitly write λ to stress that the distances $d(u, v)$ depend on the edge weights. Clearly, by taking $\lambda = 1$ for all edges, we are at unweighted case.

Remark. In the paper [7] Hosoya used the name Wiener polynomial while some authors later use the name Hosoya polynomial [3, 15]. Let us mention that also the referees gave different suggestions. We decided to use a compromise name here, namely the Hosoya-Wiener polynomial.

It is well-known that the first derivative of the Hosoya-Wiener polynomial evaluated at $x = 1$ equals the Wiener number (see, for example [13]). Higher derivatives of the Hosoya-Wiener polynomial have also been used as descriptors [4, 10].

We generalize the Hosoya-Wiener polynomial as follows. Let G be a (vertex and edge) weighted graph. $H(G, \lambda; x)$ is defined as

$$H(G, \lambda, w; x) = \sum_{u,v \in V(G)} w(u)w(v)x^{d(u,v)}. \tag{2}$$

Clearly, this definition is equivalent to the original definition if all vertex weights are equal to 1. However, note that $H(G, \lambda, w; x)$ may not be a polynomial if the edge weights are allowed to be arbitrary real numbers. Obviously, if natural numbers are used for edge weights, the function $H(G, \lambda, w; x)$ is a polynomial. Hence, with appropriate scaling factor, one can always consider $H(G, \lambda, w; x)$ to be a polynomial, for any model using rational edge weights.

Recently, [9] generalized the Hosoya-Wiener polynomial to vertex weighted graphs in two ways which slightly differ from the one given here.

Remark. Similarly, one could define, in spirit of (1)

$$\hat{H}(\lambda, w; x) = \hat{H}(G, \lambda, w; x) = \sum_{u,v \in V(G); u \neq v} w(u)w(v)x^{d(u,v)},$$

and again it holds $H(\lambda, w; x) = \hat{H}(\lambda, w; x) + \sum_{v \in V(G)} w^2(v)$. Hence the two functions differ in the costant term only.

The *weighted Wiener number* [16] of a weighted graph G is

$$W(G, \lambda, w) = \sum_{u,v \in V(G); u \neq v} w(u)w(v)d(u, v). \tag{3}$$

The definition used here is clearly a generalization of the usual definition for (unweighted) Wiener number. More precisely, if all weights of vertices are 1 and all lengths of edges are 1, then $W(G, \lambda, w)$ is the usual Wiener number $W(G)$.

It seems that the weighted Wiener number has not been studied frequently in the literature. In [16], a linear algorithm for computing the weighted Wiener number is given. A definition, analogous to (3) was used in [5] and [2] for vertex weighted graphs. A different definition in which the "weights" of atoms are added to the sum of distances is used in [14].

For a later reference, we formaly state a generalization of perhaps the most interesting property of the Hosoya-Wiener polynomial, namely

Lemma 1 $W(G, \lambda, w) = H'(G, \lambda, w; 1)$.

Proof. Clearly,

$$H^{'}(G,\lambda,w;x) = \sum_{u,v\in V(G)} w(u)w(v)d(u,v)x^{d(u,v)-1}. \tag{4}$$

which is equal to $W(G,\lambda,w)$ if evaluated at $x = 1$. □

The hyper-Wiener index was defined by Randić [12] and generalized to acyclic structures in [8]. The definition of weighted hyper-Wiener index is

$$WW(G,\lambda,w) = \frac{1}{2}\sum_{u,v\in V(G)} w(u)w(v)d(u,v)^2 + \frac{1}{2}\sum_{u,v\in V(G)} w(u)w(v)d(u,v). \tag{5}$$

We use the same name and notation because it clearly generalizes the hyper-Wiener index of unweighted graphs. (If all weights are equal 1, $WW(G,\lambda,w)$ is the standard hyper-Wiener index $WW(G)$.)

The following theorem generalizes the main result of [1]

Theorem 2

$$WW(G,\lambda,w) = H^{'}(G,w;1) + \frac{1}{2}H^{''}(G,w;1) \tag{6}$$

Proof. First note that

$$d(u,v) + d(u,v)(d(u,v)-1) = d(u,v) + d(u,v)^2 - d(u,v) = d(u,v)^2.$$

Using this, we can write

$$\begin{aligned}
&\frac{d}{dx}(xH^{'}(G,\lambda,w;x)) = H^{'}(G,\lambda,w;x) + xH^{''}(G,\lambda,w;x) = \\
&= H^{'}(G,\lambda,w;x) + x\sum_{u,v\in V(G)} w(u)w(v)d(u,v)(d(u,v)-1)x^{d(u,v)-2} = \\
&= \sum_{u,v\in V(G)} w(u)w(v)d(u,v)^2x^{d(u,v)-1}.
\end{aligned}$$

Hence

$$\sum_{u,v\in V(G)} w(u)w(v)d(u,v)^2x^{d(u,v)-1} = H^{'}(G,\lambda,w;x) + xH^{''}(G,\lambda,w;x). \tag{7}$$

From (4) and (7) at $x = 1$ we get

$$\begin{aligned}
&2WW(G,\lambda,w) = \sum_{u,v\in V(G)} w(u)w(v)d(u,v) + \sum_{u,v\in V(G)} w(u)w(v)d(u,v)^2 = \\
&= H^{'}(G,w;1) + \Big[H^{'}(G,\lambda,w;x) + xH^{''}(G,\lambda,w;x)\Big]_{x=1} = \\
&= 2H^{'}(G,w;1) + H^{''}(G,w;1)
\end{aligned}$$

as claimed. □

Finally, we wish to note that the generalization of the Hosoya-Wiener polynomial to edge and vertex weighted graphs seems to allow generalization of (at least some) algorithms. For example, $W(G,\lambda,w;x)$ on weighted trees can be computed efficiently, more precisely [17]:

Theorem 3 *The Hosoya-Wiener polynomial on a weighted tree T can be computed in $O(D\Delta^2 n)$ time, where D is the diameter of T and Δ is the maximal degree of a vertex in T.*

Furthermore, we believe that it is possible to generalize the approach outlined here to cacti, see [18]

Conjecture 4 *The Hosoya-Wiener polynomial on a weighted cactus G can be computed in $O(D\Delta^2 n)$ time, where D is the diameter of G and Δ is the maximal degree of a vertex in G.*

Acknowledgement. This work was supported in part by the Ministry of Higher Education, Science and Technology of Slovenia. We wish to thank to the referees for valuable suggestions.

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