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The Relation Between Different Versions of Hosoya Polynomial and Wiener Index

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Abstract: The Hosoya polynomial of a graph, $H(G, x)$, has the property that its first derivative, evaluated in $x = 1$, equals to Wiener index. The edge versions of Wiener index was introduced in 2008. In this paper, we obtain the relation between different versions of Hosoya polynomial and Wiener index.

Key words: Hosoya Polynomial · Wiener index · Edge Wiener indices

INTRODUCTION

The structure of a chemical compound is usually modeled as a polygonal shape, which is often called the molecular graph of this compound. Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices (e.g., distance or adjacency matrices), which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index [1, 2]. As a result, the topological index can be defined as two-dimensional descriptors that can be easily calculated from the molecular graphs and do not depend on the way the graph is depicted or labeled and no need of energy minimization of the chemical structure. It has been found that many properties of a chemical compound are closely related to some topological indices of its molecular graph by computing these indices for them, that in [3-5] you can find some of recent computations. Among these topological indices, the Wiener number is probably the most important one [6].

The Wiener number is a distance-based graph invariant, used as one of the structure descriptors for predicting physicochemical properties of organic compounds (often those significant for pharmacology, agriculture, environment protection, etc.). The Wiener index was introduced by the chemist H. Wiener about 60 years ago to demonstrate correlations between physicochemical properties of organic compounds and the topological structure of their molecular graphs. This concept has been one of the most widely used descriptors in relating a chemical compound's properties to its molecular graph. Therefore, in order to construct a compound with a certain property, one may want to build some structure that has the corresponding Wiener number [6].

In addition to the myriad applications of the Wiener number in chemistry there are many situations in communication, facility location, cryptology, etc., that are effectively modeled by a connected graph G satisfying certain restrictions [7]. The biochemical community has been using the Wiener number to correlate a compound's molecular graph with experimentally gathered data regarding the compound's characteristics. In the drug design process, one wants to construct chemical compounds with certain properties. The basic idea is to construct chemical compounds from the most common molecules so that the resulting compound has the expected Wiener number. Compounds with different structures (and different Wiener indices), even with the same chemical formula, can have different properties.

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Hence it is indeed important to study the structure (and thus also the Wiener number) of the molecular graph besides the chemical formula [6].

The Wiener index which is the sum of distances between vertices in a connected graph [8] is the first and important topological index and it has found extensive application in chemistry. For more information about the Wiener index in chemistry and mathematics see [9-10]. This version of Wiener number for a connected graph G defined as follow:

$$W(G) = W_v(G) = \sum_{\{x,y\}\subseteq V(G)} d(x,y)$$

where $d(x, y)$ is the distance between two vertices x *and* y.
Also, Wiener index can be written as

$$W(G) = W_v(G) = \sum_{k\geq 0} kd(G,k)$$

where $d(G, k)$ is the number of pairs of vertices of G that are at distance k.

Hosoya [11] introduced a distance-based graph polynomial which is

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

Nowadays it is called the Hosoya polynomial or Wiener polynomial [12]. The another form of this polynomial is

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

The edge versions of Wiener index which were introduced recently are the sum of distances between edges of a connected graph g as follow [13]:
The first edge-Wiener number is

$$W_{e0}(G) = \sum_{\{e,f\}\subseteq E(G)} d_0(e,f)$$

where $d_0(e,f) = \begin{cases} d_1(e,f)+1 & e \neq f \\ 0 & e = f \end{cases}$ and

$d_1(e, f) = \min\{d(x,u),d(x,v),d(y,u),d(y,v)\}$ such that $e = xy$ and $f = uv$.
The second edge-Wiener index is

$$W_{e4}(G) = \sum_{\{e,f\}\subseteq E(G)} d_4(e,f)$$

where $d_4(e,f) = \begin{cases} d_2(e,f) & e \neq f \\ 0 & e = f \end{cases}$ and

$d_2(e, f) = \text{mix}\{d(x,u),d(x,v),d(y,u),d(y,v)\}$ such that $e = xy$ and $f = uv$.

In [14-16], edge-Wiener indices of some graphs have been computed.

In this paper, after studying some of the elementary properties of edge Wiener polynomials, compute them for some common graphs and stating the relations between versions of Wiener index, we obtain the relation between different versions of Hosoya polynomial and Wiener index.

Some Definitions and Results: The edge Wiener polynomial is defined as follows.

If q is a parameter, then the edge Wiener polynomial of a graph G is

$$W_{ei}(G;q) = \sum_{\{e,f\}\subseteq E(G)} q^{d_i(e,f)},\ i = 0,4$$

In what follows, we use $|S|$ to describe the cardinal of a set S. Also, if $f(q)$ is a polynomial in q, then $\deg f(q)$ is its degree and $[q^i]\,f(q)$ is the coefficient of q^i.

The next theorem summarizes some of the properties of $W_{ei}(G; q)$. Its proof follows easily from the definitions and so is omitted.

Theorem 2-1: The edge Wiener polynomials satisfy the following conditions, suppose $i = 0,4$:

1. $[q^0]W_{ei}(G; q)$ = *diameter of G under dis* tan *ce* d_i.

2. $[q^0]\ W_{ei}(G; q) = 0$.

3. $\begin{cases} [q^1]W_{e0}(G;q) = |E(L(G))| \\ [q^1]W_{e0}(G;q) = \begin{cases} 0 & , \textit{if G without the triangular} \\ 3(\textit{the number of triangulars in graph G}) & , \textit{o.w.} \end{cases} \end{cases}$

4. $W_{ei}(G;1) = \binom{|E(G)|}{2}$

5. $W_{ei}{}'(G;1) = W_{ei}(G)$

We next find the edge Wiener polynomials of some specific graphs. Let K_n, $K_{a,b}$, C_n and S_n be complete graph, complete bipartite graph on parts size a and b, cycle and star. Determining the Wiener polynomials of these graphs is a matter of simple counting, so the proof of the next result is also omitted.

Theorem 2-2: Let graph G has m edge and i = 0,4, then some specific edge Wiener polynomials are as follows:

1. $W_{ei}(K_n;q) = \begin{cases} W_{e0}(K_n;q) = \frac{1}{2}\binom{n}{2}q + \frac{1}{4}\binom{n}{2}(n-2)(n-3)q^2 \\ W_{e4}(K_n;q) = \binom{m}{2}q \end{cases}$

2. $W_{ei}(K_{a,b};q) = \begin{cases} W_{e0}(K_{a.b};q) = \frac{ab}{2}(a+b-2)q + \frac{ab}{2}(ab-a-b+1)q^2 \\ W_{e4}(K_{a,b};q) = \binom{ab}{2}q^2 \end{cases}$

3. $W_{ei}(C_n;q) = \begin{cases} \begin{cases} W_{e0}(C_n;q) = \frac{n}{2}\left(2\left(q+q^2+\ldots+q^{\frac{n-2}{2}}\right)+q^{\frac{n}{2}}\right) \\ W_{e4}(C_n;q) = \frac{n}{2}\left(2\left(q^2+\ldots+q^{\frac{n}{2}}\right)+q^{\frac{n}{2}}\right) \end{cases} & , \textit{n is even} \\ \begin{cases} W_{e0}(C_n;q) = \frac{n}{2}\left(2\left(q+q^2+\ldots+q^{\frac{n-1}{2}}\right)\right) \\ W_{e4}(C_n;q) = \frac{n}{2}\left(2\left(q^2+\ldots+q^{\frac{n-1}{2}}\right)+2q^{\frac{n-1}{2}}\right) \end{cases} & , \textit{n is odd} \end{cases}$

5. $W_{ei}(S_n;q) = \begin{cases} W_{e0}(S_n;q) = \frac{n-1}{2}((n-2)q) \\ W_{e4}(S_n;q) = \frac{n-1}{2}((n-2)q^2) \end{cases}$

Combining the previous theorem with number of 5 of theorem 2-1, we obtain the well-known edge Wiener indices of theses graphs.

Conclusion 2-3: The edge Wiener indices of some graphs are:

1. $W_{ei}(K_n) = \begin{cases} W_{e0}(K_n) = \frac{1}{4}n(n-1)^2(n-2) \\ W_{e4}(K_n) = \frac{1}{8}n(n-1)(n-2)(n+1) \end{cases}$

2. $W_{ei}(K_{a,b}) = \begin{cases} W_{e0}(K_{a.b}) = \frac{ab}{2}(2ab-a-b) \\ W_{e4}(K_{a,b}) = ab(ab-1) \end{cases}$

3. $W_{ei}(C_n) = \begin{cases} \begin{cases} W_{e0}(C_n) = \frac{1}{8}n^3 \\ W_{e4}(C_n) = \frac{1}{8}n(n^2+4n-8) \end{cases} & , \ n \ is \ even \\ \begin{cases} W_{e0}(C_n) = \frac{1}{8}n(n^2-1) \\ W_{e4}(C_n) = \frac{1}{8}n(n^2+4n-13) \end{cases} & , \ n \ is \ odd \end{cases}$

4. $W_{ei}(S_n) = \begin{cases} W_{e0}(S_n) = \frac{1}{2}(n-1)(n-2) \\ W_{e4}(S_n) = (n-1)(n-2) \end{cases}$

In following, we find the relation between vertex and edge Wiener polynomials. For finding these relations, we must find the relations among distances between edges with distances between vertices that A. Iranmanesh *et al*. find them in [15] with introducing new distances between edges according to distances between vertices. We recall them and omit their proofs.

Definition 2-4: [15] Let $e = uv, f = xy$ be the edges of connected graph G. Then, we define:

$$d'(e,f) = \frac{d(u,x)+d(u,y)+d(v,x)+d(v,y)}{4}$$ and

$$d''(e,f) = \begin{cases} \lceil d'(e,f) \rceil & , \ \{e,f\} \notin C \\ d'(e,f)+1 & , \ \{e,f\} \in C \end{cases}$$

where $C = \{\{e,f\} \subseteq E(G) \mid \ if \ e = uv \ and \ f = xy \ ; \ d(u,x) = d(u,y) = d(v,x) = d(v,x)\}$ and $d_3(e,f) = \begin{cases} d''(e,f) & e \neq f \\ 0 & e = f \end{cases}$. Also, d' and d'' are not distances and $d_3 = d_0$.

In addition,. If $e, f \in E(G)$, we define:

$$d'''(e,f) = \begin{cases} \lceil d'(e,f) \rceil & , \ \{e,f\} \notin A_1 \\ d'(e,f)+1 & , \ \{e,f\} \in A_1 \end{cases} \text{ and } d_5(e,f) = \begin{cases} d'''(e,f) & e \neq f \\ 0 & e = f \end{cases}$$

The mathematical quantity d''' is not distance and $d_4 = d_5$.

In [14], due to the distance d_3, several sets have been defined.

$$A_1 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) \right\}$$

$$A_2 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) + \frac{1}{4} \right\}$$

$$A_3 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) + \frac{2}{4} \right\}$$

$$A_4 = \left\{ \{e,f\} \subseteq E(G) \middle| \; d_3(e,f) = d'(e,f) + \frac{3}{4} \right\}$$

Theorem 2-5: [15] Suppose G is a graph with m edges and A_1, A_2, A_3,A_4 *and* C are the sets which has been defined as above. Then, the first version of edge-Wiener number according to distance between vertices of graph G is:

$$W_{e0}(G) = \frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)} \deg(x)\times\deg(y)\times d(x,y) - \frac{m}{4} + \sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right) + \sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right) + \sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right) + |C|.$$

Theorem 2-6: [15] Suppose G is a graph with m edges and A_1, A_2, A_3,A_4 *and* C are the sets which has been defined in Definition 2-1 and Corollary 2-2. Then, we can repeat the second version of edge-Wiener number according to distance between vertices of graph G as follow:

$$W_{e4}(G) = \frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)} \deg(x)\times\deg(y)\times d(x,y) - \frac{m}{4} + \sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right) + \sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right) + \sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right) + |A_1|.$$

Corollary 2-7: The explicit relation between edge versions of Wiener index is

$$W_{e4}(G) = W_{e0}(G) + |A_1| - |C|.$$

□

Relation Between Different Versions of Hosoya Polynomial and Wiener Index: In the following theorem, we investigate the relations between different versions of Hosoya polynomial and Wiener index.

Theorem 3-1: The relations between different versions of Hosoya polynomial and Wiener index are as follows.

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

2. $W_{ei}(G) = H_{ei}'(G,x), \;\; i = 0,4$

3. $$W_{e0}(G)=\frac{5}{8}H'(G.x)+\frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)}\left(\deg(x)\times\deg(y)-1\right)\times d(x,y)-\frac{m}{4}+\sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right)+\sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right)+\sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right)+|C|.$$

4. $$W_{e4}(G)=\frac{5}{8}H'(G.x)+\frac{1}{8}\sum_{x\in V(G)}\sum_{y\in V(G)}\left(\deg(x)\times\deg(y)-1\right)\times d(x,y)-\frac{m}{4}+\sum_{\{e,f\}\in A_3}\left(\frac{1}{2}\right)+\sum_{\{e,f\}\in A_2}\left(\frac{1}{4}\right)+\sum_{\{e,f\}\in A_4}\left(\frac{3}{4}\right)+|A_1|.$$

5. $$W(G)=\frac{8}{5}H_{e0}'(G,x)+\frac{1}{5}\sum_{x\in V(G)}\sum_{y\in V(G)}\left(\deg(x)\times\deg(y)-1\right)\times d(x,y)+\frac{8m}{20}-\frac{4|A_3|}{5}-\frac{2|A_2|}{5}-\frac{6|A_4|}{5}-|C|$$

6. $$W(G)=\frac{8}{5}H_{e4}'(G,x)+\frac{1}{5}\sum_{x\in V(G)}\sum_{y\in V(G)}\left(\deg(x)\times\deg(y)-1\right)\times d(x,y)+\frac{8m}{20}-\frac{4|A_3|}{5}-\frac{2|A_2|}{5}-\frac{6|A_4|}{5}-|A_1|.$$

7. $$H_{e4}'(G,x)=H_{e0}'(G,x)+|A_1|-|C|.$$

Proof: Due to the definitions of versions of Wiener index and Hosoya polynomial, Theorems (2-5 and 2-6) and Corollary (2-7), the relations (1) to (7) can be concluded.

□

In the following, we would like to find the relations between some versions of Hosoya polynomial and Wiener index for nanotubes Zigzag, $TUC_4C_8(R)$ and $TUC_4C_8(S)$. For this, firstly we state the relations between versions of Wiener index for these nanotubes.

Theorem 3-2: [15] The explicit relation between vertex Wiener number and the first edge-Wiener number for zig-zag nanotubes which have been consisted of vertices with degrees 3 and 2 is

$$W_{e0}(G)=\frac{9}{4}W_v(G)+\frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}d(x,y)-\frac{5}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)-\frac{m}{4}+\sum_{\{e,f\}\in A_3}\frac{1}{2}.$$

Therefore we have following results.

Corollary 3-3: The relations between some versions of Hosoya polynomial and Wiener index for nanotubes Zigzag, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ are as follows. For convenience, we use the notations H for the molecular graph of mentioned nanotubes.

1. $$W_{e0}(H)=\frac{9}{4}H'(H,x)+\frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}d(x,y)-\frac{5}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)-\frac{m}{4}+\frac{|A_3|}{2}$$

2. $$W_{e4}(H)=\frac{9}{4}H'(H,x)+\frac{3}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}d(x,y)-\frac{5}{8}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)-\frac{m}{4}+\frac{|A_3|}{2}+|A_3|$$

3. $$W(H)=\frac{4}{9}H_{e0}'(H,x)-\frac{3}{18}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}d(x,y)+\frac{5}{18}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)+\frac{m}{9}-\frac{2|A_3|}{9}$$

4. $$W(H)=\frac{4}{9}H_{e4}'(H,x)-\frac{3}{18}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=3}}d(x,y)+\frac{5}{18}\sum_{\substack{x\in V(G)\\ \deg(x)=2}}\sum_{\substack{y\in V(G)\\ \deg(y)=2}}d(x,y)+\frac{m}{9}-\frac{2|A_3|}{9}-|A_1|$$

□

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