

# Wiener Matrix Sequence, Hyper-Wiener Vector, Wiener Polynomial Sequence and Hyper-Wiener Polynomial of Bi-phenylene

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**ABSTRACT:** The Wiener matrix and the hyper-Wiener number of a tree (acyclic structure), higher Wiener numbers of a tree that can be represented by a Wiener number sequence  ${}^1W, {}^2W, {}^3W, \dots$  where  ${}^1W = W$  is the Wiener index, and  $\sum_{k=1,2,\dots}^K W = R$  is the hyper-Wiener number. The concepts of the Wiener vector and hyper-Wiener vector of a graph are introduced for the molecular graph of bi-phenylene. Moreover, a matrix sequence  $W^{(1)}, W^{(2)}, W^{(3)}, \dots$ , called the Wiener matrix sequence (or distance matrix sequence), and their sum  $\sum_{k=1,2,\dots} W^k = W^{(H)}$ , called the hyper-Wiener matrix are computed, where  $W^{(1)} = D$  is the distance matrix, and the sum of the entries of upper triangle of  $W^{(k)}$  with respect to  $W^{(H)}$  is just equal to  ${}^k W$  with respect to  $R$ . A Wiener polynomial sequence and a weighted hyper-Wiener polynomial of a graph are also determined for the molecular graph of bi-phenylene.

**KEYWORDS:** Molecular graph, Wiener matrix sequence, hyper-Wiener vector; weighted Wiener polynomial; Wiener polynomial sequence;

## I. INTRODUCTION

The Wiener matrix and hyper-Wiener number of a tree  $T$  (acyclic structure) were first introduced by Randić [1]. The present work, based on Klein–Lukovits–Gutman’s definition[5] (Hyper –wiener matrix) for the hyper-Wiener number, gives a new definition of higher Wiener numbers, so that it is applicable to any Molecular graph (connected structure). The concepts of the Wiener vector and the hyper-Wiener vector of a graph are introduced. Later the definition of hyper-Wiener number was extended by Klein et al. for application to any graph (connected structure Molecular). Moreover, by using the distance matrix  $D = D(G)$  of a graph  $G$ , we introduce a Wiener matrix sequence (or distance matrix sequence)  $W^{(1)}, W^{(2)}, W^{(3)}, \dots$ , and their sum  $\sum_{k=1,2,\dots} W^k = W^{(H)}$ , is called the hyper-Wiener matrix, where

$W^{(1)} = D$  is the distance matrix, and the sum of the entries of the upper triangle of  $W^{(k)}$  (resp.  $W^{(H)}$ ) is just equal to  ${}^k W$  (resp.  $R$ ). A Wiener polynomial sequence and a weighted hyper-Wiener polynomial of a graph are also introduced. In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds. For particular purposes any of the labeling may be ignored. A hydrogen-depleted molecular graph or hydrogen-suppressed molecular graph is the molecular graph with hydrogen vertices deleted. The following Fig1:  $G$  is the molecular graph of biphenylene.

(Note that the hydrogen atoms and the double bonds are disregarded in  $G$ . This is not necessary, but has proved to be very convenient in practice). Recall that a molecular graph is necessarily connected.

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## II. CONCEPTS ON WIENER VECTOR AND HYPER WIENER VECTOR

For a connected graph G with n vertices, denoted by 1, 2... n, let  $W_k = \sum_{i < j, d_{ij}=k} d_{ij}, k = 1, 2, \dots$ . The vector  $(W_1, W_2, \dots)$  is called the **Wiener Vector** of G, denoted by WV (G). Clearly; the sum of all components of the Wiener vector of G is just equal to the Wiener number of G.

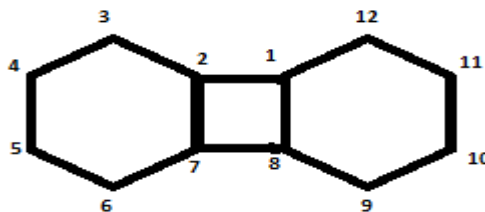
For a connected graph G with n vertices, denoted by 1, 2... n, let  $W_{ij,k} = \max\{d_{ij} - k + 1, 0\}$  where  $d_{ij}$  is the distance between vertices i and j. Then  ${}^k W = \sum_{i < j} W_{ij,k}, k = 1, 2, \dots$  are called the higher Wiener numbers of G. The vector  $({}^1 W, {}^2 W, \dots)$  is called the **hyper-Wiener vector** of G, denoted by HWV (G).

Let D be the distance matrix of a connected graph G.

A Wiener matrix Sequence  $W^{(1)}, W^{(2)}, \dots$  is defined as follows:

Let  $W^{(1)} = D$  for  $k=1, 2, \dots, W^{(k+1)}$  is obtained from  $W^{(k)}$  by leaving zeroes in place and replacing each nonzero entry x of  $W^{(k)}$  by  $x - 1$ . Let D be the distance matrix of a connected graph G, and let  $W^{(1)}, W^{(2)}, \dots$  be the Wiener matrix sequence of G. The hyper-Wiener matrix  $W^{(H)}$  of G is then defined as  $W^{(H)} = \sum_{k=1, 2, \dots} W^{(k)}$ . From the above definitions, we can see that (i, j)-entry of  $W^{(k)}$  is just equal to  $d_{ij} - k + 1$ , so the sum of entries of upper triangle of  $W^{(k)}$  is just equal to  ${}^k W$ .

Moreover, the sum of entries of upper triangle of the hyper-Wiener matrix  $W^{(H)}$  is just equal to the hyper-Wiener number R. However, the hyper-Wiener matrix is applicable for any connected structure.



**Fig 1: Molecular graph of biphenylene**

For graph G in Figure 1, its Wiener matrix sequence, Wiener vector, and hyper-Wiener vector are determined and given below.

$$W^{(1)}(G) = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 \\ 3 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 \\ 2 & 1 & 2 & 4 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 0 \end{pmatrix}$$

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$$W^{(2)}(G) = \begin{pmatrix} 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 0 & 0 & 1 & 2 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 & 4 \\ 2 & 1 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 \\ 1 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 \\ 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 2 & 1 & 0 & 0 \end{pmatrix}$$

$$W^{(3)}(G) = \begin{pmatrix} 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

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$$W^{(4)}(G) = \begin{pmatrix}
 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 \\
 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0
 \end{pmatrix}$$
  

$$W^{(5)}(G) = \begin{pmatrix}
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
 \end{pmatrix}$$

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$$W^{(6)}(G) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$W^{(H)}(G) = \begin{pmatrix} 0 & 1 & 3 & 6 & 10 & 6 & 3 & 1 & 3 & 6 & 3 & 1 \\ 1 & 0 & 1 & 3 & 6 & 3 & 1 & 3 & 6 & 10 & 6 & 3 \\ 3 & 1 & 0 & 1 & 3 & 6 & 3 & 6 & 11 & 15 & 10 & 16 \\ 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 15 & 9 \\ 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 16 \\ 6 & 3 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 10 \\ 3 & 1 & 3 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 \\ 1 & 3 & 6 & 10 & 7 & 3 & 1 & 0 & 1 & 3 & 6 & 3 \\ 3 & 6 & 10 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 7 \\ 6 & 10 & 15 & 21 & 16 & 10 & 6 & 3 & 1 & 0 & 1 & 3 \\ 3 & 6 & 10 & 15 & 21 & 16 & 10 & 6 & 3 & 1 & 0 & 0 \\ 1 & 3 & 6 & 10 & 15 & 10 & 6 & 5 & 6 & 3 & 1 & 0 \end{pmatrix}$$

WV (G) = (14, 36, 48, 40, 30, 12), HWV (G) = (180, 114, 62, 28, 10, 2)  
W = 180, R = 396

### III. WIENER POLYNOMIAL SEQUENCE AND HYPER-WIENER POLYNOMIAL

The Wiener polynomial of graph was first introduced by Hosoya[27]. Let D be the distance matrix of a graph G, let l be the largest entry of D, and let  $2d_k$  be the number of such entries of D that are equal to k. The Wiener polynomial

$W(G, x)$  of G is then given by  $W(G, x) = \sum_{k=1}^l d_k x^k$ . Later Sagan and Yeh et.al[19] defined a generating function

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$W(G, x)$  related to the Wiener index of a graph  $G$ , called the **Wiener polynomial**.  $W(G, x) = \sum_{\{u,v \subseteq V(G)\}} x^{d(u,v)}$ , where

$d(u, v)$  denotes the distance between vertices  $u$  and  $v$ . The above two formulae give the same polynomial of  $G$  that

$$W = W'(G,1), R = W'(G,1) + \frac{1}{2} W''(G,1)$$

A hyperHosoya polynomial is given by [18]  $HH(G, x) = \sum_{k=1}^l \left[ \frac{k+1}{2} \right] d_k x^k$  and showed that  $R(G) = HH'(G,1)$

It can be found that the Wiener vector  $(W_1, W_2, \dots)$  consists of the coefficients of the derivative  $W'(G, x)$  of the Wiener polynomial, where  $W_k$  is equal to the coefficient  $k d_k$  of  $x^{k-1}$  in  $W'(G, x)$ . However, the hyper-Wiener vector cannot be obtained from the hyper Hosoya polynomial  $HH(G, x)$ .

In a hyper-Wiener vector,  ${}^l W = W$  so we can call  ${}^1 W = W$  the first Wiener number and  ${}^k W$  the  $k^{\text{th}}$  Wiener number.

According to the Wiener polynomial, we will introduce a Wiener polynomial sequence  $W_1(G, x), W_2(G, x), \dots$  of a graph  $G$ , where the  $k^{\text{th}}$  Wiener polynomial of  $G$  is closely related to the  $k^{\text{th}}$  Wiener number.

Let  $G$  be a connected graph with  $n$  vertices. The  $k^{\text{th}}$  Wiener polynomial of  $G$ ,  $1 \leq k \leq \text{dia}(G)$ , is defined by

$$W_k(G, x) = \sum_{\{u,v \subseteq V(G)\}} x^{\max[d(u,v)-k+1, 0]}$$

where  $\text{dia}(G)$  is the diameter of  $G$ . The polynomial sequence  $W_1(G, x), W_2(G, x), W_3(G, x) \dots$  is called the

## IV. WIENER POLYNOMIAL SEQUENCE OF G

It is not difficult to verify that  $W_1(G, x) = W(G, x)$  and  $W_k'(G,1) = {}^k W$ . The constant term of  $W_k(G, x)$  is equal to the number of the pairs of vertices with distances less than  $k$ . For the hyper-Wiener vector of a graph  $G$ , its components  ${}^1 W$  and  ${}^k W$  might have different contributions in some research for the structure–property relationship. We can weight the  $k^{\text{th}}$  Wiener number by  $y_k$  and define a weighted hyper-Wiener number as follows.

The **weighted hyper-Wiener number**  $R_w(G)$  of a graph  $G$  is defined a  $R_w(G) = \sum_{k=1,2,\dots} {}^k W y_k$ , Where  $y_k$  is the

weight of  ${}^k W$ . In addition; we will introduce a novel weighted hyper-Wiener polynomial  $HW(G, x, y)$  of a graph  $G$ , so that the hyper-Wiener vector and the weighted hyper-Wiener number can be obtained from the polynomial.

The **weighted hyper-Wiener polynomial**  $HW(G, x, y)$  of a graph  $G$  is defined as

$$HW(G, x, y) = \sum_{k=1,2,\dots} W_k(G, x) \cdot y_k, \text{ where } y = (y_1, y_2, \dots). \text{ From the above definition we have that}$$

$$\frac{d}{dx} [HW(G, x, y)] / x = 1 = R_w(G) = \sum_{k=1,2,\dots} {}^k W y_k \text{ where the coefficients of } y_k \text{ in the weighted hyper Wiener}$$

number  $R_w(G)$  are equal to the  $k^{\text{th}}$  Wiener number. Hence, the hyper-Wiener vector can be given by coefficients of

$$\frac{d}{dx} [HW(G, x, y)] / x = 1. \text{ In particular, we have } \frac{d}{dx} [HW(G, x, y)] / x = 1, y = (1, 1, 1, \dots) = R(G) \text{ For graph}$$

$G$  in Figure 1, the Wiener vector, the Wiener polynomial sequence, the weighted hyper Wiener polynomial of  $G$  is given

$$W'(G, x) = 12x^5 + 30x^4 + 40x^3 + 48x^2 + 36x + 14$$

$$WV(G) = (14, 36, 48, 40, 30, 12), W = 180$$

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$$W^{(1)}(G, x) = 2x^6 + 6x^5 + 10x^4 + 16x^3 + 18x^2 + 14x$$

$$W^{(2)}(G, x) = 2x^5 + 6x^4 + 10x^3 + 16x^2 + 18x + 14$$

$$W^{(3)}(G, x) = 2x^4 + 6x^3 + 10x^2 + 16x + 32$$

$$W^{(4)}(G, x) = 2x^3 + 6x^2 + 10x + 48$$

$$W^{(5)}(G, x) = 2x^2 + 6x + 58$$

$$W^{(6)}(G, x) = 2x + 64$$

$$HW(G, x, y) = (2x^6 + 6x^5 + 10x^4 + 16x^3 + 18x^2 + 14x)y_1$$

$$+ (2x^5 + 6x^4 + 10x^3 + 16x^2 + 18x + 14)y_2$$

$$+ (2x^4 + 6x^3 + 10x^2 + 16x + 32)y_3$$

$$+ (2x^3 + 6x^2 + 10x + 48)y_4$$

$$+ (2x^2 + 6x + 58)y_5 + (2x + 64)y_6$$

$$\frac{d}{dx} [HW(G, x, y)] / x = 1 = 180y_1 + 114y_2 + 62y_3 + 28y_4 + 10y_5 + 2y_6$$

$$\frac{d}{dx} [HW(G, x, y)] / x = 1, y = (1,1,1,\dots) = R(G) = 396$$

From the above example, it can be found that if the  $k^{\text{th}}$  Wiener polynomial is given, the  $(k + 1)^{\text{th}}$  Wiener polynomial can be obtained from  $W^{(k)}(G, x)$  by replacing exponent  $k$  of  $x^k$  by  $k - 1$  for  $k = 1, 2, \dots$

## V. CONCLUSION

In the present work, we intended a series of novel topological invariants such as the Wiener vector, the hyper-Wiener vector, the Wiener matrix sequence, the Wiener polynomial sequence, the weighted hyper-Wiener number, and the weighted hyper-Wiener polynomial for molecular graph bi-phenylene. These sequences will be helpful for similarity research analysis and multiply regression analysis in the study of structure-property relationship.

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