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# Generalized Wiener indices of zigzagging pentachains

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The "*pentachains*" studied in this paper are graphs formed of concatenated 5-cycles. Explicit formulas are obtained for the Schultz and modified Schultz indices of these graphs, as well as for generalizations of these indices. In the process we give a more refined version of the procedure that earlier was reported for the ordinary Wiener index.

**KEY WORDS:** Wiener index, Schultz index, pentagonal chains

## 1. Introduction

Finding general expressions for Wiener indices of classes of polycyclic graphs, especially those with multiple odd-length cycles, was considered as an intractable problem until the explicit formula of Yang and Yeh was found in 1995 [1]. Some time ago one of the authors [2] studied two extensions of the Wiener index, derived from, and related to, the "molecular topological index" of Schultz [3]. We shall refer to these molecular-graph-based structure descriptors as *the Schultz* and *the modified Schultz* indices, and denote them as $\mathcal{W}_+$ and $\mathcal{W}_*$, respectively.

Recently, Eu et al. [4] generalized an earlier result [5] about catacondensed benzenoid chains (concatenated 6-cycles, or hex chains) to the Schultz indices and other indices of the same general type. Ideas from these derivations are now combined to find an explicit formula for all Schultz-type indices (defined below) for graphs formed of concatenated 5-cycles (pentachains). Doing this we

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elaborate a more refined version of the procedure [1], that earlier was applied to the ordinary Wiener index.

## 2. Introduction to the problem at hand

**Definition 1** (Wiener [6,7]). Let $G$ be a connected graph with vertex set $V(G)$. Let $d_G$ be the distance function on $G$. The WIENER INDEX of $G$ is

$$\mathcal{W}(G) := \sum_{\{u,v\}\in\binom{V(G)}{2}} d_G(u, v).$$

**Definition 2** [2]. Let $\deg_G v$ be the degree of the vertex $v$ of the graph $G$. With the same notation as in Definition 1, the THE SCHULTZ INDEX and the MODIFIED SCHULTZ INDEX of $G$ are

$$\mathcal{W}_+(G) := \sum_{\{u,v\}\in\binom{V(G)}{2}} \big(\deg_G u + \deg_G v\big)\ d_G(u, v)$$

$$\mathcal{W}_*(G) := \sum_{\{u,v\}\in\binom{V(G)}{2}} \big(\deg_G u \cdot \deg_G v\big)\ d_G(u, v),$$

respectively.

**Problem.** Determine $\mathcal{W}_+$ and $\mathcal{W}_*$ for an arbitrary pentachain, specified by a binary string. The way in which such a string is associated to the pentachain should be evident from the examples depicted in figure 1.

## 3. A brief survey of Wiener index and its generalizations

The Wiener index of a molecular graph provides a rough measure of the compactness of the underlying molecule. It was demonstrated [8] that the Wiener index is related to the molecular surface area. As a result, the Wiener index is

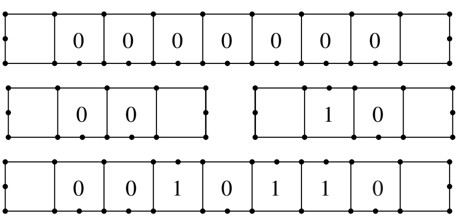



Figure 1. Examples illustrating the construction of the binary string that uniquely determines a pentachain.

reasonably well-correlated with many physical and chemical properties of organic compounds, and chemists are hence interested in computing it for a variety of classes of graphs. There are other chemically useful quantities associated with a molecular graph (see, for instance [9]), but the Wiener index is one of the best known and most thoroughly examined among them. For further details on the mathematical properties and chemical applications of the Wiener index see the reviews [10–13] and the references cited therein. For further details on distances in graphs see the book [14].

Researches concerned with the computing the Wiener index of a generic chain-like polygonal system showed up in print the late 1980s; [15–17] for more details see the review [12]. Doing this for an arbitrary hexagonal chain was considered a hard problem until the solution was found in 1993 [5]. Eventually, this approach was extended to 2-dimensional hexagonal patterns, pentagonal chains, and motley (mixed) chains [1,18–20].

**Definition 3a** (Motley chain [19]). Given $n$ ordered pairs of non-negative integers $S = (a_1, b_1), \ldots, (a_n, b_n)$, we construct a graph as follows: Start with the graph $P_2 \times P_{n+1}$ (noting that it is composed of $n$ adjacent squares, joined up side by side) and subdivide the $j$th upper and lower edges by inserting $a_j$ and $b_j$ extra vertices, respectively. This is the MOTLEY CHAIN associated with $S$, denoted $M(S)$ or (context permitting) just $S$.

**Definition 3b.** As long as the two sequences specified in Definition 3a differ only in the first and last pairs, with the sums $a_1 + b_1$ and $a_n + b_n$ being identical, the associated graphs will remain the same. Hereafter, we will represent such a equivalence class as:

$$\left\langle (a_1 + b_1) \begin{matrix} a_2 \; a_3 \cdots a_{n-1} \\ b_2 \; b_3 \cdots b_{n-1} \end{matrix} (a_n + b_n) \right\rangle .$$

This representation of a motley chain is unique up to top–bottom and left–right reflections.

An example of a motley chain is shown in figure 2.

In a less rigorous manner we may describe a motley chain as a graph of linearly concatenated polygons (cycles that connect only by sharing an edge), in which no three cycles meet at any vertex.

**Definition 4** [1,5,21]. For a vertex $u \in V(G)$ and a subsets of vertices $U \subset V(G)$; $U' \subset V(G)$, we have the following PARTIAL WIENER INDICES:

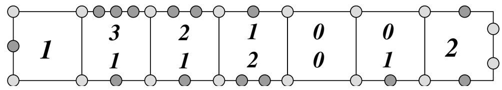



Figure 2. A motley chain; the numerals inscribed in the cycles correspond to the sequence specified in Definition 3b.

$$\mathcal{W}(U, U'; G) := \sum_{u\in U,\, u'\in U'} d_G(u, u')$$

$$\mathcal{W}(u, U; G) := \sum_{v\in U} d_G(u, v)$$

$$\mathcal{W}(U; G) := \sum_{\{u,u'\}\in\binom{U}{2}} d_G(u, u')$$

$$\mathcal{W}(u; G) := \sum_{v\in V(G)} d_G(u, v).$$

The computation of the Wiener indices of motley chains (including hex chains and pentachains) is based on the following:

**Lemma 1.** (Shelling lemma [1,19]). If $V(G) = \uplus_{i=1}^{k} U_i$ ($\uplus$ stands for disjoint union), then

$$\begin{aligned}\mathcal{W}(G) &= \sum_{j=1}^{k} \mathcal{W}(U_i; G) + \sum_{1\leqslant i<j\leqslant k} \mathcal{W}(U_i, U_j; G)\\ &= \mathcal{W}(U_1; G) + \sum_{j=2}^{k} \Big[\mathcal{W}\left(\left(\uplus_{1\leqslant i\leqslant j} U_i\right), U_j; G\right) - \mathcal{W}(U_j; G)\Big].\end{aligned}$$

Divide-and-conquer is a standard approach in combinatorics, and by means of it we derived most of our results on Wiener indices as well as Wiener polynomials [21,22].

Meanwhile, several generalizations of the Wiener index were put forward in the chemical literature [2,3,23–38]. In this work we focus our attention to Schultz-type indices (Definition 2) and their further generalizations, (Definition 5).

Earlier, Eu et al. [4] made an explicit computation of Schultz-type indices for one family of polycyclic graphs. Indeed, for hex chains they found a general formula not only for $\mathcal{W}_+$ and $\mathcal{W}_*$, but also for the following even more generalized variations on Wiener indices analogous to the those of the Schultz-type:

**Definition 5.** Let $G$ be a connected graph and the notation same as in Definitions 1 and 2. Let $\alpha$ be a real number. Then,

$$\mathcal{W}_{\ddagger}^{(\alpha)}(G) := \sum_{\{u,v\}\in\binom{V(G)}{2}} \left[\left(\deg_G u\right)^{\alpha} + \left(\deg_G v\right)^{\alpha}\right] d_G(u,v)$$

$$\mathcal{W}_{+}^{(\alpha)}(G) := \sum_{\{u,v\}\in\binom{V(G)}{2}} \left(\deg_G u + \deg_G v\right)^{\alpha} d_G(u,v)$$

$$\mathcal{W}_{*}^{(\alpha)}(G) := \sum_{\{u,v\}\in\binom{V(G)}{2}} \left(\deg_G u\right)^{\alpha} \cdot \left(\deg_G v\right)^{\alpha} d_G(u,v).$$

Evidently, for $\alpha = 1$ the quantities $\mathcal{W}_{\ddagger}^{(\alpha)}$, $\mathcal{W}_{+}^{(\alpha)}$, and $\mathcal{W}_{*}^{(\alpha)}$ reduce to $\mathcal{W}_{+}$, $W_{+}$, and $W_{*}$, respectively. In what follows we refer to them as the GENERALIZED SCHULTZ-TYPE INDICES. An approach similar to what has been used in Ref. [4] provides a unified way to compute explicitly all these generalized Schultz-type indices for an arbitrary polygonal chain.

At this point it should be noted that any motley chain has only vertices of degree 2 or 3.

**Lemma 2** (Splitting a generalized Schultz-type index of a motley chain). Consider a motley chain and let $V_2$ and $V_3$ be the sets of its vertices of degree two and degree three, respectively. In view of the notation introduced via Definition 4, let

$$\mathcal{W}_1(G) := \mathcal{W}(V_2, V_3; G), \quad \mathcal{W}_2(G) := \mathcal{W}(V_2; G), \quad \mathcal{W}_3(G) := \mathcal{W}(V_3; G).$$

Then for all motley chains,

$$\begin{aligned}
\mathcal{W} &= \mathcal{W}_1 + \mathcal{W}_2 + \mathcal{W}_3 \\
\mathcal{W}_{\ddagger}^{(\alpha)} &= (2^{\alpha} + 3^{\alpha})\, \mathcal{W}_1 + 2 \cdot 2^{\alpha}\, \mathcal{W}_2 + 2 \cdot 3^{\alpha}\, \mathcal{W}_3 \\
\mathcal{W}_{+} &= 5\, \mathcal{W}_1 + 4\, \mathcal{W}_2 + 6\, \mathcal{W}_3 \\
\mathcal{W}_{+}^{(\alpha)} &= 5^{\alpha}\, \mathcal{W}_1 + 4^{\alpha}\, \mathcal{W}_2 + 6^{\alpha}\, \mathcal{W}_3 \\
\mathcal{W}_{*} &= 6\, \mathcal{W}_1 + 4\, \mathcal{W}_2 + 9\, \mathcal{W}_3 \\
\mathcal{W}_{*}^{(\alpha)} &= 6^{\alpha}\, \mathcal{W}_1 + 4^{\alpha}\, \mathcal{W}_2 + 9^{\alpha}\, \mathcal{W}_3.
\end{aligned}$$

We can say even more:

**Lemma 3.** Lemma 1 holds even if $d_G$ is replaced by any $f_G$ symmetric in its two arguments.

We refer to Lemma 3 as to the *Extended shelling lemma*We use it to deduce explicit formulas for generalized Schultz-type indices for any pentachain, and some useful corollaries as well.

## 4. Wiener index of pentachains, a new derivation

We first specify our notation to describe a pentachain. Let $n \in \mathbf{N}$ be a non-negative integer and $S \in \{0,1\}^n = (s_1, s_2, \ldots, s_n)$ be a binary $n$-string. Consider the motley chain

$$\left\langle 1 \; \begin{matrix} s_1 \\ 1-s_1 \end{matrix} \; \begin{matrix} s_2 \\ 1-s_2 \end{matrix} \; \begin{matrix} \cdots \\ \cdots \end{matrix} \; \begin{matrix} s_n \\ 1-s_n \end{matrix} \; 1 \right\rangle.$$

with $(n+2)$ pentagons, and denote this pentachain by $P(S)$.

Then $P(\overbrace{0\cdots0}^{n})$ will be called our "base" chain of $n+2$ pentagons, which we will shorten write as $P(0^n)$.

**Proposition 4** [1]. The minimum Wiener index for a fixed value of $n$ is

$$\mathcal{W}(P(0^n)) = (3n^3 + 39n^2 + 114n + 110)/3 = 9\binom{n}{3} + 48\binom{n}{2} + 78n + 55.$$

**Proposition 5.** [1]. For $S = s_1 s_2 \cdots s_n \in \{0,1\}^n$ being an $n$-bit string, we define

$$\begin{aligned} B = B_S &:= \{j : s_j = s_{j+1} \text{ or } j = n\} \\ \bar{j} = \bar{j}_S &:= \min\{i \geqslant j : i \in B_S\} \\ C = C_S &:= \{j : 2 \nmid (\bar{j}_S - j)\}. \end{aligned}$$

We may think of a segment 01 or 10 as zigzagging, and 00 or 11 as bending to one direction, so $B$ marks the positions that bends, and $C$ the positions that precedes an odd number (at least one) of zigzags. Given these definitions,

$$\mathcal{W}(P(S)) - \mathcal{W}(P(0^n)) = \sum_{j \notin C_S} (3j-1) \cdot 3 \binom{\frac{\bar{j}_S - j}{2}}{2} + \sum_{j \in C_S} (3j-1) \left[ 3 \left( n - \frac{1}{2}(\bar{j}_S + j - 1) \right) - 1 \right]. \quad (1)$$

*Proof.* We give a proof that is shorter and somewhat improved than the one given in Ref. [1]. Let $B = B_S = \{j_1 < j_2 < \cdots < j_k\}$. We define a sequence of strings $S := S_0,\ S_1, \ldots,\ 0^n$ or $1^n$, such that $S_i$ is created by flipping $S_{i-1}$ between the positions $j_i$ and $(j_i + 1)$:

$$\text{(the } \ell\text{th binary digit of } S_i) = \begin{cases} \text{(the } \ell\text{-th binary digit of } S_{i-1}) & \text{if } \ell \leqslant i \\ 1 - \text{(the } \ell\text{-th binary digit of } S_{i-1}) & \text{if } \ell > i. \end{cases}$$

For example, if $S = 110110$ then $S_0 = S$, $S_1 = 111001$, $S_2 = 111110$, $S_3 = 1^6$. Clearly,

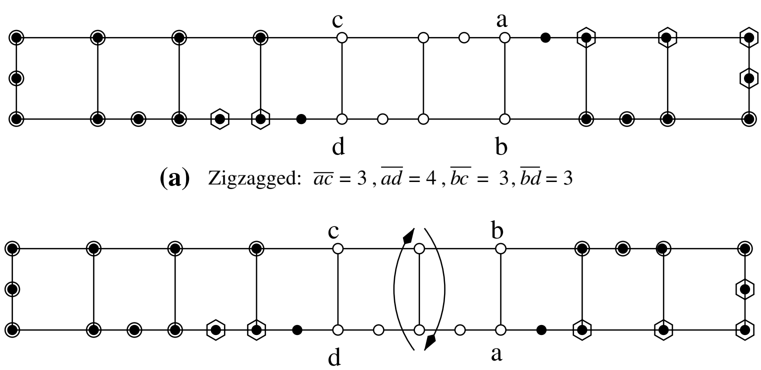
$$\mathcal{W}(P(S)) - \mathcal{W}(P(0^n)) = \sum_{i=1}^{k} \left(\mathcal{W}(P(S_{i-1})) - \mathcal{W}(P(S_i))\right).$$

We can view $P(S_i)$ as comprising $j_i + 1$ "curled" pentagons, then $\bar{\jmath} - j_i$ zigzagging pentagons, then curling to the remaining $n + 1 - \bar{\jmath}$ pentagons that may be drawn in any way (cf. figure 3).

**Claim.** We may define $j_{k+1} := n + 1$ so as to take care of the boundary case. Then for each $i$,

$$\mathcal{W}(P(S_{i-1})) - \mathcal{W}(P(S_i)) = \begin{cases} 3\left(\frac{\bar{\jmath}-j_i}{2}\right)(3j_i - 1) & \text{if } j_i \notin C_S \\ \left(3\left(n - \frac{1}{2}(\bar{\jmath} + j_i - 1)\right) - 1\right)(3j_i - 1) & \text{if } j_i \notin C_S. \end{cases}$$

This implies equation (1). To prove it, split the pentachain into left, middle (marked in white, the portion that is twisted) and right sets of vertices, then use the shelling lemma and write




**(a)** Zigzagged: $\overline{ac} = 3$, $\overline{ad} = 4$, $\overline{bc} = 3$, $\overline{bd} = 3$

**(b)** Curled: $\overline{ac} = 3$, $\overline{ad} = 4$, $\overline{bc} = 2$, $\overline{bd} = 3$

Figure 3. Changing the zigzagging after location $j_i$ to a curl.

$$\mathcal{W}(P(S)) = \mathcal{W}(\text{right side}; P(S)) + \mathcal{W}(\text{left side}; P(S)) + \mathcal{W}(\text{twisted link}; P(S)) + \mathcal{W}(\text{twisted link, right side}; P(S)) + \mathcal{W}(\text{twisted link, left side}; P(S)) + \mathcal{W}(\text{left side, right side}; P(S)). \quad (2)$$

We see that with the twisting action that we perform, only one term in equation (2) changes.

Before: $\overline{ac}=3$, $\overline{ad}=4$, $\overline{\mathbf{bc}}=\mathbf{3}$, $\overline{bd}=3$; after: $\overline{ac}=3$, $\overline{ad}=4$, $\overline{\mathbf{bc}}=\mathbf{2}$, $\overline{bd}=3$. Since in either case $\overline{ac} \leqslant \overline{ad}$ and $\overline{bc} \leqslant \overline{bd}$, we know that

**for any vertex on the left that is closer to *c* than to *d*, or equally close to *c* and to *d*, at least one shortest path to the left side of the pentachain goes through *c*.**

The result is that to the left of the twisted segment, except the one single (small, unmarked) vertex that is closer to $d$, every vertex, even one of the two vertices (marked by a hexagon) that is equidistant to $c$ and $d$, has one shortest path to the right side that runs through $c$. There is a total of $3j_i - 1$ such vertices. Similarly, we have $\overline{ac} \geqslant \overline{bc}$, $\overline{ad} > \overline{bd}$, hence

**for any vertex on the right that is closer to *b* than to *a*, or equally close to *b* and to *a*, at least one shortest path to the left side of the pentachain goes through *b*.**

So the difference is $(3j_i - 1)$ times the number of vertices to the right of the twisted segment that are either closer to $b$ or equidistant to $a$ and $b$. Three cases need to be distinguished.

1. There is at least one further zigzag following the one that is twisted back into a curl. In this case the extra point in the next pentagon is at the side of $b$ and not $a$, and it will be the single vertex that is closer to $b$ than to $a$. If $j_i \notin C_S$, then there will be $(\bar{\jmath} - j_i)/2$ pairs of pentagons zigging and zagging back and forth (with three vertices that are equidistant to $a$ and $b$ for every pair of pentagons). Eventually, there will be an extra vertex along the lower edge, and every vertex thereafter will be closer to $a$. The resulting difference is hence $(3j_i - 1) \cdot \frac{3}{2}(\bar{\jmath} - j_i)$.

2. If $j_i \in C_S$, then there will be $(\bar{\jmath} - j_i - 1)/2$ pairs of pentagons zigzagging back and forth (again with 3 vertices on the "$b$" side per pair). Eventually there will be an extra vertex along the "$a$"-side edge, and every vertex thereafter will be equidistant to $a$ and $b$. The resulting difference is hence $(3j_i - 1)\left[\frac{3}{2}(\bar{\jmath} - j_i - 1) + 3(n + 1 - j_{j+1}) - 1\right]$.

3. There may be a "curl" position directly following the "zigzag" position that is unzagged, as in figure 3a. In this situation, only one vertex (unmarked) is closer to $a$, the rest are either closer to $b$ (circled) or equidistant to $a$ and $b$ (marked by a hexagon). The resulting difference is hence $(3j_i - 1)(3(n - j_i) - 1)$.

We have proved the claim and hence the proposition. □

## 5. Generalized Schultz-type indices of a pentachain

When working with a pentachain, there is a handicap that is not present in the case of hex chains. As we bend a hex chain around, generalized Schultz-type indices of two hex chains of the same length always differ by some multiple of a fairly large integer [4]. The same phenomenon is not present at the pentachains. However, we have the following:

**Lemma 6.** For any string $S \in \{0, 1\}^n$:

$$\mathcal{W}_2(P(S)) - \mathcal{W}_2(P(0^n)) = \sum_{j \notin C_S} j \left( \frac{\bar{\jmath}_S - j}{2} \right) + \sum_{j \in C_S} j \left( n - \tfrac{1}{2} (\bar{\jmath}_S + j - 1) \right) \quad (3)$$

$$\mathcal{W}_3(P(S)) - \mathcal{W}_3(P(0^n)) = \sum_{j \notin C_S} (2j - 1)(\bar{\jmath}_S - j) + \sum_{j \in C_S} (2j - 1)\,(2n - \bar{\jmath}_S - j)\,. \quad (4)$$

*Proof.* We redraw figure 3b again with degree-3 vertices in black and degree-2 vertices in white:

We first verify the easier equation (4). It is no longer true that two pentagons whose join is twisted have no effect on $\mathcal{W}_2$ and $\mathcal{W}_3$, as is the case with $\mathcal{W}$ in the proof of Theorem 2. The reason is that the relative locations of black and white vertices now change. However, the center (the two boxed black vertices) is still an invariant section. Thus,

$$\begin{aligned} \mathcal{W}_3(P(S)) = \; & \mathcal{W}_3(\text{right side}; P(S)) + \mathcal{W}_3(\text{left side}; P(S)) + \mathcal{W}_3(\text{center}; P(S)) \\ & + \mathcal{W}_3(\text{center, right side}; P(S)) + \mathcal{W}_3(\text{center, left side}; P(S)) \\ & + \mathcal{W}_3(\text{left side, right side}; P(S)). \end{aligned}$$

When using Lemma 4, we need the function

$$f_G(x, y) = \begin{cases} d_G(x, y) & \text{if } \deg x = \deg y = 3 \\ 0 & \text{else.} \end{cases}$$

We construct $S = S_0, \ldots, S_k$ as in Proposition 5 and try to find $\mathcal{W}_3(P(S_{i-1})) - \mathcal{W}_3(P(S_i))$ by comparing each of the six terms above as we change the zigzag at location $j_i$. Again, any differences will be created in the last term only, and we can summarize those as follows:

- The distance of any vertex on the right side to the vertex $d$ does not change.
- The distance of any vertex on the left side to the vertex $a$, as well as to any deg-3 vertex on the right that is closer to $a$ than to $b$ (unmarked black vertices), does not change.

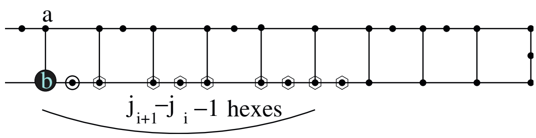



Figure 4. The case when the number of consecutive zigzags is even.

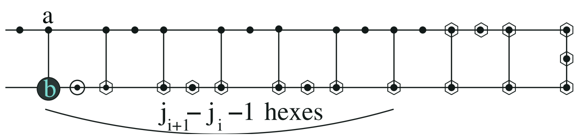



Figure 5. The case when the number of consecutive zigzags is odd.

- The distance of any black vertex on the left side (as marked, including $c$ but excluding $d$) to any black vertex on the right side that is either closer to $b$ than to $a$ (marked by a large circle), or equidistant to $a$ and $b$ (marked by a hex), decreases by 1.

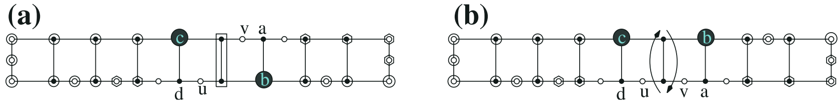
So the difference as we eliminate the zigzag after position $j_i$ is $(2j_i - 1)$ times the number of marked black vertices to the right of the twist. Again there are three cases:

- If there is a single zigzag (i.e., $\bar{j} = j_i + 1$), then we count 2 vertices for each pentagon to the right of $\overline{ab}$, which is equal to $(n - j_i)$, minus one (for $a$); cf. figure 6.
- If there is an even number of zigzags, then by inspection of figure 4 we count $\bar{j} - j_i$ vertices on the "$b$"-side that are either closer to $b$ (circled) or equidistant to $a$ and $b$ (hexed).
- If there is an odd number of zigzags, according to figure 5 we count from $(\bar{j} - j_i)$ vertices on the "$b$"-side until after the curl at position $\bar{j}$, then 2 black vertices for each of the remaining $(n - \bar{j})$ pentagons, for a total of $(2n - j_i - \bar{j})$, which is compatible with the first point above.

Summarizing the above results we get

$$\mathcal{W}_3(P(S_{i-1})) - \mathcal{W}_3(P(S_i)) = \begin{cases} (\bar{j} - j_i)(2j_i - 1) & \text{if } j_i \notin C_S \\ (n - \bar{j} - j_i)\,(2j_i - 1) & \text{if } j_i \in C_S. \end{cases}$$

and equation (4) is proved.




Zigzagged: $\overline{ac} = 3, \overline{ad} = 4, \overline{\boldsymbol{bc}} = \mathbf{3}, \overline{bd} = 3$

Curled: $\overline{ac} = 3, \overline{ad} = 4, \overline{\boldsymbol{bc}} = \mathbf{2}, \overline{bd} = 3$

Figure 6. Another view at the change of the zigzagging after location $j_i$ to a curl.

We now use the extended shelling lemma to do the same for $\mathcal{W}_2$:

$$\begin{aligned}\mathcal{W}_2(P(S)) = {}& \mathcal{W}_2(\text{right side; } P(S)) \\ & + \mathcal{W}_2(\text{left side; } P(S)) + \mathcal{W}_2(\text{twisted link; } P(S)) \\ & + \mathcal{W}_2(\text{twisted link, right side; } P(S)) \\ & + \mathcal{W}_2(\text{twisted link, left side; } P(S)) \\ & + \mathcal{W}_2(\text{left side, right side; } P(S)).\end{aligned}$$

Here, the function

$$f_G(x, y) = \begin{cases} d_G(x, y) & \text{if } \deg x = \deg y = 2 \\ 0 & \text{else} \end{cases}$$

will be used.

Twisting after location $j_i$ creates the following terms in $\mathcal{W}_2(P(S_{i-1})) - \mathcal{W}_2(P(S_i))$:

- *On the left and the right sides*none.
- *The twisted link* $+1$, as $d(u, v) = 3$ in figure 6a, but $= 2$ in figure 6b.
- *From twisted link to the left*$v$ moves 1 further away from each deg-2 vertex that is either closer to $c$ or equidistant to $c$ and $d$ (marked by white vertices). The net difference is $-(j_i + 1)$.
- *From twisted link to the right*As above, $u$ moves 1 further away from each deg-2 vertex that is either closer to $b$ or equidistant to $a$ and $b$ (marked by white vertices), so creating a net difference of -(number of marked white vertices on the right).
- *Between the left and the right sides*$+1$ for any pair that consists of exactly one deg-2 vertex on the right that is either closer to $c$ or equidistant to $c$ and $d$ (marked by white vertices on the left), and one deg-2 vertex on the left that is either closer to $b$ or equidistant to $a$ and $b$ (marked by white vertices on the left), for a total of

$$(j_i + 1)(\text{number of marked white vertices on the right}).$$

So if the number of marked white vertices on the right is $m$, then we have

$$\begin{aligned} \mathcal{W}_2(P(S_{i-1})) - \mathcal{W}_2(P(S_i)) &= 1 - (j_i + 1) - m + (j_i + 1)\, m \\ &= 2\,(m-1)\,((j_i+1)-1) = (m-1)\, j_i\,. \end{aligned}$$

In order to find $m$, we look at the same three cases as above (cf. figure 6):

- If there is a single zigzag, then we count one deg-2 (white) vertex in every pentagon after the twist (except for the one next to $a$) and three in the last pentagon, which adds up to $m = n + 1 - j_i$ pertinent vertices when $\bar{\jmath} = j_i + 1$.
- If there is an odd number of zigzags, then for every pair of zigzags, one more deg-2 (white) vertex turns closer to $a$, and we count $m = n + 1 - j_i - \frac{1}{2}(\bar{\jmath} - j_i - 1)$.
- Finally, if there is an even number of zigzags, then in an analogous manner, $m = 1 + \frac{1}{2}(\bar{\jmath} - j_i)$.

Hence we now know that

$$\mathcal{W}_2(P(S_{i+1})) - \mathcal{W}_2(P(S_i)) = \begin{cases} \frac{1}{2} j_i(\bar{\jmath} - j_i) & j_i \notin C_S \\ j_i \left[ (n + 1 - \bar{\jmath}) + \frac{1}{2}(\bar{\jmath} - j_i - 1) \right] & j_i \in C_S. \end{cases}$$

By this we have verified all of Eq. (3) and thus the proof of Lemma 6 is completed. □

By means of Lemma 6, we can find $\mathcal{W}_+ = 5\,\mathcal{W} + \mathcal{W}_3 - \mathcal{W}_2$ and $\mathcal{W}_* = 6\,\mathcal{W} + 3\,\mathcal{W}_3 - 2\,\mathcal{W}_2$, viz.:

**Lemma 7.** For straight pentachains consisting of $n + 2$ pentagons,

$$\begin{aligned} \mathcal{W}_2(P(0^n)) &= (n^3 + 39n^2 + 104n + 204)/6; \\ \mathcal{W}_3(P(0^n)) &= (2n^3 + 12n^2 + 10n + 3)/3. \end{aligned}$$

*Proof.* We do this via mathematical induction. By inspection of figure 7 it follows that:

$$f_3(n) := \sum_{x \in V_3} d(v, x) = [1 + \cdots + (n+1)] + [2 + \cdots + (n+2)] = n^2 + 4n + 3$$

$$f_2(n) := \sum_{x \in V_2} d(v, x) = [1 + \cdots + (n+3)] + (n+2) + (n+3) = \frac{1}{2}\,(n^2 + 11\,n + 22)$$

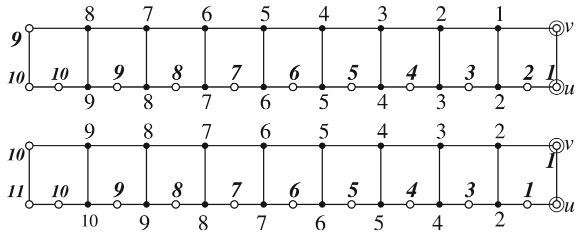


Figure 7. Distances from the leading vertices in the pentachain $P(0^n)$; (here $n = 7$).

$$g_3(n) := \sum_{x \in V_3} d(u, x) = [2 + \cdots + (n+2)] + 2 + [4 + \cdots + (n+3)] = n^2 + 6n + 6$$

$$g_2(n) := \sum_{x \in V_2} d(v, x) = 1 + 1 + [3 + \cdots + (n+3)] + (n+3) + (n+4)$$
$$= \frac{1}{2}(n^2 + 11n + 24).$$

It can be shown that the formulas given above satisfy the recurrence relations

$$\mathcal{W}_3(P(0^{n+1})) - \mathcal{W}_3(P(0^n))$$
$$= 1 + f_2(n) + g_2(n) \quad \text{(terms corresponding to } u \text{ and } v\text{)}$$
$$= n^2 + 10n + 10$$

$$\mathcal{W}_2(P(0^{n+1})) - \mathcal{W}_2(P(0^n))$$
$$= -[f_3(n) + g_3(n) - 1] \quad \text{(deduct terms for } u \text{ and } v\text{)}$$
$$+ [f_3(n+1) + g_3(n+1) - 1] \quad \text{(terms for the "new" } u \text{ and } v\text{)}$$
$$+ g_3(n) - 1 + (n+4) + 1 + 2 \quad \text{(add vertex to the right of } u\text{)}$$

the last of which simplifies to $\frac{1}{2}n^2 + 27/2\,n + 24$. □

We may combine the above with the result from Ref. [1]:

$$\mathcal{W}(P(0^n) = 55 + 78n + 48\binom{n}{2} + 9\binom{n}{3} = 55 + 57n + \frac{39}{2}n^2 + \frac{3}{2}n^3$$

by means of which we get the desired result:

**Theorem 8.** Let

$$\tilde{j}_S := \begin{cases} (\bar{j} - j)/2 & j \notin C_S \\ n - \frac{1}{2}(\bar{j} + j - 1) & j \in C_S. \end{cases}$$

Then

$$\mathcal{W}_{+}(P(S)) = 265 + \frac{952}{3}n + 116n^2 + \frac{32}{3}n^3 + \sum_{j \notin C_S} \tilde{j}_S(48j - 17) + \sum_{j \in C_S} (48j\tilde{j}_S - 17\tilde{j}_S - 17j + 6)$$

$$\mathcal{W}_{*}(P(S)) = 242 + 271n + 95n^2 + 8n^3 + \sum_{j \notin C_S} \tilde{j}_S(64j - 24) + \sum_{j \in C_S} (64j\tilde{j}_S - 24\tilde{j}_S - 24j + 9).$$

*Proof.* We can write

$$\mathcal{W}(P(S)) - \mathcal{W}(P(0^n)) = \sum_{j \notin C_S} (3j-1)(3\tilde{j}_S) + \sum_{j \in C_S} (3j-1)(3\tilde{j}_S - 1)$$

$$\mathcal{W}_2(P(S)) - \mathcal{W}_2(P(0^n)) = \sum_{j \notin C_S} j\tilde{j}_S + \sum_{j \in C_S} j\tilde{j}_S$$

$$\mathcal{W}_3(P(S)) - \mathcal{W}_3(P(0^n)) = \sum_{j \notin C_S} (2j-1)(2\tilde{j}_S) + \sum_{j \in C_S} (2j-1)(2\tilde{j}_S - 1). \square$$

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