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On Extensions of Wiener Index

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Abstract

The n-th order Wiener index of a molecular graph G was put forward by Estrada et al. [*New J. Chem*. **22** (1998) 819] as ${}^{n}W = H^{(n)}(G,x)\big|_{x=1}$ where $H(G,x)$ is the Hosoya polynomial. Recently Brückler et al. [*Chem. Phys. Lett.* **503** (2011) 336] considered a related graph invariant, $W^{(n)} = (1/n!)\, d^n (x^{n-1} H(G,x)) / d\,x^n\big|_{x=1}$. For n=1, both ${}^{n}W$ and $W^{(n)}$ reduce to the ordinary Wiener index. The aim of this paper is to obtain closed formulas for these two extensions of the Wiener index. It is proved that $W^{(n)} = (1/n!)\sum_{k=1}^{n} c(n,k) W_k$ and ${}^{n}W = \sum_{k=1}^{n} s(n,k) W_k$, where $c(n,k)$, $s(n,k)$, and W_k stand for the unsigned Stirling number of the first kind, Stirling number of the first kind, and the k-th distance moment of G, respectively.

1. Introduction

Throughout this paper we are concerned with molecular graphs. Let $G = (V(G), E(G))$, be such a graph, where $V(G)$ and $E(G)$ are its vertex and edge sets. The distance $d_G(u,v)$ between the vertices u and v of G is the length of a shortest path connecting u and v; if misunderstanding is avoided, then this distance will be written as $d(u,v)$ for short. The diameter of G is the maximum distance between any pair of vertices, and is denoted by $diam(G)$.

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The Wiener index is the oldest and one of the most studied distance-based topological indices in chemistry. It was introduced by Harold Wiener [1] in 1947, equal to the sum of distances between all pairs of vertices of the graph under consideration. For details on the theory of Wiener index consult the reviews [2-4].

The distance moments of a graph G are defined as $W_k = W_k(G) = \sum_{\{u,v\} \in V(G)} d_G(u,v)^k$, where k is a positive integer; in this case W_k is the k-th distance moment of G [5]. Also the generalization of the distance moments, viz. $W_\lambda = W_\lambda(G) = \sum_{\{u,v\} \in V(G)} d_G(u,v)^\lambda$ was considered [6,7], in which case λ may be a real number. However, if $\lambda < 0$, then the summation must be restricted to pairs of *different* vertices u and v. The cases of λ = 1, −1 and −2 pertain, respectively, to the ordinary Wiener index [1], Harary (or reciprocal Wiener) index [8-10] and the old variant of the Harary index [11]. Other much studied distance-based topological indices are $WW = (1/2)[W_1 + W_2]$ and $TSZ = (1/6)W_3 + (1/2)W_2 + (1/3)W_1$, referred to as the hyper−Wiener index [12] and the Tratch−Stankevich−Zefirov index [13], respectively.

In [14], Hosoya introduced the generating function of distances that he termed the "Wiener polynomial". Eventually, it was re-named into "Hosoya polynomial" [15], which name is nowadays most frequently used in the mathematical and mathematico-chemical literature; for further details and references see [16]. The Hosoya polynomial is defined as

$$H(G,x) = \sum_{k \geq 0} d(G,k)\, x^k \tag{1}$$

where $d(G,k)$ denotes the number of pairs of vertices of the graph G whose distance is k. Evidently, $d(G,0)$ and $d(G,1)$ are, respectively, equal to the number of vertices and edges of G, and $H(G,x)$ is a polynomial in the variable x, of degree $diam(G)$.

Another equivalent way to write the Hosoya polynomial is

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

The n-th order Wiener index, denoted by ${}^nW(G)$, seems to be the oldest extensions of the ordinary Wiener index.. It was introduced by Estrada et al. in 1998 [17] as:

$${}^nW(G) = \left. \frac{d^n H(G,x)}{dx^n} \right|_{x=1} \quad ; \quad n = 1,2,3,\ldots .$$

It has been noticed recently [18] that the Hosoya polynomial satisfies also the following conditions:

$$\left.\frac{d\big(H(G,x)\big)}{dx}\right|_{x=1} = W(G) \tag{3}$$

$$\left.\frac{1}{2}\frac{d^2\big(xH(G,x)\big)}{dx^2}\right|_{x=1} = WW(G) \tag{4}$$

$$\left.\frac{1}{6}\frac{d^3\big(x^2H(G,x)\big)}{dx^3}\right|_{x=1} = TSZ(G)\,. \tag{5}$$

Eqs. (3)–(5) are special cases for n=1,2,3, of the following graph invariant, which was mentioned in the paper [18], but not further investigated:

$$W^{(n)} := \left.\frac{1}{n!}\frac{d^n\big(x^{n-1}H(G,x)\big)}{dx^n}\right|_{x=1}$$

In the next section we show how all these extensions and generalizations of the Wiener index are mutually related, and how these can be expressed in terms of distance moments. Throughout this paper our notation is standard and taken mainly from [19,20].

2. Main Results and Discussion

The Stirling numbers of the first kind are the coefficients in the expansion

$$x(x-1)(x-2)\cdots(n-n+1) = \sum_{k=0}^{n} s(n,k)\,x^k\,.$$

The unsigned Stirling numbers of the first kind, $c(n,k)$, are defined as $c(n,k) = (-1)^{n-k}\,s(n,k)$. Recall [19], that $c(n,k)$ is the number of permutations of n elements with k disjoint cycles. As well known [19], the generating functions of these sequences are $(t)_{(n)} = t(t-1)\cdots(t-n+1)$ and $(t)^{(n)} = t(t+1)\cdots(t+n-1)$, respectively. This means that:

$$(t)_{(n)} = \sum_{k=1}^{n} s(n,k)\,t^k \qquad \text{and} \qquad (t)^{(n)} = \sum_{k=1}^{n} c(n,k)\,t^k$$

We are now ready to state our main result:

Theorem 2.1. For any positive integer n,

$$W^{(n)} = \frac{1}{n}\sum_{k=1}^{n} c(n,k)\,W_k \tag{6}$$

$${}^{n}W = \sum_{k=1}^{n} s(n,k)\,W_k\,. \tag{7}$$

Proof. We compute the n-th derivative of $x^{n-1}H(G,x)$, using the form (2) of the Hosoya polynomial. This yields:

$$\frac{1}{n!}\frac{d^n(x^{n-1}H(G,x))}{dx^n} = \frac{1}{n!}\sum_{\{u,v\}\subseteq V(G)} (d(u,v)+n-1)(d(u,v)+n-2)\ldots(d(u,v)+1)d(u,v)x^{d(u,v)-1}$$

$$= \frac{1}{n!}\sum_{\{u,v\}\subseteq V(G)} (d(u,v))^{(n)}x^{d(u,v)-1}$$

$$= \frac{1}{n!}\sum_{\{u,v\}\subseteq V(G)} \sum_{k=1}^{n} c(n,k)\,d(u,v)^k x^{d(u,v)-1}$$

By evaluating $1/n!\times d^n/dx^n(x^{n-1}H(G,x))$ at $x = 1$, we arrive at Eq. (6).

In order to prove Eq. (7), we notice that

$$\frac{d^n(H(G,x))}{dx^n} = \sum_{\{u,v\}\subseteq V(G)} d(u,v)(d(u,v)-1)\ldots(d(u,v)-n+1)x^{d(u,v)-n}$$

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

$$= \sum_{\{u,v\}\subseteq V(G)} \sum_{k=1}^{n} s(n,k)\,d(u,v)^k\,x^{d(u,v)-n} \quad .$$

By evaluating $d^nH(G,x)/dx^n$ at $x=1$, the Eq. (7) is obtained. ■

Notice that in the second part of Theorem 2.1, the upper bound in the summation is *diam*(*G*).

As a direct consequence of Theorem 2.1 we have:

Corollary 2.2. (see also [17,18,20]). If n = 1, 2, 3, 4 or 5, then,

1) $W^{(1)} = W_1 = W$, $W^{(2)} = \frac{1}{2}W_2 + \frac{1}{2}W_1 = WW$, $W^{(3)} = \frac{1}{6}W_3 + \frac{1}{2}W_2 + \frac{1}{3}W_1 = TSZ$,

$W^{(4)} = \frac{1}{24}W_4 + \frac{1}{4}W_3 + \frac{11}{24}W_2 + \frac{1}{4}W_1$, $W^{(5)} = \frac{1}{120}W_5 + \frac{1}{12}W_4 + \frac{1}{24}W_3 + \frac{5}{12}W_2 + \frac{1}{5}W_1$

2) ${}^{1}W = W_1 = W$, ${}^{2}W = \frac{1}{2}W_2 - \frac{1}{2}W_1$, ${}^{3}W = \frac{1}{6}W_3 - \frac{1}{2}W_2 + \frac{1}{3}W_1$,

${}^{4}W = \frac{1}{24}W_4 - \frac{1}{4}W_3 + \frac{11}{24}W_2 - \frac{1}{4}W_1$, ${}^{5}W = \frac{1}{120}W_5 - \frac{1}{12}W_4 + \frac{1}{24}W_3 - \frac{5}{12}W_2 + \frac{1}{5}W_1$

Corollary 2.3. Since the diameter of the complete graph K_p is equal to 1, and its Hosoya polynomial is equal to $H(K_p,x) = p + \binom{p}{2}x$, we get $W^{(n)}(K_p) = \binom{p}{2}$ for any $n \geq 1$, whereas ${}^{1}W(K_p) = \binom{p}{2}$ and ${}^{n}W(K_p) = 0$ for $n > 1$.

The Stirling number of the second kind, $S(n,k)$, is the number of partitions of n elements into k non-empty parts. It is well known that $t^n = \sum_{k=1}^{n} S(n,k)(t)_{(k)}$.

Theorem 2.4. For any positive integer n,

$$W_n = \sum_{k=1}^{n} S(n,k) \left. \frac{d^k H(G,x)}{dx^k} \right|_{x=1}.$$

Proof. Suppose that u and v are arbitrary vertices of G. Then $(d(u,v))_{(n)} = \sum_{k=1}^{n} s(n,k)\, d(u,v)^k$ and so $d(u,v)^n = \sum_{k=1}^{n} S(n,k)(d(u,v))_{(k)}$. Therefore,

$$\begin{aligned}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^n &= \sum_{\{u,v\}\subseteq V(G)} \sum_{k=1}^{n} S(n,k)(d(u,v))_{(k)} \\ &= \sum_{k=1}^{n} S(n,k) \sum_{\{u,v\}\subseteq V(G)} (d(u,v))_{(k)}\end{aligned}$$

proving the theorem. ■

Corollary 2.5. If n = 1, 2, 3, 4 or 5 then,

$$W_1 = H'(G,1)$$

$$W_2 = H'(G,1) + H''(G,1)$$

$$W_3 = H'''(G,1) + 3H''(G,1) + H'(G,1),$$

$$W_4 = H^{(4)}(G,1) + 6H'''(G,1) + 7H''(G,1) + H'(G,1)$$

$$W_5 = H^{(5)}(G,1) + 10H^{(4)}(G,1) + 25H'''(G,1) + 15H''(G,1) + H'(G,1)$$

The number of r-permutations of a collection of s distinct objects is denoted by $P(s,r)$. This number is equal to 0 when $r \geq s$ and otherwise $P(s,r) = s!/(s-r)!$. Obviously, $P(s,r) = (s)_{(r)}$.

Theorem 2.6. Let G be any graph. Then,

$$W^{(n)}(G) = \frac{1}{n!}\left(\sum_{k=1}^{diam(G)} P(n+k-1,n)\, d(G,k)\right) \tag{8}$$

where n is a positive integer, and

$$^{n}W(G) = \sum_{k=n}^{\dim a(G)} P(k,n) d(G,k) \tag{9}$$

where $1 \le n \le diam(G)$.

Proof. We rewrite $H(G,x)$ and $x^{n-1}H(G,x)$ according to Eq. (1):

$$H(G,x) = \sum_{1\le k\le diam(G)} d(G,k)\,x^k \text{ and } x^{n-1}H(G,k) = \sum_{1\le k\le diam(G)} d(G,k)\,x^{n+k-1}.$$

Then

$$\frac{1}{n!}\frac{d^n(x^{n-1}H(G,x))}{dx^n} = \frac{1}{n!}\Big((n\times(n-1)\times\ldots\times 2\times 1)d(G,1) + ((n+1)\times n\times\ldots\times 2)d(G,2)x^1 + \cdots$$

$$+ ((n+diam(G)-1)\times\ldots\times b)d(G,diam(G))x^{diam(G)-1}\Big)$$

$$= \frac{1}{n!}\sum_{k=1}^{diam(G)}\big((n+k-1)\times(n+k-2)\times\ldots\times k\big)d(G,k)x^{k-1}$$

$$= \frac{1}{n!}\sum_{k=1}^{diam(G)}\frac{(n+k-1)!}{(k-1)!}d(G,k)x^{k-1}$$

By evaluating $(1/n!)d^n(x^{n-1}H(G,x))/dx^n$ at $x=1$, we arrive at (8). In order to prove (9), we notice that

$$\frac{d^n(H(G,x))}{dx^n} = (n\times(n-1)\times\ldots\times 2\times 1)d(G,n) + ((n+1)\times n\times\ldots\times 2)d(G,n+1)x^1 + \cdots$$

$$+ (diam(G)\times(diam(G)-1)\times\ldots\times(diam(G)-n+1))d(G,diam(G))x^{diam(G)-n}$$

$$= \sum_{k=n}^{diam(G)}\big(k\times(k-1)\times\ldots\times(k-n+1)\big)d(G,k)x^{k-n}$$

$$= \sum_{k=n}^{diam(G)}\frac{k!}{(k-n)!}d(G,k)x^{n-k}$$

Eq. (9) in Theorem 2.6 is obtained by evaluating $\dfrac{d^nH(G,x)}{dx^n}$ at $x=1$. ■

Suppose that G is a connected graph. It is easy to restate Theorem 2.1, Eq. (7), by a matrix equation $BX = Y$, where

$$B = [s_{ij}];\ s_{ij} = s(i,j),$$

is a matrix of dimension $diam(G) \times diam(G)$ and X and Y are column vectors defined as follows:

$$X = \begin{pmatrix} W_1 \\ W_2 \\ W_3 \\ \vdots \\ W_{diam(G)} \end{pmatrix}, \; Y = \begin{pmatrix} H^{(1)}(1) \\ H^{(2)}(1) \\ H^{(3)}(1) \\ \vdots \\ H^{(diam(G))}(1) \end{pmatrix}$$

Since B is lower triangular and $\det(B) = 1$, B is invertible. On the other hand, by orthogonality relation $\sum_k S(n,k)\, s(k,m) = \delta_{n,m}$ where $\delta_{n,m}$ denotes the Kronecker delta, it is $B^{-1} = [S(i,j)]$. Therefore, $X = B^{-1}Y$ is equivalent to Theorem 2.4.

In a similar way, by Theorem 2.6, Eq. (9), we obtain the matrix equation $PD = H$, where $P = [P_{ij}]$ is a square matrix of dimension $diam(G)$ and $P_{ij} = P(i,j)$. Obviously, P is upper triangular, $\det(P) = \prod_{i=1}^{diam(G)} \frac{1}{i!}$ and we have:

$$P^{-1} = \begin{pmatrix} \frac{1}{1!}\frac{(-1)^0}{0!} & \frac{1}{1!}\frac{(-1)^1}{1!} & \frac{1}{1!}\frac{(-1)^2}{2!} & \cdots & \frac{1}{1!}\frac{(-1)^{diam(G)-1}}{(diam(G)-1)!} \\ 0 & \frac{1}{2!}\frac{(-1)^0}{0!} & \frac{1}{2!}\frac{(-1)^1}{1!} & \cdots & \frac{1}{2!}\frac{(-1)^{diam(G)-2}}{(diam(G)-2)!} \\ 0 & 0 & \frac{1}{3!}\frac{(-1)^0}{0!} & \cdots & \frac{1}{3!}\frac{(-1)^{diam(G)-3}}{(diam(G)-3)!} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{diam(G)!}\frac{(-1)^0}{0!} \end{pmatrix}.$$

Thus, from the matrix equation $D = P^{-1}H$, we obtain

$$d(G,n) = \sum_{k=0}^{diam(G)-n} \frac{1}{n!}\frac{(-1)^k}{k!} \cdot H^{(k+n)}(1)\,,\; n = 1, 2, \ldots, diam(G).$$

This interesting identity is, of course, of little practical value, since if the Hosoya polynomial is known, cf. Eq. (1), then each $d(G,n)$, $n = 1,2,\ldots,diam(G)$, is also known.

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