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[GTN XXXII:2] WIENER NUMBER OF SOME POLYCYCLIC GRAPHS

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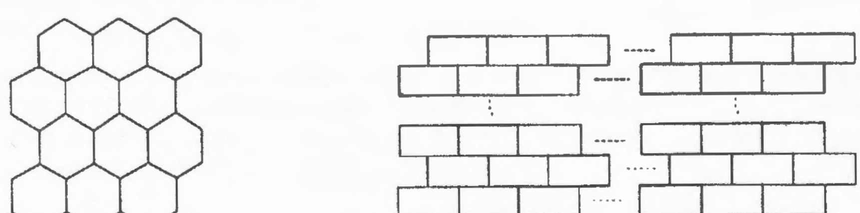
Abstract

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 rectangle is called an $n \times m$ hexagonal rectangle. Similarly, a graph consisting of hexagonal chains forming the shape of an equilateral triangle is called a hexagonal triangle. In this paper, we obtain the Wiener number of an $n \times m$ hexagonal rectangle and of a hexagonal triangle.

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 the respective graph. American physico-chemist Harold Wiener first examined this invariant in 1947. He conceived this index in an attempt to formulate a mathematical model capable of describing molecular shapes. Wiener, and after him numerous researchers, reported the existence of correlation between W and a variety of physico-chemical properties of alkanes. For recent reviews on this subject and references to previous work, see **[1][2]**. The Wiener number has also been studied in the mathematical literature (see, for instance, **[3]–[6]**). For a generalization of the Wiener number, refer to **[7][8]**.

Despite this large body of work on the theory of the Wiener number, some basic problems remain open. For example, no recursive method is known for the calculation of W for a general graph, especially for 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 by designing a method for finding an 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 much examined in the theory of benzenoid hydrocarbons (see, for instance, **[10]–[12]**).



$R_{3,4}$ $R_{n,m}$

Figure 1

It is natural to consider other types of hexagonal systems. In **[13]**, the following type of hexagonal system was considered. 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 $n \times m$ *hexagonal parallelogram*, which we denoted by $Q_{n,m}$ (in **[13]** it is denoted by $Q_{m,n}$). This is another molecular graph of importance in the theory of benzenoid hydrocarbons **[12]**. In this paper, we consider other types of hexagonal systems. A graph consisting of m n-hexagonal chains forming the shape of a rectangle is called an $n \times m$ *hexagonal rect-*

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angle, which we denoted by $R_{n,m}$, see Figure 1. It should be noted that $R_{1,n}$ and $R_{n,1}$ are not isomorphic. A graph with n k-hexagonal chains, where k ranges from 1 to n, in the shape of an equilateral triangle is called an *n-hexagonal triangle* and is denoted by T_n, see Figure 2.

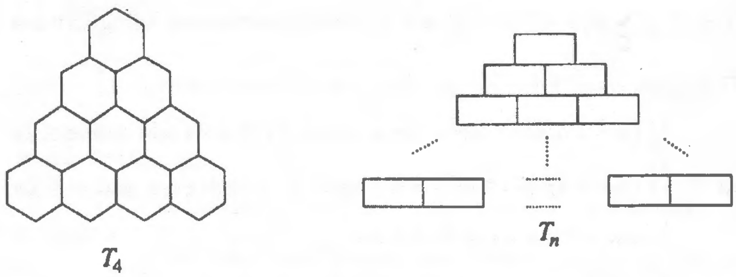

Figure 2

We shall obtain expressions for $W(R_{n,m})$ and for $W(T_n)$. In section 2, we derive some preliminary results. In section 3, we obtain the Wiener number of $R_{n,m}$, using the same technique as was employed in **[9]** and **[13]**. In section 4, where another type of technique for handling Wiener number of polycyclic graphs is introduced, we obtain the Wiener number of T_n.

In this paper, $\mathbb{Z}$ denotes the set of integers. Graph theory terminology not defined in this paper can be found in Bondy and Murty **[14]**.

2. Preliminary Results

Definition: Let $G = (V, E)$ be a graph. For $v, w \in V$ let $\rho(v, w)$ denote 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 was previously defined in **[9]** where it was called *wall*. The $n \times m$ hexagonal rectangle $R_{n,m}$ is a subgraph of G. Thus, we may describe the set of vertices of $R_{n,m}$ as

$$\{(x, y) \in \mathbb{Z}\times\mathbb{Z} : 0 \le x \le 2n+1, 0 \le y \le m\}\setminus\{(2n+1, 0), (0, m)\} \text{ if } m \text{ is even,}$$
$$\{(x, y) \in \mathbb{Z}\times\mathbb{Z} : 0 \le x \le 2n+1, 0 \le y \le m\}\setminus\{(2n+1, 0), (2n+1, m)\} \text{ if } m \text{ is odd.}$$

Similarly, we identify the order n-hexagonal triangle T_n as a subgraph of G and describe the vertex set of T_n as $\{(c, d) \in \mathbb{Z}\times\mathbb{Z} : 0 \le d \le n, d-1 \le c \le 2n-d+1 \text{ for } d \ne 0, 0 \le c \le 2n \text{ for } d = 0\}$.

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, (a, b) and (c, d), in the wall is

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

3. Wiener Number of a Hexagonal Rectangle

Consider the hexagonal rectangle, $R_{n,m}$. Let $A = \{(a, 0) : 0 \le a \le 2n\} \cup \{(0, 1)\}$ and let $R'_{n,m-1} = R_{n,m} - A$. Then by reflection $R'_{n,m-1}$ is isomorphic to $R_{n,m}$. Thus

$$W_{n,m} = W_{n,m-1} + \sum_{\substack{v \in A \\ w \in V\setminus A}} \rho(v, w) + \sum_{v, w \in A} \rho(v, w) = W_{n,m-1} + \sum_{v \in A} T(v) + W(P_{2n+1}),$$

where $T(v) = \sum_{w \in V\setminus A}\rho(v, w)$.

To calculate $T(v)$ of $v \in A$ we first obtain $T_0(v) = \sum_{w \in V_0 \setminus A} \rho(v, w)$, where $V_0 = V \cup \{v_0\}$ and $v_0 = (2n+1, m)$ if m is odd and $v_0 = (0, m)$ if m is even. Then

$$\sum_{v \in A} T(v) = \sum_{v \in A} T_0(v) - \sum_{v \in A} \rho(v, v_0)$$

Note that $T_0((0, 1)) = T_0((\underset{0}{\cancel{1}}, 0)) - 2(n+1)m + 1$. Direct calculation, using Lemma A gives

Lemma 3.1:

$$\sum_{v \in A} \rho(v, v_0) = \begin{cases} \frac{1}{2}(m^2 + 4mn + 4n^2 + 4m + 10n + 1) & \text{if } m \text{ is odd and } m \le 2n \\ \frac{1}{2}(m^2 + 4mn + 4n^2 + 8m + 2n - 2) & \text{if } m \text{ is even and } m \le 2n \\ 4mn + 4m + n - 1 & \text{if } m > 2n \end{cases}$$

■

To obtain the Wiener number of $R_{n,m}$ we need only calculate $T_0((a, 0))$ for $0 \le a \le 2n$. To do this we separate the range of m into three cases: $1 \le m \le n$, $n \le m \le 2n$ and $m \ge 2n$

For $1 \le m \le n$, there are three cases: (a), (b), and (c)

(a) $0 \le a \le m - 1$. $T_0((a, 0)) + \rho((a, 0), \underset{(0,1)}{(\cancel{1, 0})})$ is the sum of the following four summands:

For $a = 2k$

(1) $$\sum_{y=1}^{2k} \sum_{x=0}^{2k-y} 2k - x + y = 4k^3 + 4k^2 + k$$

(2) $$\sum_{y=1}^{2k} \sum_{x=2k+y}^{2n+1} x - 2k + y = \tfrac{1}{2}m(4n^2 + 2mn - 8kn - m^2 - 2km + 4k^2 + 8n + m - 8k + 4)$$

(3) $$\sum_{y=1}^{2k} \sum_{x=2k-y+1}^{2k+y-1} \rho((2k, 0), (x, y)) = \sum_{y=1}^{2k} (2y(2y-1) - y) = \tfrac{1}{3}k(32k^2 + 6k - 5)$$

(4) $$\sum_{y=2k+1}^{m} \sum_{x=0}^{2k+y-1} \rho((2k, 0), (x, y)) = \sum_{y=2k+1}^{m} \{2y(2k+y) - \lceil \tfrac{2k+y}{2} \rceil\}$$

$$= \begin{cases} \frac{1}{12}(8m^3 + 24m^2 - 160k^3 + 9m^2 + 12km - 60k^2 - 2m + 4k - 3) & \text{if } m \text{ is odd} \\ \frac{1}{12}(8m^3 + 24m^2 - 160k^3 + 9m^2 + 12km - 60k^2 - 2m + 4k) & \text{if } m \text{ is even} \end{cases}$$

that is not less than x

where $\lceil x \rceil$ is the least integer that ~~does not exceed~~ x.

which is ~~greater than or equal to x.~~

For $a = 2k + 1$

(1) $$\sum_{y=1}^{2k+1} \sum_{x=0}^{2k+1-y} 2k + 1 - x + y$$

(2) $$\sum_{y=1}^{m} \sum_{x=2k+1+y}^{2n+1} x - 2k - 1 + y$$

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

(4) $$\sum_{y=2k+2}^{m} \sum_{x=0}^{2k+y} \rho((2k+1, 0), (x, y)) = \sum_{y=2k+2}^{m} \{2y(2k+y+1) + \lceil \tfrac{2k+y+1}{2} \rceil\}.$$

Hence,

$$T_0((0,1))+\sum_{a=0}^{m-1}T_0((a,0)) = \begin{cases}\frac{1}{24}(15m^4+48m^2n^2+14m^3+144m^2n+48mn^2+78m^2+48mn-26m-9) & \text{if } m \text{ is odd}\\ \frac{1}{24}(15m^4+48m^2n^2+14m^3+144m^2n+48mn^2+90m^2+48mn-8m-9) & \text{if } m \text{ is even.}\end{cases}$$

(b) $m \le a \le 2n-m+1$. Similarly,

$$\sum_{a=m}^{2n-m+1} T_0((a,0)) = \frac{1}{3}(-4m^4+2m^3n-6m^2n^2+8mn^3-m^3-15m^2n+30mn^2-8m^2+41mn-6n^2+22m-15n-9).$$

(c) $2n-m+2 \le a$. In this case,

$$\sum_{a=2n-m+2}^{2n} T_0((a,0)) = \begin{cases}\frac{1}{8}(m-1)(5m^3+16mn^2+7m^2+32mn+23m-16n-15) & \text{if } m \text{ is odd}\\ \frac{1}{8}(5m^3+16mn^2+2m^2+32m^2n+16mn^2+12m^2-48mn-44m+16n+16) & \text{if } m \text{ is even.}\end{cases}$$

Consequently,

$$\sum_{v\in A} T_0(v) = \begin{cases}\frac{1}{12}(-m^4+8m^3n+24m^2n^2+32mn^3+6m^3+60m^2n+120mn^2+31m^2+116mn-24n^2+18m-36n-18), & m \text{ odd}\\ \frac{1}{12}(-m^4+8m^3n+24m^2n^2+32mn^3+6m^3+60m^2n+120mn^2+31m^2+116mn-24n^2+18m-36n-12), & m \text{ even.}\end{cases}$$

By applying Lemma 3.1 we obtain

$$\sum_{v\in A} T_0(v) = \begin{cases}\frac{1}{12}(-m^4+8m^3n+24m^2n^2+32mn^3+6m^3+60m^2n+120mn^2+25m^2+92mn-48n^2+6m-96n-24), & m \text{ odd}\\ \frac{1}{12}(-m^4+8m^3n+24m^2n^2+32mn^3+6m^3+60m^2n+120mn^2+25m^2+92mn-48n^2-30m-48n), & m \text{ even.}\end{cases}$$

Consequently,

$$W_{n,m}-W_{n,m-1} = \begin{cases}\frac{1}{12}(-m^4+8m^3n+24m^2n^2+32mn^3+6m^3+60m^2n+120mn^2+16n^3+25m^2+92mn-6m-52n-12), & m \text{ odd}\\ \frac{1}{12}(-m^4+8m^3n+24m^2n^2+32mn^3+6m^3+60m^2n+120mn^2+16n^3+25m^2+92mn-30m-4n+12), & m \text{ even.}\end{cases}$$

When $n \le m \le 2n$, using a similar calculation, we obtain an identical expression for $W_{n,m}-W_{n,m-1}$. For more details, refer to [16]. By solving the difference (recurrence) equations with initial values $W_{n,1} = \frac{1}{3}(16n^3+36n^2+26n+3)$, for $n \ge 1$; and $W_{n,2} = 12n^3+40n^2+49n+8$, for $n \ge 2$, we obtain:

Theorem 3.2: For $1 \le m \le 2n$ the Wiener number of $R_{n,m}$ is

$$\begin{cases}\frac{1}{60}(-m^5+10m^4n+40m^3n^2+80m^2n^3+5m^4+120m^3n+120m^3n+360m^2n^2+160mn^3\\ \quad +55m^3+390m^2n+320mn^2+80n^3+25m^2+140mn+6m-140n-30) \text{ if } m \text{ is odd}\\ \frac{1}{60}(-m^5+10m^4n+40m^3n^2+80m^2n^3+5m^4+120m^3n+120m^3n+360m^2n^2+160mn^3\\ \quad +55m^3+390m^2n+320mn^2+80n^3+25m^2+140mn-54m-20n) \text{ if } m \text{ is even.}\end{cases}$$

■

Corollary 3.3: The Wiener number of $R_{n,n}$ is

$$\begin{cases}\frac{1}{60}(129n^5+645n^4+845n^3+165n^2-134n-30) \text{ if } n \text{ is odd}\\ \frac{1}{60}(129n^5+645n^4+845n^3+165n^2-74n) \text{ if } n \text{ is even.}\end{cases}$$ ■

Corollary 3.4: The Wiener number of $R_{n,2n}$ is
$\frac{1}{15}(192n^5+700n^4+680n^3+95n^2-32n)$. ■

For the case $m \ge 2n$, we obtain (see [16])

$$W_{n,m}-W_{n,m-1} = \frac{1}{3}(12m^2n^2+4n^4+24m^2n+12mn^2+16n^3+12m^2+23n^2-12m+8n+3).$$

Solving the difference equations with the initial value for $W_{n,2n}$ we obtain the following theorem.

Theorem 3.5: The Wiener number of $R_{n,m}$ for $m \ge 2n$ is
$\frac{1}{15}(20m^3n^2+20mn^4-8n^5+40m^3n+60m^2n^2+80mn^3-20n^4+20m^3+60m^2n+155mn^2-30n^3+60mn-25n^2-5m-22n)$.

■

4. Wiener Number of a Hexagonal Triangle

An n-hexagonal triangle contains the vertex set

$$V_n = V(T_n) = \{(c,d) : 0 \le d \le n, d-1 \le c \le 2n-d+1 \text{ for } d \ne 0, 0 \le c \le 2n \text{ for } d = 0\},$$

which can be partitioned as follows, $V_n = V'_n \cup L_n$, where
$V'_n = \{(c,d) \in \mathbb{Z}\times\mathbb{Z} : 1 \le d \le n, d-1 \le c \le 2n-d+1\}$, and $L_n = \{(c,0) \in \mathbb{Z}\times\mathbb{Z} : 0 \le c \le 2n\}$.
Moreover $V'_n = V(\hat{T}_{n-1}) \cup \{(0,1), (2n,1)\}$ where

$$\hat{V}_{n-1} = V(\hat{T}_{n-1}) = \{(c,d) : 1 \le d \le n, d-1 \le c \le 2n-d+1 \text{ for } d \ne 1, 1 \le c \le 2n-1 \text{ for } d = 1\}.$$

Thus we have split the n-hexagonal triangle into three parts: L_n is the base line; $\{(0,1), (2n,1)\}$, are the two end points on the line above the base line; and $\hat{T}_{n-1}$, which is isomorphic to an $(n-1)$-hexagonal triangle. In particular,

$$\rho(\hat{T}_{n-1}, \hat{T}_{n-1}) = W_{n-1} = W(T_{n-1}),$$

the Wiener number of an $(n-1)$-hexagonal triangle. (Here we have extended the meaning of $\rho(S_1, S_2)$ to denote the sum of distances between all vertices in set S_1 and all vertices in set S_2.)

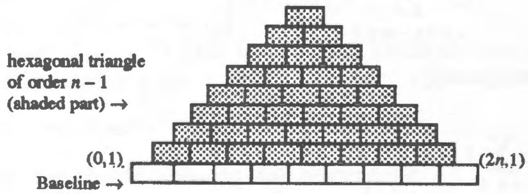

Figure 3

Therefore

$$\begin{aligned}
W_n = W(T_n) &= \rho(V'_n \cup L_n, V'_n \cup L_n) = \rho(V'_n, V'_n) + \rho(L_n, V'_n) + \rho(L_n, L_n) \\
&= W_{n-1} + \rho((0,1), \hat{V}_{n-1}) + \rho((2n-1), \hat{V}_{n-1}) + \rho((0,1), (2n-1)) + \rho(L_n, T'_n) + \rho(L_n, L_n) \\
&= W_{n-1} + \rho(L_n, L_n) + 2\rho((0,1), V'_n) - 2n + \rho(L_n, V'_n)
\end{aligned}$$

Clearly $\rho(L_n, L_n) = \frac{2}{3}n(n+1)(2n+1)$, and

$$2\rho((0,1), V'_n) = 2\sum_{d=1}^{n}\sum_{c=d-1}^{2n-d+1}\rho((0,1),(c,d)) = 2\sum_{d=1}^{n}\sum_{c=d-1}^{2n-d+1}(c+d-1) = \tfrac{1}{3}n(8n^2+15n-5).$$

Now let us consider the term $\rho(L_n, V'_n)$. For convenience, we classify contributions to the distance sum (see Lemma A) into two types: Type I contributions are those for which $|c-a| < |d-b|$, and Type II contributions are those for which $|c-a| \ge |d-b|$. Therefore $\rho(L_n, V'_n) = \rho_{\mathrm{I}}(L_n, V'_n) + \rho_{\mathrm{II}}(L_n, V'_n)$.

Type I contributions $\rho_{\mathrm{I}}(L_n, V'_n)$, are essentially of the form $2|d-0| = 2d$ but some vertices acquire a ± 1 correction depending on parity considerations (see Lemma A).

We evaluate the basic contributions first, and return to the corrections later. Each vertex (c,d) on the d^{th} layer will only contribute $2d-1$ times since there are precisely $2d-1$ vertices on the base line which satisfy the condition for Type I, namely: $(c-d+1, 0), (c-d+2, 0), \ldots, (c, 0), (c+1, 0), \ldots, (c+d-1, 0)$. Hence each vertex (c,d) acquires a multiplicity of $2d-1$. Thus the sum of basic Type I contributions is

$$\sum_{d=1}^{n}(2d-1)(2d) = \tfrac{1}{3}n(n+1)(4n-1).$$

To deal with the parity corrections, we consider each layer in the triangular structure. The first vertex in the d^{th} layer is $(d-1, d)$ and it will contribute with the vertices $(0,0), \ldots, (2d-2, 0)$ on the base line. Since $d-1+d = 2d-1$ is odd, the first term, $(0,0)$, picks up a negative correction, the second term no correction, the third term a negative correction, and so on. In other words, the vertex $(d-1, d)$ acquires a correction of $-d$. Similarly, since the next vertex in the d^{th} layer, (d,d), has opposite parity to $(d-1,d)$, it requires a positive correction of d. These corrections cancel in pairs except for the last term. Thus the net correction for the d^{th} layer is $-d$, and hence the total correction for the entire structure is $\sum_{d=1}^{n}(-d) = -\frac{1}{2}n(n+1)$. Thus,

$$\rho_I(L_n, V'_n) = \tfrac{1}{3}n(n+1)(4n-1) - \tfrac{1}{2}n(n+1) = \tfrac{1}{6}n(n+1)(8n-5) .$$

The Type II contributions, $\rho_{II}(L_n, V'_n)$, occur when $|c-d| \geq d$, where $(c, d) \in V'_n$, and $(a, 0)$ is a vertex on the base line L_n. The corresponding contribution is $|c-a| + d$. Fixing d and c, the condition implies that $0 \leq a \leq c-d$ if $c-d \geq 0$ or $c+d \leq a \leq 2n$ if $c+d \leq 2n$. The total of these contributions is

$$(*) \qquad \sum_{d=1}^{n} \sum_{c=d-1}^{2n-d+1} \left(\sum_{a=0}^{c-d} (|c-a|+d) + \sum_{a=c+d}^{2n} (|c-a|+d) \right) = \tfrac{1}{3}n(n+1)(4n^2+10n+7) .$$

Remark: In the first term of (*), the condition $c-d \geq 0$ implies that the summation on c starts from d instead of $d-1$. In the second term, the condition $c+d \leq 2n$ implies that the summation on c ends at $c = 2n-d$ instead of $2n-d+1$. Collecting all the terms, we have $W_n = W_{n-1} + \tfrac{1}{2}(4n^3+24n^2+29n-3)$. Using the initial condition $W_1 = 27$, the difference equation can be solved to give the following theorem.

Theorem 4.1: The Wiener number of an n-hexagonal triangle is
$W_n = \tfrac{1}{10}n(n+1)(4n^3+36n^2+79n+16)$. ■

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