Wiener numbers of random pentagonal chains

HONG-YONG WANG\textsuperscript{1}, JIANG QIN\textsuperscript{1} and IVAN GUTMAN\textsuperscript{2,*}

\textsuperscript{1}School of Mathematics and Physics, University of South China, Hengyang 421001, Hunan, P. R. China
\textsuperscript{2}Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia

(Received April 7, 2013; Accepted April 25, 2013)

\textbf{ABSTRACT}

The Wiener index is the sum of distances between all pairs of vertices in a connected graph. In this paper, explicit expressions for the expected value of the Wiener index of three types of random pentagonal chains (cf. Fig. 1) are obtained.

\textbf{Keywords:} Wiener index, pentagonal chain.

1. \textbf{INTRODUCTION}

The Wiener index is the oldest molecular structure descriptor, invented as early as in 1947 by Harold Wiener [18]. Initially it was ignored by the chemical community, and so it happened that Rouvray [16] independently re-invented it in 1975. The precise mathematical definition of the Wiener index (in terms of distance in graphs) was given in 1971 by Hosoya [9]. Mathematicians arrived at the very same idea somewhat later [5], but also independently.

Eventually, the Wiener index attracted the attention of chemists, due to its correlation with a large number of physico–chemical properties of organic molecules. It also attracted the attention of mathematicians due to its interesting and non-trivial mathematical properties.

Anyway, in the last 20-30 years an enormous amount of work was done on the study of the Wiener index. Ante Graovac also participated in these researches (see, for instance, [7, 11]). It is particularly worth noting that in the years that preceded his untimely death, the study of Wiener index and other distance–based structure descriptors, as well as

\*Corresponding author (Email: gutman@kg.ac.rs)
their applications to fullerenes and nanomolecules, was Ante Graovac’s main scientific interest [1–4, 6, 10, 12, 13, 17].

Let $G$ be a connected graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The distance $d(v_r, v_s)$ between the vertices $v_r$ and $v_s$ in $G$ is the number of edges of a shortest path between $v_r$ and $v_s$. The Wiener index is the sum of distances between all pairs vertices and is defined by

$$W(G) = \sum_{r<s} d(v_r, v_s) = \frac{1}{2} \sum_{r=1}^{n} \sum_{s=1}^{n} d(v_r, v_s) = \frac{1}{2} \sum_{r=1}^{n} d(v_r, G)$$

where $d(v_r, G)$ is the distance number of the vertex $v_r$, defined by

$$d(v_r, G) = \sum_{s=1}^{n} d(v_r, v_s).$$

Motivated by the works [8] and [19], in the present paper we establish explicit expressions for the expected value of the Wiener index of three types of random pentagonal chains, shown as Fig. 1.

Fig. 1. The three types of pentagonal chains (pentachains) examined in this paper: alpha (1), beta (2), and gamma (3).

The following lemma is the main tool in the proof of our results.

**Lemma 1.** Let $\{t_n\}$ be a real number sequence satisfying

$$t_n = q \cdot t_{n-1} + d \cdot n^3 + a \cdot n^2 + b \cdot n + c \quad ; \quad n \geq 1.$$  \hspace{1cm} (1)

If $t_0 = 0$ and $q \neq 1$, then

$$t_n = d \cdot I_0 + a \cdot I_1 + b \cdot I_2 + c \cdot I_3$$  \hspace{1cm} (2)

where

$$I_0 = \frac{1}{(1-q)^4} \left[ n^3 - (3n^3 + 3n^2 - 3n + 1)q + (3n^3 + 6n^2 - 4)q^2 ight.$$

$$\quad \left. - (n^3 + 3n^2 + 3n + 1)q^3 + q^{n+1} + 4q^{n+2} + q^{n+3} \right]$$
Wiener numbers of random Pentagonal Chains

\[ I_1 = \frac{1}{(q-1)^3} \left[ -n^2 + (2n^2 + 2n - 1)q - (n^2 + 2n + 1)q^2 + q^{n+1} + q^{n+2} \right] \]

\[ I_2 = \frac{1}{(1-q)^2} \left[ n - (n+1)q + q^{n+1} \right] \]

\[ I_3 = \frac{1-q^n}{1-q} \]

**Proof.** From (1), we have

\[ t_n = q t_{n-1} + d n^3 + a n^2 + bn + c \]

\[ t_{n-1} = q t_{n-2} + d(n-1)^3 + a(n-1)^2 + b(n-1) + c \]

\[ t_{n-2} = q t_{n-3} + d(n-2)^3 + a(n-2)^2 + b(n-2) + c \]

\[ t_2 = q t_1 + d 2^3 + a 2^2 + 2b + c \]

\[ t_1 = q t_0 + d 1^3 + a 1^2 + 1b + c \]

The above formulas imply

\[ t_n = d n^3 + d q(n-1)^3 + d q^2(n-2)^3 + \cdots + d q^{n-2}2^3 + d q^{n-1}1^3 \]

\[ + a n^2 + a q(n-1)^2 + a q^2(n-2)^2 + \cdots + a q^{n-2}2^2 + a q^{n-1}1^2 \]

\[ + b n + b q(n-1) + b q^2(n-2) + \cdots + b q^{n-2}2 + b q^{n-1} \]

\[ + c + c q + c q^2 + \cdots + c q^{n-2} + c q^{n-1} = d I_0 + a I_1 + b I_2 + c I_3. \]

\[ I_3 \] is a geometric sequence with the common ratio \( q \). Hence,

\[ I_3 = \frac{1-q^n}{1-q}. \quad (3) \]

From the definition of \( I_2 \), we have

\[ I_2 = n + q(n-1) + q^2(n-2) + \cdots + q^{n-2}2 + q^{n-1} \quad (4) \]

and

\[ q I_2 = q n + q^2(n-1) + q^3(n-2) + \cdots + q^{n-1}2 + q^n. \quad (5) \]

Taking into account the difference between equations (5) and (4), we conclude that

\[ I_2 = \frac{n - q \left( 1 - q^{n+1} \right)}{1-q}, \quad \frac{1}{1-q} = \frac{n - (n+1)q + q^{n+1}}{(1-q)^2}. \quad (6) \]
For $I_1$, we rewrite its expression as follows:

$$I_1 = n^2 + q(n-1)^2 + q^2(n-2)^2 + \cdots + q^{n-2}2^2 + q^{n-1}1^2$$

$$= q^{n-1} \left[ 1^2 + 2^2 \left( \frac{1}{q} \right) + \cdots + (n-2)^2 \left( \frac{1}{q} \right)^{n-3} \right.\left. + (n-1)^2 \left( \frac{1}{q} \right)^{n-2} + n^2 \left( \frac{1}{q} \right)^{n-1} \right] = q^{n-1}J.$$  

In order to compute $J$, consider the formula:

$$\sum_{k=1}^{n} k^2 x^{k-1} = 1^2 + 2^2 x + \cdots + (n-2)^2 x^{n-3} + (n-1)^2 x^{n-2} + n^2 x^{n-1}.$$  

Noticing that

$$k^2 = k(k-1) + k$$

we have

$$\sum_{k=1}^{n} k^2 x^{k-1} = \sum_{k=1}^{n} [k(k-1) + k] x^{k-1} = \sum_{k=1}^{n} k(k-1) x^{k-1} + \sum_{k=1}^{n} k x^{k-1}.$$  

Furthermore, it is not hard to verify the identities:

$$\sum_{k=1}^{n} k(k-1) x^{k-2} = (1 + x + x^2 + x^3 + \cdots + x^n)^{\prime}\left( 1 - x \right)^{\prime} = \frac{1 - x^{n+1}}{1 - x}.$$  

(7)

$$\sum_{k=1}^{n} k x^{k-1} = (1 + x + x^2 + \cdots + x^{n-1} + x^n)^{\prime}\left( 1 - x \right)^{\prime} = \frac{1 - x^{n+1}}{1 - x}.$$  

(8)

Combining (7) and (8) we arrive at

$$\sum_{k=1}^{n} k^2 x^{k-1} = - \frac{n^2 x^{n+2} + (2n^2 + 2n - 1)x^{n+1} - (n^2 + 2n + 1)x^n + x+1}{(1-x)^3}.$$  

(9)

After replacing $x$ by $1/q$ in (9), we establish
Wiener numbers of random Pentagonal Chains

\[ I_1 = \frac{-n^2 + (2n^2 + 2n - 1)q - (n^2 + 2n + 1)q^2 + q^{n+1} + q^{n+2}}{(q-1)^3}. \] (10)

For \( I_0 \), we rewrite its expression as:

\[ I_0 = n^3 + q(n-1)^3 + q^2(n-2)^3 + \cdots + q^{n-2}2^3 + q^{n-1}1^3 \]

\[ = q^{n-1}\left[1^3 + 2^3\left(\frac{1}{q}\right) + \cdots + (n-2)^3\left(\frac{1}{q}\right)^{n-3} \right] 
+ (n-1)^3\left(\frac{1}{q}\right)^{n-2} + n^3\left(\frac{1}{q}\right)^{n-1}\right] = q^{n-1}K. \]

In order to compute \( K \), consider the following representation

\[
\sum_{k=1}^{n} k^3 x^{k-1} = \sum_{k=1}^{n} [k(k-1)(k-2) + 3k(k-1) + k]x^{k-1} \\
= \sum_{k=3}^{n} k(k-1)(k-2)x^{k-1} + 3 \sum_{k=2}^{n} k(k-1)x^{k-1} + \sum_{k=1}^{n} kx^{k-1} \\
= K_1 + K_2 + K_3.
\]

By applying the following formulas, which are not hard to derive,

\[ K_3 = \left( \sum_{k=0}^{n} x^k \right)^{'} = \left( \frac{1-x^{n+1}}{1-x} \right)^{'} = \frac{nx^{n+1} - (n+1)x^n + 1}{(1-x)^2} \]

\[ K_2 = 3x \left( \sum_{k=0}^{n} x^k \right)^{''} = 3x \left( \frac{1-x^{n+1}}{1-x} \right)^{''} = 3x \left( \frac{(n-n^2)x^{n+1} + (2n^2-2)x^n - (n^2+n)x^{n-1} + 2}{(1-x)^3} \right) \]

\[ K_1 = x^2 \left( \frac{1-x^{n+1}}{1-x} \right)^{'''} = \frac{x^2}{(1-x)^4} [(n^3 - 3n^2 + 2n)x^{n+1} - (3n^3 - 6n^2 - 3n + 6)x^n + (3n^3 - 3n^2 - 6n)x^{n-2} + 6] \]

we arrive at
\[ K = \frac{1}{(1-x)^3} \left[ n^3 x^{n+3} - (3n^3 + 3n^2 - 3n + 1) x^{n+2} + (3n^3 + 6n^2 - 4) x^{n+1} ight. \\
\left. - (3n^3 + 3n^2 + 3n + 1) x^n + x^2 + 4x + 1 \right]. \] (11)

Replacing $x$ by $1/q$ in (11), we obtain

\[ I_0 = \frac{1}{(1-q)^3} \left[ n^3 - (3n^3 + 3n^2 - 3n + 1) q + (3n^3 + 6n^2 - 4) q^2 ight. \\
\left. - (3n^3 + 3n^2 + 3n + 1) q^3 + q^{n+1} + 4q^{n+2} + q^{n+3} \right]. \] (12)

Eqs. (3), (6), (10), combined with Eqs. (12) lead to (2).

2. **ALPHA-TYPE PENTACHAINS**

The alpha-pentachains for $n = 1, 2,$ and $n = 3$ are depicted in Fig. 2. More generally, an alpha-pentachain $B_n$ with $n$ pentagons (see Fig. 3) can be obtained by attaching a pentagon, by means of an edge, to $B_{n-1}$ which has $n-1$ pentagons. However, for $n \geq 2$, there are two ways to arrange the terminal pentagon, leading to the local arrangements $B_{n+1}^1$ and $B_{n+1}^2$ as shown in Fig. 4.

![Fig. 2. The alpha-pentachains with one, two, and three pentagons.](image)

![Fig. 3. An alpha-pentachain with $n$ pentagons.](image)
Wiener numbers of random Pentagonal Chains

Due to the random selection from $B_{k-1}$ to $B_k$, $k = 3, 4, 5, \ldots$, we may regard an alpha-pentachain obtained by stepwise addition of terminal pentagon as a random alpha-pentachain, denoted by $R_n^{(\alpha)}$ if it has $n$ pentagons, $n > 2$. Furthermore, at each step $k = 3, 4, \ldots, n$, a random selection is emerged from one of the two possible constructions:

1. $B_k \rightarrow B^1_{k+1}$ with probability $p$, and
2. $B_k \rightarrow B^2_{k+1}$ with probability $1 - p$. Here we assume that the construction described is a zeroth–order Markov process, which means that the probability $p$ is constant and independent of the step parameter $k$.

Denote by $E(\Xi)$ the expected value of a random variable $\Xi$.

**Theorem 1.** For $n \geq 1$,

$$E(W(R_n^{(\alpha)})) = \frac{5}{6} (15 - 5p)n^3 + (5 + \frac{25}{2}p)n^2 - (\frac{5}{2} + \frac{25p}{3})n.$$  \hfill (13)

**Proof.** As shown in Fig. 3, the pentachain $B_n$ is constructed by adding a pentagon to $B_{n-1}$ by means of a new edge. Based on this construction, it is easily to prove the following relations.

1. For any $v \in B_{n-1}$,
   $$d(x_k, v) = d(u_{n-1}, v) + k, \quad k = 1, 2, 3$$

   and
   $$d(x_4, v) = d(u_{n-1}, v) + 3, \quad d(x_5, v) = d(u_{n-1}, v) + 2.$$

2. $B_{n-1}$ has $5(n - 1)$ vertices.
\[ 3^* \cdot \sum_{i=1}^{5} d(x_k, x_1) = 6, \quad \forall k \in \{1, 2, 3, 4, 5\}. \]

Then we have

\[ d(x_1|B_n) = d(u_{n-1}|B_{n-1}) + 1 \times 5(n-1) + 6 \]  
\[ (14) \]

\[ d(x_2|B_n) = d(u_{n-1}|B_{n-1}) + 2 \times 5(n-1) + 6 \]  
\[ (15) \]

\[ d(x_3|B_n) = d(u_{n-1}|B_{n-1}) + 3 \times 5(n-1) + 6 \]  
\[ (16) \]

\[ d(x_4|B_n) = d(u_{n-1}|B_{n-1}) + 3 \times 5(n-1) + 6 \]  
\[ (17) \]

\[ d(x_5|B_n) = d(u_{n-1}|B_{n-1}) + 2 \times 5(n-1) + 6 \]  
\[ (18) \]

and

\[ W(B_n) = W(B_{n-1}) + 5d(u_{n-1}|B_{n-1}) + 55n - 40 \]  
\[ (19) \]

with the boundary condition \( W(B_1) = d(u_1|B_1) = 15 \). Thus from (19), we obtain the recursive relation

\[ W(B_{n+1}) = W(B_n) + 5d(u_n|B_n) + 55n + 15. \]  
\[ (20) \]

For a random chain \( R_n^{(\alpha)} \), the distance number \( d(u_n|R_n^{(\alpha)}) \) is a random variable and we denote its expected value by

\[ U_n^{(\alpha)} = E(d(u_n|R_n^{(\alpha)})). \]

There are two cases to be distinguished:

Case 1: \( B_n \rightarrow B_{n+1}^1 \). In this case, the vertex \( u_n \) coincides with the vertex labeled \( x_2 \) or \( x_5 \).

Then, \( d(u_n|B_n) \) is given by (15) or (18).

Case 2: \( B_n \rightarrow B_{n+1}^2 \). In this case, the vertex \( u_n \) coincides with the vertex labeled \( x_3 \) or \( x_4 \).

Then, \( d(u_n|B_n) \) is given by (16) or (17).

Since the above two cases occur with probabilities \( p \) and \( 1 - p \), respectively, we have
Wiener numbers of random Pentagonal Chains

\[ U_n^{(\alpha)} = p \left[ d(u_{n-1}|R_{n-1}^{(\alpha)}) + 2 \times 5(n-1) + 6 \right] + (1 - p) \left[ d(u_{n-1}|R_{n-1}^{(\alpha)}) + 3 \times 5(n-1) + 6 \right] \]  

(21)

Simplifying (21), the recursion formula for \( U_n^{(\alpha)} \) becomes

\[ U_n^{(\alpha)} = U_{n-1}^{(\alpha)} + (15 - 5p)n + 5p - 9 \]  

(22)

with the boundary condition

\[ U_1^{(\alpha)} = E(d(u_1|R_1^{(\alpha)}) = 1 + 2 + 1 + 2 = 6 \]  

(23)

Eq. (22) combined with Eq. (23) provides the explicit expression of \( U_n^{(\alpha)} \), that is

\[ U_n^{(\alpha)} = \frac{1}{2}(15 - 5p)n^2 + \frac{1}{2}(5p - 3)n \]

By applying the expectation operator to equation (19), we get

\[ E(W(R_{n+1}^{(\alpha)})) = E(W(R_n^{(\alpha)})) + 5 \left[ \frac{1}{2}(15 - 5p)n^2 + \frac{1}{2}(5p - 3)n \right] + 55n + 15 \]

with the boundary condition \( E(W(R_1^{(\alpha)})) = 15 \). From the above recurrence relation, we arrive at Eq. (13), by which Theorem 1 is proven.

3. Beta-type Pentachains

A beta-pentachain is a graph consisting of pentagonal rings, every two successive rings having a common edge, see Fig. 5. More generally, a beta-pentachain \( C_n \) with \( n \) pentagons (see Fig. 6) can be regarded as a beta-pentachain \( C_{n-1} \) with \( n-1 \) pentagons to which a new terminal pentagon \( \{w_{n-1}, v_{n-1}, y_1, y_2, y_3\} \) has been adjoined. However, this terminal pentagon can be added in two ways, resulting in the local arrangements described as \( C_{n+1}^1 \) and \( C_{n+1}^2 \) and shown in Fig. 7.
**Fig. 5.** The beta-pentachains with one, two, and three pentagons.

**Fig. 6.** A beta-pentachain with $n$ pentagons.

**Fig. 7.** The two types of local arrangements in beta-pentachains.

A random beta-pentachain $R_n^{(β)}$ is a beta-pentachain obtained by stepwise addition of terminal pentagons. At each step $k = 3, 4, \ldots, n$, a random selection is made from one of the two possible constructions: (1) $C_k \rightarrow C_{k+1}^1$ with probability $p$, and (2) $C_k \rightarrow C_{k+1}^2$ with probability $1 - p$. Here we also assume that this construction is a zeroth–order Markov
Wiener numbers of random Pentagonal Chains

Earlier, Rao and Prasanna considered the Wiener indices of beta-pentachains [14, 15]. In what follows, we provide an explicit formula for the expected value of the Wiener index of a random beta-pentachain.

**Theorem 2.** For \( n \geq 1 \),

\[
W_{n+1}^{(\beta)} = \frac{a_1}{3} I_0 + \left(\frac{a_1}{2} + \frac{b_1}{2}\right) I_1 + \left(\frac{a_1}{6} + \frac{b_1}{2} + c_1\right) I_2 + I_3 \left((2 - p) n^3 + (12 - p) n^2 + 22n + 12\right)
\]

with \( I_0 \), \( I_1 \), \( I_2 \), and \( I_3 \) given in Lemma 1 whereas \( a_1 \), \( b_1 \), and \( c_1 \) defined as

\( q = 1 - p \), \( a_1 = \frac{1}{2} p (6 - 3p) \), \( b_1 = \frac{7}{2} p^2 + 3 \), \( c_1 = -2p^2 - 2p + 2 \).

**Proof.** As seen from Figs. 5–7, the beta-pentachain is a graph consisting of pentagonal rings, every two successive rings having a common edge. Taking into account this construction, we get the following basic relations:

1. For any \( v \in C_{n-1} \),

\[ d(y_k, v) = d(w_{n-1}, v) + k \quad k = 1, 2 \quad \text{and} \quad d(y_3, v) = d(v_{n-1}, v) + 1. \]

2. \( C_{n-1} \) has \( 3n - 1 \) vertices.

3. \( \sum_{i=1}^{3} d(y_k, y_i) = 3 \), \( \forall k \in \{1, 3\} \), \( \sum_{i=1}^{3} d(y_2, y_i) = 2. \)

Then it is straightforward to establish that

\[
d(y_1|C_n) = d(w_{n-1}|C_{n-1}) + 1 \times (3n - 1) + 3 \quad (25)
\]

\[
d(y_2|C_n) = d(w_{n-1}|C_{n-1}) + 2 \times (3n - 1) + 2 \quad (26)
\]

\[
d(y_3|C_n) = d(v_{n-1}|C_{n-1}) + 1 \times (3n - 1) + 3 \quad (27)
\]

and

\[
W(C_n) = W(C_{n-1}) + 2d(w_{n-1}|C_{n-1}) + d(v_{n-1}|C_{n-1}) + 12n \quad (28)
\]

with the boundary conditions

\( W(C_0) = d(w_0|C_0) = d(v_0|C_0) = 0. \)

Clearly, equation (28) implies

\[
W(C_{n+1}) = W(C_n) + 2d(w_n|C_n) + d(v_n|C_n) + 12n + 12. \quad (29)
\]
There are two cases to investigate:

Case 1: $C_n \rightarrow C_{n+1}^1$. In this case, $w_n$ and $v_n$ coincide with $x_1$ and $x_2$. Hence, $d(w_n|C_n)$ and $d(v_n|C_n)$ are given by (25) and (26).

Case 2: $C_n \rightarrow C_{n+1}^2$. In this case, $w_n$ and $v_n$ coincide with $x_2$ and $x_3$. Hence, $d(w_n|C_n)$ and $d(v_n|C_n)$ are given by (26) and (27).

If the expected values of $d(w_n|R_n^{(\beta)})$ and $d(v_n|R_n^{(\beta)})$ are denoted by, respectively,

$$U_n^{(\beta)} = E(d(w_n|R_n^{(\beta)})) \quad \text{and} \quad V_n^{(\beta)} = E(d(v_n|R_n^{(\beta)}))$$

then the recursion formulas for $U_n^{(\beta)}$ and $V_n^{(\beta)}$ are given by,

$$U_n^{(\beta)} = p \left[ d(w_{n-1}|R_{n-1}^{(\beta)}) + 3n + 2 \right] + (1 - p) \left[ d(w_{n-1}|R_{n-1}^{(\beta)}) + 6n \right]$$

$$= U_{n-1}^{(\beta)} + (6 - 3p)n + 2p \tag{30}$$

and

$$V_n^{(\beta)} = p \left[ d(v_{n-1}|R_{n-1}^{(\beta)}) + 6n \right] + (1 - p) \left[ d(v_{n-1}|R_{n-1}^{(\beta)}) + 3n + 2 \right]$$

$$= pU_{n-1}^{(\beta)} + (1 - p)V_{n-1}^{(\beta)} + (3 + 3p)n + 2 - 2p \tag{31}$$

Meanwhile, from Eq. (29) we get

$$W(R_{n+1}^{(\beta)}) = W(R_n^{(\beta)}) + 2U_n^{(\beta)} + V_n^{(\beta)} + 12n + 12 \tag{32}$$

with the boundary conditions

$$W(C_0^{(\beta)}) = d(w_0|C_0^{(\beta)}) = d(v_0|C_0^{(\beta)}) = 0.$$ 

By applying the expectation operator to (32), and noting that $E(U_n^{(\beta)}) = U_n^{(\beta)}$ and $E(V_n^{(\beta)}) = V_n^{(\beta)}$, we get

$$W_{n+1}^{(\beta)} = W_n^{(\beta)} + 2U_n^{(\beta)} + V_n^{(\beta)} + 12n + 12 \tag{33}$$

where $W_n^{(\beta)} = E(W(R_n^{(\beta)}))$.

The aim of this subsection is to calculate the expected value of $W_n^{(\beta)}$. To this end, usually one computes the expression for $U_n^{(\beta)}$ by means of Eq. (30) and for $V_n^{(\beta)}$ by means of Eq.
Wiener numbers of random Pentagonal Chains

(31). Then, by making use of Eq. (33), one would arrive at the desired result. In what follows, instead of this usual way, we employ another direct approach to do so.

From Eq. (33) we conclude that $W_{n+1}^{(\beta)}$ can also be expressed as

$$W_{n+1}^{(\beta)} = 2(U_n^{(\beta)} + U_{n-1}^{(\beta)} + \cdots + U_0^{(\beta)}) + (V_n^{(\beta)} + V_{n-1}^{(\beta)} + \cdots + V_0^{(\beta)}) + 12(n + 1 + n + n - 1 + \cdots + 2 + 1).$$

(34)

Hence, it remains to determine the values of the two sums in the bracket on the right–hand side of Eq. (34). Noting that $U_0^{(\beta)} = 0$, by a direct calculation we find

$$U_n^{(\beta)} = \frac{6 - 3p}{2} n^2 + (3 + \frac{1}{2}p)n$$

implying

$$U_n^{(\beta)} + U_{n-1}^{(\beta)} + \cdots + U_0^{(\beta)} = (1 - \frac{1}{2}p)n^3 + (3 - \frac{1}{2}p)n^2 + 2n.$$  (35)

On the other hand, Eq. (31) can be rewritten as

$$V_n^{(\beta)} = q V_{n-1}^{(\beta)} + a_n^2 + b_n n + c_1$$  (36)

where

$$q = 1 - p, \quad a_n = \frac{1}{2} p (6 - 3p), \quad b_n = \frac{7}{2} p^2 + 3, \quad c_1 = -2p^2 - 2p + 2.$$

If we introduce an auxiliary quantity $H_n$ defined by

$$H_n = V_n^{(\beta)} + V_{n-1}^{(\beta)} + \cdots + V_0^{(\beta)}$$

then Eq. (36) implies that $H_n$ satisfies the recursion relation:

$$H_n = q H_{n-1} + \frac{a_n}{6} n(n + 1)(2n + 1) + \frac{b_n}{2} n(n + 1) + nc_1$$

$$= q H_{n-1} + \frac{a_n}{3} n^3 + (\frac{a_1}{2} + b_n) n^2 + (\frac{a_1}{6} + b_n + c_1)n.$$  (37)

By virtue of Eq. (2) in Lemma 1, we obtain the following representation of $H_n$:

$$H_n = \frac{a_1}{3} I_0 + \left(\frac{a_1}{2} + \frac{b_1}{2}\right) I_1 + \left(\frac{a_1}{6} + \frac{b_1}{2} + c_1\right) I_2 + I_3$$  (38)

where $I_0, I_1, I_2,$ and $I_3$ are defined in Lemma 1. Combining Eqs. (34), (35), and (38), one can derive the equation (24). This completes the proof of Theorem 2.
4. **Gamma-Type Pentachains**

The gamma-pentachains for \( n = 1, 2, \) and \( n = 3 \) are depicted in Fig. 8. More generally, a gamma-pentachain \( D_n \) with \( n \) pentagons can be obtained by attaching a pentagon by means of two edges to \( D_{n-1} \) which has \( n - 1 \) pentagons (see Fig. 9). However, for \( n \geq 2 \), there are two ways to attach the terminal pentagon, leading to the local arrangements \( D_{n+1}^1 \) and \( D_{n+1}^2 \) shown in Fig. 10.

A random gamma-pentachain is constructed analogously to the above-described random alpha- and beta-pentachains.

**Fig. 8.** The gamma-pentachains with one, two, and three pentagons.

**Fig. 9.** A gamma-pentachain with \( n \) pentagons.
Wiener numbers of random Pentagonal Chains

Fig. 10. The two types of local arrangements in gamma-pentachains.

**Theorem 3.** For \( n \geq 1 \),

\[
W_{n+1}^{(y)} = \frac{2a_2}{3} I_0 + (a_2 + b_2) I_1 + \left( \frac{a_2}{3} + b_2 + 2c_2 \right) I_2 + 2 I_3 + \frac{1}{2} (15 - 5p) n^3 \\
+ \frac{63}{2} n^2 + (39 + \frac{5}{2} p) n + 15
\]  

(39)

where \( I_0, I_1, I_2, \) and \( I_3 \) are given in Lemma 1 and \( q, a_2, b_2, \) and \( c_3 \) are given by

\[
q = 1 - p \ , \ a_2 = \frac{1}{2} (15p - 5p^2) \ , \ b_2 = \frac{15}{2} p^2 - \frac{23}{2} p + 10 \ , \ c_2 = -(5p^2 - 4p + 4).
\]

**Proof.** As see from Figs. 8–10, the gamma-pentachain is a graph consisting of pentagonal rings, every two successive rings connected by two edges. In view of this construction, we find the following basic facts:

1’. For any \( v \in D_{n-1} \),

\[
d(z_k, v) = d(r_{n-1}, v) + k, \quad k = 1, 2, 3
\]

\[
d(z_4, v) = d(t_{n-1}, v) + 2
\]

\[
d(z_5, v) = d(t_{n-1}, v) + 1.
\]

2’. \( D_{n-1} \) has \( 5n - 1 \) vertices.

3’. \( \sum_{i=1}^{5} d(z_k, z_i) = 6 \ , \ \forall k \in \{1, 2, 3, 4, 5\} \).

Hence we have
\[
d(z_1|D_n) = d(r_{n-1}|D_{n-1}) + 1 \times 5(n-1) + 6
\]
(40)
\[
d(z_2|D_n) = d(r_{n-1}|D_{n-1}) + 2 \times 5(n-1) + 6
\]
(41)
\[
d(z_3|D_n) = d(r_{n-1}|D_{n-1}) + 3 \times 5(n-1) + 6
\]
(42)
\[
d(z_4|D_n) = d(t_{n-1}|D_{n-1}) + 2 \times 5(n-1) + 6
\]
(43)
\[
d(z_5|D_n) = d(t_{n-1}|D_{n-1}) + 1 \times 5(n-1) + 6
\]
(44)
and
\[
W(D_n) = W(D_{n-1}) + 3d(r_{n-1}|D_{n-1}) + 2d(t_{n-1}|D_{n-1}) + 45 \, n - 30
\]
(45)
with the boundary conditions
\[
W(D_0) = d(r_0|D_0) = d(t_0|D_0) = 0
\]
Replacing \(n\) by \(n + 1\), we get from Eq. (45)
\[
W(D_{n+1}) = W(D_n) + 3d(r_n|D_n) + 2d(t_n|D_n) + 45 \, n + 15
\]
(46)

There are two cases to be considered:

Case 1: \(D_n \rightarrow D_{n+1}^1\). In this case, \(r_n\) and \(t_n\) coincide with \(z_2\) and \(z_3\). Hence, \(d(r_n|C_n)\) and \(d(t_n|C_n)\) are given by Eqs. (40) and (41).

Case 2: \(D_n \rightarrow D_{n+1}^2\). In this case, \(r_n\) and \(t_n\) coincide with \(z_3\) and \(z_4\). Hence, \(d(r_n|C_n)\) and \(d(t_n|C_n)\) are given by Eqs. (41) and (42).

If we introduce the notation
\[
U_n^{(\gamma)} = E(d(r_n|R_{n-1}^{(\gamma)})) \quad , \quad V_n^{(\gamma)} = E(d(t_n|R_{n-1}^{(\gamma)}))
\]
then we can obtain the following recursions for \(U_n^{(\gamma)}\) and \(V_n^{(\gamma)}\):

\[
U_n^{(\gamma)} = p \left[ d(r_{n-1}|R_{n-1}^{(\gamma)}) + 10(n-1) + 6 \right] + (1-p) \left[ d(r_{n-1}|R_{n-1}^{(\gamma)}) + 15(n-1) + 6 \right] = U_{n-1}^{(\gamma)} + (15 - 5p)n + 5p - 9
\]
(47)
\[
V_n^{(\gamma)} = p \left[ d(r_{n-1}|R_{n-1}^{(\gamma)}) + 15(n-1) + 6 \right] + (1-p) \left[ d(t_{n-1}|R_{n-1}^{(\gamma)}) + 10(n-1) + 6 \right] = p U_{n-1}^{(\gamma)} + (1-p) V_{n-1}^{(\gamma)} + (5p + 10)n - 4 - 5p
\]
(48)
Furthermore, it also can be shown that \(W_n^{(\gamma)} = E(W(R_{n-1}^{(\gamma)}))\) satisfies
Wiener numbers of random Pentagonal Chains

\[ W_{n+1}^{(\gamma)} = W_n^{(\gamma)} + 3U_n^{(\gamma)} + 2V_n^{(\gamma)} + 45n + 15 \]  \hspace{1cm} (49)

with the boundary conditions

\[ U_0^{(\gamma)} = V_0^{(\gamma)} = W_0^{(\gamma)} = 0. \]

Noticing that Eqs. (47), (48), and (49) differ from Eqs. (31), (32), and (34) only by the coefficients, the remaining discussion and calculations follows closely the proof of the Theorem 2, and the final result, Eq. (39), is obtained in a similar way.

\[ \square \]

REFERENCES


