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Wiener numbers of random pentagonal chains

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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.

Keywords: Wiener index, pentagonal chain.

1. 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

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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 $V = \{v_1, v_2, \dots, v_n\}$. 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.

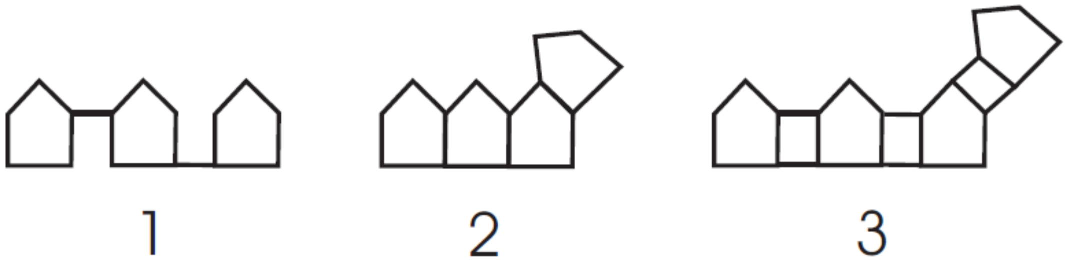

Fig. 1. The three types of pentagonal chains (pentachains) examined in this paper: alpha (1), beta (2), and gamma (3).

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

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

$$t_n = q\, t_{n-1} + d\, n^3 + a\, n^2 + bn + c\, ;\, n \ge 1\, . \tag{1}$$

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

$$t_n = d\, I_0 + a\, I_1 + b\, I_2 + c\, I_3 \tag{2}$$

where

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

$$I_1 = \frac{1}{(q-1)^3}[-n^2 + (2n^2 + 2n - 1)q - (n^2 + 2n + 1)q^2 + q^{n+1} + q^{n+2}]$$
$$I_2 = \frac{1}{(1-q)^2}[n - (n+1)q + q^{n+1}]$$
$$I_3 = \frac{1-q^n}{1-q}.$$

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

$$\begin{aligned} t_n = {} & d\, n^3 + d\, q(n-1)^3 + d\, q^2(n-2)^3 + \cdots + d\, q^{n-2}2^3 + d\, q^{n-1}1^3 \\ & + a\, n^2 + a\, q(n-1)^2 + a\, q^2(n-2)^2 + \cdots + a\, q^{n-2}2^2 + a\, q^{n-1}1^2 \\ & + b\, n + b\, q(n-1) + b\, q^2(n-2) + \cdots + b\, q^{n-2}2 + b\, q^{n-1}1 \\ & + c + c\, q + c\, q^2 + \cdots + c\, q^{n-2} + c\, q^{n-1} = d\, I_0 + a\, I_1 + b\, I_2 + c\, I_3\, . \end{aligned}$$

I_3 is a geometric sequence with the common ratio q. Hence,

$$I_3 = \frac{1-q^n}{1-q}. \tag{3}$$

From the definition of I_2 , we have

$$I_2 = n + q(n-1) + q^2\,(n-2) + \cdots + q^{n-2}\, 2 + q^{n-1} \tag{4}$$

and

$$q\, I_2 = qn + q^2\,(n-1) + q^3\,(n-2) + \cdots + q^{n-1}\, 2 + q^n. \tag{5}$$

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

$$I_2 = (n - \frac{q-q^{n+1}}{1-q})\frac{1}{1-q} = \frac{n-(n+1)q+q^{n+1}}{(1-q)^2}. \tag{6}$$

For I_1 , we rewrite its expression as follows:

$$\begin{aligned} I_1 &= n^2 + q(n-1)^2 + q^2(n-2)^2 + \cdots + q^{n-2}2^2 + q^{n-1}1^2 \\ &= q^{n-1}\left[1^2 + 2^2\left(\frac{1}{q}\right) + \cdots + (n-2)^2\left(\frac{1}{q}\right)^{n-3}\right. \\ &\quad \left. + (n-1)^2\left(\frac{1}{q}\right)^{n-2} + n^2\left(\frac{1}{q}\right)^{n-1}\right] = q^{n-1}J. \end{aligned}$$

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

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

Furthermore, it is not hard to verify the identities:

$$\begin{aligned} \sum_{k=1}^{n} k(k-1) x^{k-2} &= (1 + x + x^2 + x^3 + \cdots + x^n)'' = \left(\frac{1-x^{n+1}}{1-x}\right)'' \\ &= \frac{(n-n^2)x^{n+1} + (2n^2-2)x^n - (n^2+n)x^{n-1} + 2}{(1-x)^3} \end{aligned} \tag{7}$$

$$\begin{aligned} \sum_{k=1}^{n} k x^{k-1} &= (1 + x + x^2 + \cdots + x^{n-1} + x^n)' = \left(\frac{1-x^{n+1}}{1-x}\right)' \\ &= \frac{1-(n+1)x^n + nx^{n+1}}{(1-x)^2}. \end{aligned} \tag{8}$$

Combining (7) and (8) we arrive at

$$\sum_{k=1}^{n} k^2 x^{k-1} = \frac{-n^2 x^{n+2} + (2n^2+2n-1)x^{n+1} - (n^2+2n+1)x^n + x + 1}{(1-x)^3}. \tag{9}$$

After replacing *x* by $1/q$ in (9), we establish

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

For I_0, we rewrite its expression as:

$$\begin{aligned} I_0 &= n^3 + q(n-1)^3 + q^2(n-2)^3 + \cdots + q^{n-2}2^3 + q^{n-1}1^3 \\ &= q^{n-1}\left[1^3 + 2^3\left(\frac{1}{q}\right) + \cdots + (n-2)^3\left(\frac{1}{q}\right)^{n-3}\right. \\ &\quad \left. + (n-1)^3\left(\frac{1}{q}\right)^{n-2} + n^3\left(\frac{1}{q}\right)^{n-1}\right] = q^{n-1}K. \end{aligned}$$

In order to compute K, consider the following representation

$$\begin{aligned} \sum_{k=1}^{n} k^3 x^{k-1} &= \sum_{k=1}^{n}[k(k-1)(k-2) + 3k(k-1) + k]x^{k-1} \\ &= \sum_{k=3}^{n} k(k-1)(k-2)x^{k-1} + 3\sum_{k=2}^{n} k(k-1)x^{k-1} + \sum_{k=1}^{n} k\,x^{k-1} \\ &= K_1 + K_2 + K_3. \end{aligned}$$

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

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

$$\begin{aligned} K_2 &= 3x\left(\sum_{k=0}^{n} x^k\right)'' = 3x\left(\frac{1-x^{n+1}}{1-x}\right)'' \\ &= 3x\frac{(n-n^2)x^{n+1} + (2n^2-2)x^n - (n^2+n)x^{n-1} + 2}{(1-x)^3} \end{aligned}$$

$$\begin{aligned} K_1 &= x^2\left(\frac{1-x^{n+1}}{1-x}\right)''' = \frac{x^2}{(1-x)^4}[(n^3 - 3n^2 + 2n)x^{n+1} \\ &\quad - (3n^3 - 6n^2 - 3n + 6)x^n + (3n^3 - 3n^2 - 6n)x^{n-2} + 6] \end{aligned}$$

we arrive at

$$K = \frac{1}{(1-x)^4}[n^3 x^{n+3} - (3n^3 + 3n^2 - 3n + 1)x^{n+2} + (3n^3 + 6n^2 - 4)x^{n+1} \\ - (n^3 + 3n^2 + 3n + 1)x^n + x^2 + 4x + 1]. \tag{11}$$

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

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

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.

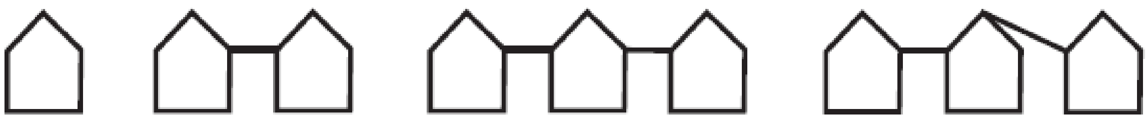

Fig. 2. The alpha-pentachains with one, two, and three pentagons.

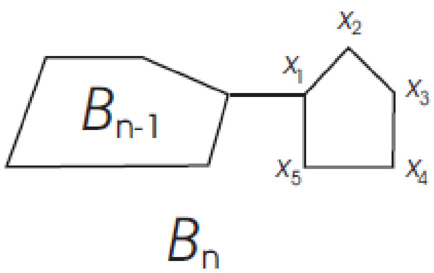

Fig. 3. An alpha-pentachain with n pentagons.

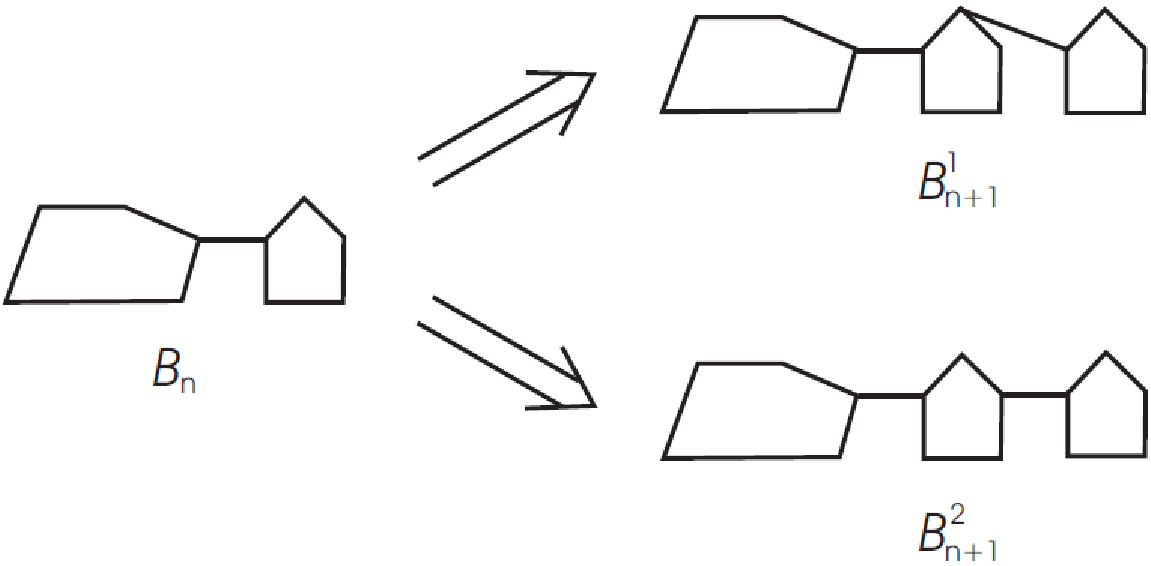

Fig. 4. The two types of local arrangements in alpha-pentachains.

Due to the random selection from B_{k-1} to B_k , $k = 3, 4, 5, \dots,$ 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 $k = 3, 4, \dots, n$, 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 Ξ.

Theorem 1. For $n \geq 1$,

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

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 $v \in B_{n-1}$,

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

and

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

2°. B_{n-1} has $5(n - 1)$ vertices.

$3^\circ \cdot \sum_{i=1}^{5} d(x_k, x_i) = 6, \quad \forall k \in \{1,2,3,4,5\}.$

Then we have

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

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

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

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

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

and

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

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

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

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: $B_n \to B_{n+1}^1$. 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: $B_n \to B_{n+1}^2$. 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

$$U_n^{(\alpha)} = p\left[d(u_{n-1}\middle|R_{n-1}^{(\alpha)}) + 2\times 5(n-1) + 6\right] \\ +(1-p)\left[d(u_{n-1}\middle|R_{n-1}^{(\alpha)}) + 3\times 5(n-1) + 6\right]. \tag{21}$$

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

$$U_n^{(\alpha)} = U_{n-1}^{(\alpha)} + (15-5p)n + 5p - 9 \tag{22}$$

with the boundary condition

$$U_1^{(\alpha)} = E(d(u_1\middle|R_1^{(\alpha)}) = 1+2+1+2 = 6 \tag{23}$$

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.

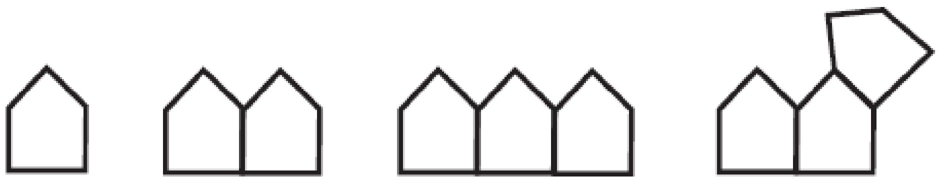

Fig. 5. The beta-pentachains with one, two, and three pentagons.

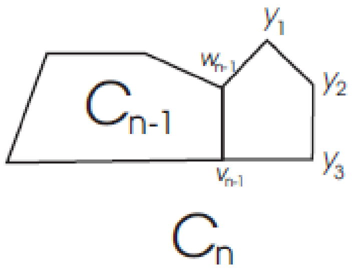

Fig. 6. A beta-pentachain with n pentagons.

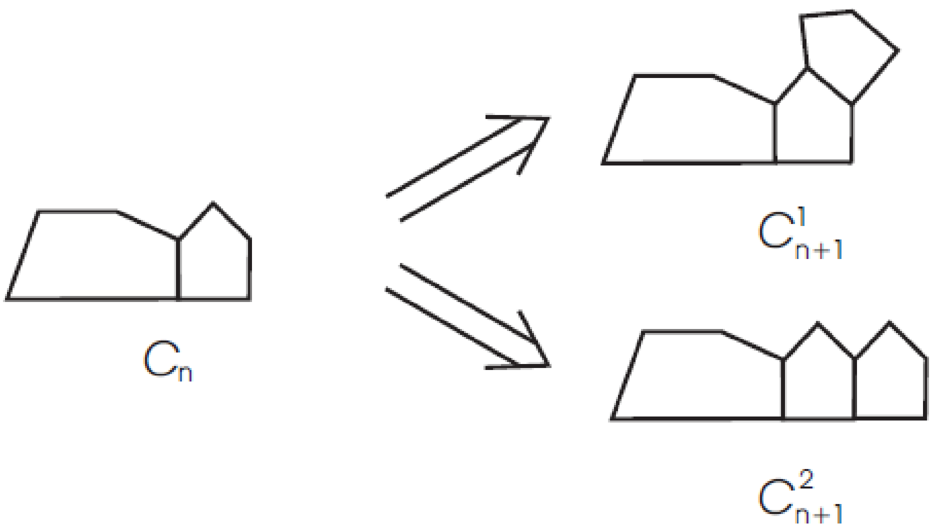

Fig. 7. The two types of local arrangements in beta-pentachains.

A random beta-pentachain $R_n^{(\beta)}$ 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) $C_k \to C^1_{k+1}$ with probability p, and (2) $C_k \to C^2_{k+1}$ with probability $1 - p$. Here we also assume that this construction is a zeroth–order Markov process. 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 $n \geq 1$,

$$W_{n+1}^{(\beta)} = \frac{a_1}{3} I_0 + (\frac{a_1}{2} + \frac{b_1}{2}) I_1 + (\frac{a_1}{6} + \frac{b_1}{2} + c_1) I_2 \\ + I_3 + (2-p)n^3 + (12-p)n^2 + 22n + 12 \tag{24}$$

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

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

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 $v \in C_{n-1}$,

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

2°. C_{n-1} has $3n - 1$ vertices.

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

Then it is straightforward to establish that

$$d(y_1 | C_n) = d(w_{n-1} | C_{n-1}) + 1 \times (3n-1) + 3 \tag{25}$$

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

$$d(y_3 | C_n) = d(v_{n-1} | C_{n-1}) + 1 \times (3n-1) + 3 \tag{27}$$

and

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

with the boundary conditions

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

Clearly, equation (28) implies

$$W(C_{n+1}) = W(C_n) + 2d(w_n | C_n) + d(v_n | C_n) + 12n + 12. \tag{29}$$

There are two cases to investigate:

Case 1: $C_n \to C_{n+1}^1$. 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: $C_n \to C_{n+1}^2$. 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 $d(w_n \left| R_n^{(\beta)}\right.)$ and $d(v_n \left| R_n^{(\beta)}\right.)$ are denoted by, respectively,

$$U_n^{(\beta)} = E(d(w_n \left| R_n^{(\beta)}\right.)) \qquad \text{and} \qquad V_n^{(\beta)} = E(d(v_n \left| R_n^{(\beta)}\right.))$$

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

$$\begin{aligned} U_n^{(\beta)} &= p\left\lfloor d(w_{n-1} \left| R_{n-1}^{(\beta)}\right.) + 3n + 2 \right\rfloor + (1-p)\left\lfloor d(w_{n-1} \left| R_{n-1}^{(\beta)}\right.) + 6n \right\rfloor \\ &= U_{n-1}^{(\beta)} + (6-3p)n + 2p \end{aligned} \tag{30}$$

and

$$\begin{aligned} V_n^{(\beta)} &= p\left\lfloor d(w_{n-1} \left| R_{n-1}^{(\beta)}\right.) + 6n \right\rfloor + (1-p)\left\lfloor d(v_{n-1} \left| R_{n-1}^{(\beta)}\right.) + 3n + 2 \right\rfloor \\ &= pU_{n-1}^{(\beta)} + (1-p)V_{n-1}^{(\beta)} + (3+3p)n + 2 - 2p. \end{aligned} \tag{31}$$

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

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

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.

(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

$$\begin{aligned} W_{n+1}^{(\beta)} &= 2(U_n^{(\beta)} + U_{n-1}^{(\beta)} + \cdots + U_0^{(\beta)}) + (V_n^{(\beta)} + V_{n-1}^{(\beta)} + \cdots + V_0^{(\beta)}) \\ &\quad + 12(n+1+n+n-1+\cdots+2+1). \end{aligned} \tag{34}$$

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

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

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

$$V_n^{(\beta)} = q V_{n-1}^{(\beta)} + a_1 n^2 + b_1 n + c_1 \tag{36}$$

where

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

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:

$$\begin{aligned} H_n &= q H_{n-1} + \frac{a_1}{6}n(n+1)(2n+1) + \frac{b_1}{2}n(n+1) + nc_1 \\ &= q H_{n-1} + \frac{a_1}{3}n^3 + (\frac{a_1}{2} + \frac{b_1}{2})n^2 + (\frac{a_1}{6} + \frac{b_1}{2} + c_1)n. \end{aligned} \tag{37}$$

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

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

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 $n \geq 2$, three 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.

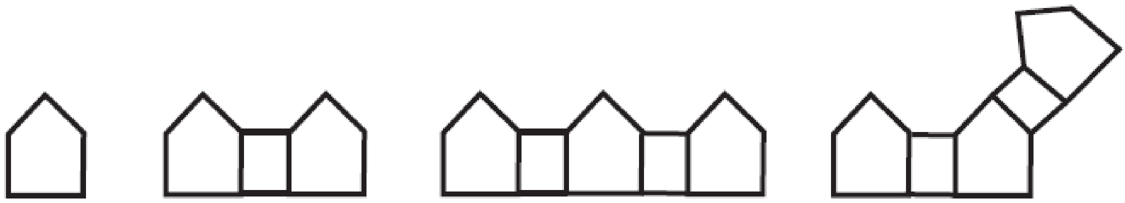

Fig. 8. The gamma-pentachains with one, two, and three pentagons.

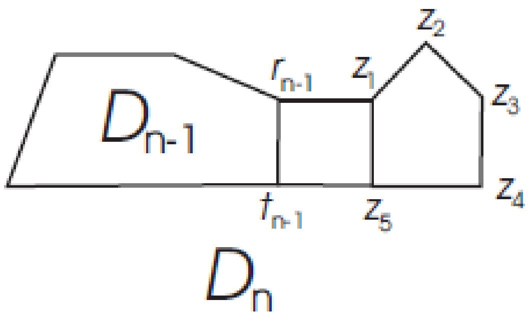

Fig. 9. A gamma-pentachain with n pentagons.

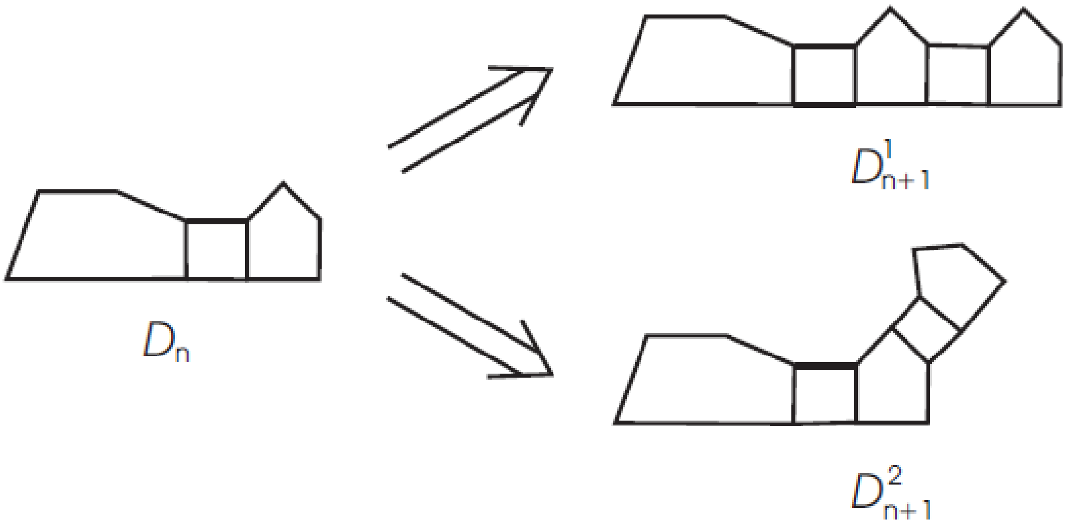

Fig. 10. The two types of local arrangements in gamma-pentachains.

Theorem 3. For n ≥ 1,

$$\begin{aligned} W_{n+1}^{(\gamma)} &= \frac{2a_2}{3} I_0 + (a_2 + b_2) I_1 + (\frac{a_2}{3} + b_2 + 2c_2) I_2 + 2I_3 + \frac{1}{2}(15 - 5p) n^3 \\ &+ \frac{63}{2} n^2 + (39 + \frac{5}{2} p) n + 15 \end{aligned} \tag{39}$$

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 $v \in D_{n-1}$,

$$d(z_k, v) = d(r_{n-1}, v) + k, \qquad k = 1, 2, 3$$
$$d(z_4, v) = d(t_{n-1}, v) + 2$$
$$d(z_5, v) = d(t_{n-1}, v) + 1 .$$

2°. D_{n-1} has $5(n - 1)$ vertices.

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

Hence we have

$$d(z_1|D_n) = d(r_{n-1}|D_{n-1}) + 1\times 5(n-1) + 6 \tag{40}$$

$$d(z_2|D_n) = d(r_{n-1}|D_{n-1}) + 2\times 5(n-1) + 6 \tag{41}$$

$$d(z_3|D_n) = d(r_{n-1}|D_{n-1}) + 3\times 5(n-1) + 6 \tag{42}$$

$$d(z_4|D_n) = d(t_{n-1}|D_{n-1}) + 2\times 5(n-1) + 6 \tag{43}$$

$$d(z_5|D_n) = d(t_{n-1}|D_{n-1}) + 1\times 5(n-1) + 6 \tag{44}$$

and

$$W(D_n) = W(D_{n-1}) + 3d(r_{n-1}|D_{n-1}) + 2d(t_{n-1}|D_{n-1}) + 45\,n - 30 \tag{45}$$

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)

$$W(D_{n+1}) = W(D_n) + 3d(r_n|D_n) + 2d(t_n|D_n) + 45\,n + 15\,. \tag{46}$$

There are two cases to be considered:

Case 1: $D_n \to D_{n+1}^1$. 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: $D_n \to D_{n+1}^2$. 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

$$U_n^{(\gamma)} = E(d(r_n|R_n^{(\gamma)})) \quad , \quad V_n^{(\gamma)} = E(d(t_n|R_n^{(\gamma)}))$$

then we can obtain the following recursions for $U_n^{(\gamma)}$ and $V_n^{(\gamma)}$:

$$\begin{aligned} U_n^{(\gamma)} &= p\left[d(r_{n-1}|R_{n-1}^{(\gamma)}) + 10(n-1) + 6\right] + (1-p)\left[d(r_{n-1}|R_{n-1}^{(\gamma)}) + 15(n-1) + 6\right] \\ &= U_{n-1}^{(\gamma)} + (15-5p)n + 5p - 9 \end{aligned} \tag{47}$$

$$\begin{aligned} V_n^{(\gamma)} &= p\left[d(r_{n-1}|R_{n-1}^{(\gamma)}) + 15(n-1) + 6\right] + (1-p)\left[d(t_{n-1}|R_{n-1}^{(\gamma)}) + 10(n-1) + 6\right] \\ &= pU_{n-1}^{(\gamma)} + (1-p)V_{n-1}^{(\gamma)} + (5p+10)n - 4 - 5p. \end{aligned} \tag{48}$$

Furthermore, it also can be shown that $W_n^{(\gamma)} = E(W(R_n^{(\gamma)}))$ satisfies

$$W_{n+1}^{(\gamma)} = W_n^{(\gamma)} + 3U_n^{(\gamma)} + 2V_n^{(\gamma)} + 45n + 15 \tag{49}$$

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. □

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