Graph Theory Notes of New York XXX, 21–25 (1996)
New York Academy of Sciences.

[GTN XXX:6] WIENER NUMBER OF HEXAGONAL PARALLELOGRAMS

Wai Chee Shiu, Peter Che Bor Lam†
Department of Mathematics
Hong Kong Baptist University
224 Waterloo Road
Kowloon, HONG KONG

Ivan Gutman‡
Institute of Physical Chemistry
Attila Jozef University
H-6701 Szeged, HUNGARY

Abstract

The Wiener number of a connected graph is equal to the sum of the distances between all pairs of its vertices. A graph formed by a row of n hexagonal cells is called an n-hexagonal chain. A graph consisting of m n-hexagonal chains forming the shape of a parallelogram is called an $m \times n$ hexagonal parallelogram. We obtain the Wiener number of the $n \times n$ hexagonal parallelogram and then more generally, of the $m \times n$ hexagonal parallelogram.

1. Introduction

An important invariant of connected graphs is called the Wiener number (or Wiener index) W. This number is equal to the sum of the distances between all pairs of vertices of a graph. The quantity W was first examined by the American physico-chemist Harold Wiener in 1947 and 1948. He conceived this index within an effort to formulate a mathematical model capable of describing molecular shapes. Wiener, and after him numerous other researchers, reported the existence of correlation between W and a variety of physico-chemical properties of alkanes; for recent reviewers on this matter see **[1][2]**, where further references to previous work in this area can be found. The Wiener number (also called *status*, *graph distance*, *transmittance*) has been extensively studied in mathematical literature (see, for instance, **[3]–[6]**). For a generalization of the Wiener number, refer to **[7][8]**.

In spite of the many works on the theory of the Wiener number, some basic problems still remain open. For example, no recursive method is known for the calculation of W of a general graph, especially of polycyclic graphs. This is particularly frustrating in chemical applications, where the majority of molecular graphs are polycyclic. Two of the present authors **[9]** made a significant breakthrough with regard to this problem by designing a method for finding the expression for $W(H_n)$, where H_n is a *hexagonal system* consisting of one central hexagon, surrounded by $(n-1)$ layers of hexagonal cells, $n \geq 2$. Note that H_n is a molecular graph, corresponding to benzene ($n = 1$), coronene ($n = 2$), circumcoronene ($n = 3$), etc. H_n has been extensively studied in the theory of benzenoid hydrocarbons (see, for instance, **[10]–[12]**).

In this paper, we consider another type of hexagonal system. A graph formed by a row of n hexagonal cells is called an n-hexagonal chain. A graph consisting of m n-hexagonal chains forming the shape of a parallelogram is called an $m \times n$ *hexagonal parallelogram*, and is denoted by $Q_{m,n}$. This is another molecular graph of great importance in the theory of benzenoid hydrocarbons **[12]**. In this paper, we obtain expressions for $W(Q_{n,n})$ and of $W(Q_{m,n})$. In section 2, we derive some preliminary results. In section 3, we obtain the Wiener number of $Q_{n,n}$. In section 4 we obtain the Wiener number of $Q_{m,n}$.

In this paper, $\mathbb{Z}$ denotes the set of integers. Graph theory notation and terminology not defined in this paper is as described in the book of Bondy and Murty **[13]**.

---

† This work is partially supported by the Hong Kong Baptist University Faculty Research Grant.

‡ On leave from Faculty of Science, University of Kragujevac, Kragujevac, Yugloslavia.

2. Preliminary Results

Definition: Let $G = (V, E)$ be a graph. For $v, w \in V$ let $\rho(v, w)$ be the distance between v and w. The *Wiener number* of G is defined by $W(G) = \frac{1}{2}\sum_{v, w \in V} \rho(v, w)$. ■

Let $G = (V, E)$ be an infinite graph where $V = \mathbb{Z} \times \mathbb{Z}$ and $\{(x_1, y_1), (x_2, y_2)\} \in E$ if (1) $y_1 = y_2$ and $|x_1 - x_2| = 1$, or, (2) $x_1 = x_2$, $|y_1 - y_2| = 1$ and $x_1 + y_1 + x_2 + y_2 \equiv 1 \pmod 4$. The graph G is called the *wall*, and was first defined in **[9]**.

We identify the $m \times n$ hexagonal parallelogram (see Figure 1) $Q_{m,n}$ as a subgraph of G, with vertex set

$$\left(\bigcup_{y=0}^{m} \{(x+y, y) \in \mathbb{Z} \times \mathbb{Z} : -1 \le x \le 2n\}\right) \backslash \{(-1, 0), (2n+m, m)\}.$$

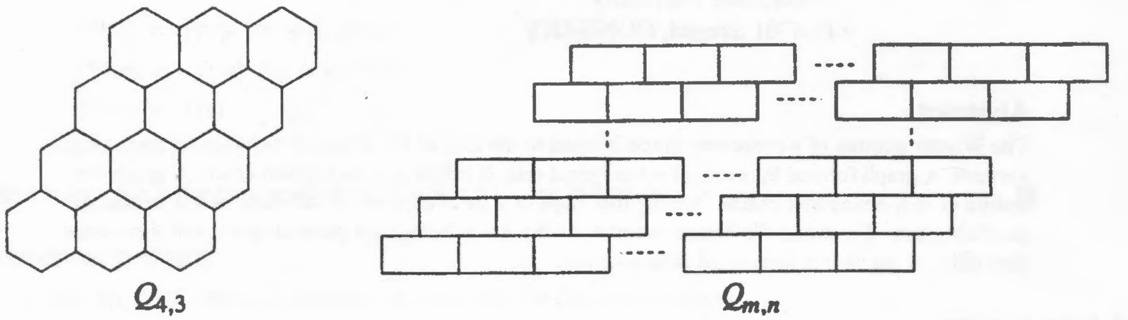

Figure 1

By symmetry we may assume $m \ge n$. In this paper, we intend to find the Wiener number $W_{m,n} = W(Q_{m,n})$. Let $A = \{(a, 0) : 0 \le a \le 2n-1\} \cup \{(0, 1)\}$. Suppose $\rho(v, w)$ is the distance between v and w for $v \in A$, as defined in **[9]**. We need to compute $T(v) = \sum_{w \in V(Q_{m-1,n})} \rho(v, w)$.

The following lemma is a useful tool for computing the distance between two vertices in the wall. It was proved by Shiu and Lam **[9]**.

Lemma A: Suppose $d \ge b$. The distance between two vertices in the wall (a, b) and (c, d) is

$$\rho((a, b), (c, d)) = \begin{cases} 2(d-b) & \text{if } |c-a| \le (d-b) \text{ and } c+d \equiv a+b \pmod 2 \\ 2(d-b)+1 & \text{if } |c-a| \le (d-b),\ c+d \equiv 0 \text{ and } a+b \equiv 1 \pmod 2 \\ 2(d-b)-1 & \text{if } |c-a| \le (d-b),\ c+d \equiv 1 \text{ and } a+b \equiv 0 \pmod 2 \\ (d-b)+|c-a| & \text{if } |c-a| \ge (d-b) \end{cases}$$

■

Now consider $v = (a, 0)$, $0 \le a \le 2n-1$ and separate $Q_{m-1,n}$ into four regions as shown in Figure 2.

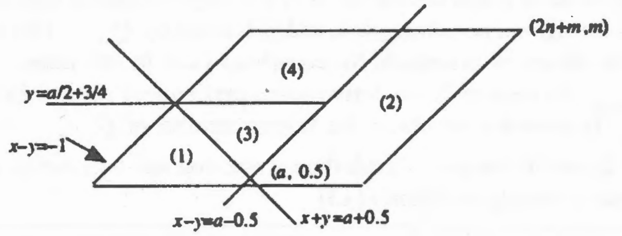

Figure 2

Apply Lemma A to compute the total distances from $(a, 0)$ to each vertex in each region as follows:

Case 1: $a = 2k, 0 \le k < n$.

$$\text{(1)}\quad \left(\sum_{y=1}^{k}\sum_{x=y-1}^{2k-y} 2k-x+y\right)-\rho((2k,0),(0,1)) = \left(\sum_{y=1}^{k}\sum_{x=y-1}^{2k-y} 2k-x+y\right)-(2k+1),$$

$$\text{(2)}\quad \left(\sum_{y=1}^{m}\sum_{x=2k+y}^{2n+y} x-2k+y\right)-\rho((2k,0),(2n+m,m)) = \left(\sum_{y=1}^{m}\sum_{x=2k+y}^{2n+y} x-2k+y\right)-2(m+n-k),$$

$$\text{(3)}\quad \sum_{y=1}^{k}\sum_{x=2k-y+1}^{y+2k-1}\rho((2k,0),(x,y)) = \sum_{y=1}^{k}\{2y(2y-1)-y\},$$

$$\text{(4)}\quad \sum_{y=k+1}^{m}\sum_{x=y-1}^{y+2k-1}\rho((2k,0),(x,y)) = \sum_{y=k+1}^{m}\{2y(2k+1)-(k+1)\}.$$

Case 2: $a = 2k+1, 0 \le k < n$.

$$\text{(1)}\quad \left(\sum_{y=1}^{k+1}\sum_{x=y-1}^{2k+1-y} 2k+1-x+y\right)-\rho((2k+1,0),(0,1)) = \left(\sum_{y=1}^{k+1}\sum_{x=y-1}^{2k+1-y} 2k+1-x+y\right)-(2k+2),$$

$$\text{(2)}\quad \left(\sum_{y=1}^{m}\sum_{x=2k+1+y}^{2n+y} x-2k-1+y\right)-\rho((2k+1,0),(2n+m,m)) = \left(\sum_{y=1}^{m}\sum_{x=2k+1+y}^{2n+y} x-2k-1+y\right)-(2m+2n-2k-1),$$

$$\text{(3)}\quad \sum_{y=1}^{k+1}\sum_{x=2k+2-y}^{y+2k}\rho((2k+1,0),(x,y)) = \sum_{y=1}^{k+1}\{2y(2y-1)+y\},$$

$$\text{(4)}\quad \sum_{y=k+2}^{m}\sum_{x=y-1}^{y+2k}\rho((2k+1,0),(x,y)) = \sum_{y=k+1}^{m}\{2y(2k+2)+(k+1)\}.$$

Finally we consider $v = (0,1)$. $T((0,1)) = \left(\sum_{y=1}^{m}\sum_{x=y-1}^{2n+y} y-1+x\right)-\rho((0,1),(2n+m,m))$.

Let $T'(v) = T(v)+\rho(v,(2n,0))$. Note that $\rho(v,(2n,0)) = 2n-a$ and $2n+1$ when $v = (a,0)$ and $(0,1)$, respectively. We have

Lemma 1: With the notation described above,

$$T(v)=\begin{cases} 2m^2n+2mn^2-4mnk+2mk^2+\frac{2}{3}k^3+2m^2+3mn-2mk+k^2-m-2n+\frac{1}{3}k-1 & \text{if } v=(2k,0)\\ 2m^2n+2mn^2-4mnk+2mk^2+\frac{2}{3}k^3+2m^2+mn-2mk+k^2+m-2n+\frac{1}{3}k-1 & \text{if } v=(2k+1,0)\\ 2m^2n+2mn^2+2m^2+mn-3m-2n+1 & \text{if } v=(0,1)\end{cases}$$

and

$$T'(v)=\begin{cases} 2m^2n+2mn^2-4mnk+2mk^2+\frac{2}{3}k^3+2m^2+3mn-2mk+k^2-m-\frac{5}{3}k-1 & \text{if } v=(2k,0)\\ 2m^2n+2mn^2-4mnk+2mk^2+\frac{2}{3}k^3+2m^2+mn-2mk+k^2+m-\frac{5}{3}k-2 & \text{if } v=(2k+1,0)\\ 2m^2n+2mn^2+2m^2+mn-3m+2 & \text{if } v=(0,1)\end{cases}$$

■

Remark: The formulæ in Lemma 1 also hold when $v = (2n,0)$.

3. Wiener Number of $Q_{n,n}$

In this section we assume that $m = n$. Let W_n stand for the Wiener number of $Q_{n,n}$ and A be the set defined in Section 2. Further, let

$$B = \{(2n+y, y) : 0 \le y \le n-1\} \cup \{(2n+y, y+1) : 0 \le y \le n-1\} \cup \{(3n-2, n)\}.$$

Then

$$W_n = W_{n-1} + 2\sum_{v \in A} T'(v) + 2W(P_{2n+1}) - \sum_{v \in A}\sum_{u \in B} \rho(v, u),$$

where P_{2n+1} is the path with $2n+1$ vertices. It is easy to see that

$$\sum_{v \in A} T'(v) = \frac{17n^4 + 42n^3 + 4n^2 - 12n + 6}{3}.$$

Also

$$\begin{aligned}
\sum_{v \in A}\sum_{u \in B} \rho(v, u) &= \sum_{a=0}^{2n-1}\sum_{y=0}^{n-1} \{\rho((a,0), (2n+y, y)) + \rho((a,0), (2n+y, y+1))\} \\
&\quad + \sum_{a=0}^{2n-1} \rho((a,0), (3n-2, n)) \\
&\quad + \sum_{y=0}^{n-1} \{\rho((0,1), (2n+y, y)) + \rho((0,1), (2n+y, y+1))\} \\
&\quad + \rho((0,1), (3n-2, n)) \\
&= \sum_{a=0}^{2n-1}\sum_{y=0}^{n-1} (4n + 4n - 2a + 1) + \sum_{a=0}^{2n-2} (4n - a - 2) + (2n+1) \\
&\quad + \sum_{y=0}^{n-1} (4n + 3y + |y-1|) + (4n-3) \\
&= 8n^3 + 12n^2 - 2n + 1.
\end{aligned}$$

It is known that $W(P_r) = \frac{1}{6}(r-1)r(r+1)$ [4]. Therefore

$$W_n = W_{n-1} + \frac{34n^4 + 68n^3 - 16n^2 - 14n + 9}{3}.$$

Solving the above difference equation with initial value $W_1 = 27$ we get the following theorem:

Theorem 2: The Wiener number of the $n \times n$ hexagonal parallelogram $Q_{n,n}$ is

$$\frac{n(34n^4 + 170n^3 + 200n^2 + 10n - 9)}{15}, \quad n \ge 1. \qquad \blacksquare$$

4. Wiener Number of $Q_{m,n}$

In this section we fix m. Let A be the set defined in Section 2. Then $Q_{m,n} - (A \cup \{(2n, 0)\})$ is isomorphic to $Q_{m-1,n}$. For convenience we identify these two graphs. It is clear that $Q_{m,n} - Q_{m-1,n}$ is a path P_{2n+2}. It is easy to get the following equation:

$$W_{m,n} = W_{m-1,n} + W(P_{2n+2}) + \sum_{v \in A \cup \{(2n,0)\}} T(v), \quad m > n.$$

By Lemma 1 we have, for $m > n$

$$W_{m,n} = W_{m-1,n} + \frac{12(n+1)^2m^2 + (4n^3 + 24n^2 + 8n - 12)\,m + (n^4 + 6n^3 + 2n^2 - 6n + 3)}{3}$$

Solving the above difference equation with initial value $W_{n,n} = \frac{1}{15}n(34n^4 + 170n^3 + 200n^2 + 10n - 9)$ we get the following theorem:

Theorem 3: For $m \geq n \geq 1$ the Wiener number of the $m \times n$ hexagonal parallelogram $Q_{m,n}$ is

$$\frac{20(n+1)^2m^3 + 10n(n^2 + 9n + 8)\,m^2 + 5(n^4 + 8n^3 + 16n^2 + 2n - 1)\,m - n(n^4 - 20n + 4)}{15}.$$

■

As a corollary of Theorem 3 we get the Wiener number of a hexagonal chain, a previously known result [14].

Corollary 4: The Wiener number of the n-benzenoid chain $(n \geq 1)$ is $\frac{1}{3}(16n^3 + 36n^2 + 26n + 3)$. ■

References

[1] I. Gutman, Y.N. Yeh, S.L. Lee and Y.L. Luo; Some recent results in the theory of the Wiener number, *Indian J. Chem.*, **32A**, 651–661(1993).

[2] S. Nikolić, N. Trinajsić and Z. Mihalić; The Wiener index: Developments and Applications, *Croat. Chem. Acta*, **68**, 105–129 (1995).

[3] F. Harary; Status and contrastatus, *Sociometry*, **22**, 23–43 (1959).

[4] R.C. Entringer, D.E. Jackson and D.A. Snyder; Distance in graphs, *Czech. Math. J.*, **26**, 283–296 (1976).

[5] J. Plesnik; On the sum of distances in a graph or digraph, *J. Graph Theory*, **8**, 1–21 (1984).

[6] Y.N. Yeh and I. Gutman; On the sum of all distances in composite graphs, *Discrete Appl. Math.*, **135**, 359–365 (1994).

[7] I. Gutman; A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes of New York*, **XXVII:2**, New York Academy of Sciences, 9–15 (1994).

[8] A. Dobrynin and I. Gutman; Solving a problem connected with distances in graphs, *Graph Theory Notes of New York*, **XXVIII:5**, New York Academy of Sciences, 21–23 (1995).

[9] W.C. Shiu and P.C.B. Lam; The Wiener number of a hexagonal net, *Discrete Appl. Math.*, — in press.

[10] I. Gutman; Topological resonance energy of very large benzenoid hydrocarbons, *Z. Naturforsch*, **36a**, 128–131 (1981).

[11] O. Bodroža, I. Gutman, S.J. Cyvin and R. Tošić; Number of Kekulé structures of hexagon shape benzenoids, *J. Math. Chem.*, **2**, 287–298 (1988).

[12] I. Gutman and S.J. Cyvin; *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer-Verlag, Berlin (1989).

[13] J.A. Bondy and U.S.R. Murty; *Graph Theory with Applications*, Macmillan, New York (1976).

[14] I. Gutman and O.E. Polansky; Wiener numbers of polyacenes and related benzenoid molecules, *Commun. Math. Chem. (MATCH)*, **20**, 115–123 (1986).

Received: October 30, 1995