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Zigging and Zagging in Pentachains

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We answer Ivan Gutman's open problem of systematically evaluating the Wiener indices of pentagonal chains by a compact formula. This enables speedy evaluations by hand as well as easy automated checking. The general algorithm is also suitable for treating chains involving polygons with odd number of sides other than five in general. We also obtain independent and consequent results of all-around relevance, both analogous to and widely divergent from that for hexagonal chains.

1. INTRODUCTION

DEFINITION 1 (Wiener index). For a connected graph $G = (V, E)$, we define

$$\mathscr{W} = \mathscr{W}(G) \equiv \sum_{\{u,v\} \subset V} d(u,v),$$

where $d\colon V \times V \to \mathbb{N} = \{0, 1, 2, 3, \dots\}$ is the distance function on G. For any given point u in $V = V(G)$, we also define

$$\mathscr{W}(u|G) \equiv \sum_{v \in V} d(u,v),$$

which is sometimes called the *partial Wiener index* of u (with respect to G).

This seemingly innocuous "topological index" introduced by Harold H. Wiener in 1947 and used in his seminal article [22] later proved to be strongly correlated to motley physicochemical properties of organic

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molecules and polymers of many types, including the boiling points, heats of vaporization and isomerization, specific dispersion, and surface energy of alkanes or π-electron characteristics of conjugated polymers (like total π-electron energy and HOMO–LUMO separation). In its earliest days it was called simply "the sum of topological distances," defined by counting number of carbon–carbon bonds and only for non-cyclic alkanes, where the molecular graph is nothing more complex than a tree. However, in its general form the name has stuck, even though graph theorists already have terms such as *transmission* and *gross status* (the former being twice the Wiener index).

In short, the Wiener index of a graph is the sum of all topological (graph-theoretical) distances between pairs of its vertices. Obviously we have $\mathscr{W} = \frac{1}{2}\Sigma_{u \in V}\mathscr{W}(u|G)$. Intuitively, Wiener indices are a measure of just how apart the average pair of vertices are in a graph and, hence, measure the *compactness* of the graph. Indeed, the physical properties mentioned above all depend principally on the compactness of the individual molecules, or equivalently that of its molecular graphs.

Much water has gone under the bridge and today there is a rich selection of material on the properties of Wiener indices, both mathematically and chemically, References [8, 17] should be sufficient for a background, and we also recommend for the serious student at least this limited selection of material of interest from some of the pioneers and notables in this area: [1, 2, 11, 12, 19].

The mathematical properties of Wiener numbers have been examined in some detail (see [9, 10, 16, 18, 20, and 21] for detailed treatments and useful techniques). However, for the most part the subject of systematic study has been *trees*. The Wiener indices of *linear benzenoid systems*, graphs that can be drawn as a planar figure of a chain of hexagons and have found utility in modelling several classes of conjugated polymers, is one conspicuous exception which has been studied in some depth (e.g., in [5]), and an algorithm to evaluate the Wiener index of any given linear benzenoid, while cumbersome and not easily manageable, has been known for some time (see [6, 7]). The Wiener numbers of graphs involving polygons with numbers of edges other than six, meanwhile, remains virgin territory, despite some continued interest. In fact, even the problem of systematically evaluating the Wiener indices of a graph of a fused chain of pentagons (henceforth referred to as a *pentachain*) remains open since being posed and studied by I. Gutman *et al.* some years ago. This is in stark contrast to the detailed treatments now available for benzenoid chains [14] and even two-dimensional hexagonal patterns [13]!

In Section 2, we will establish a fundamental recursion relation for Wiener indices of pentachains and discuss its similarities and differences with hex chains. In Section 3 we will use this relation to obtain some probabilistic results. In Section 4, we deduce an explicit formula for evaluating any given pentachain. Finally we will discuss some other topics and derive a few other useful results in Section 5.

2. The Fundamental Recursion

As usual, to handle the properties of something systematically requires its expression as some mathematical structure, and a pentachain is special enough that *two* such possibilities in encryption actually exists! First, we need some definitions.

Definition 2. Given any set Σ we associate with it the set of *strings* (otherwise known as the free monoid over Σ) Σ^* based on the *character set* (*or alphabet*) Σ as

$$\Sigma^* = \bigcup_{n=0}^{\infty} \Sigma^n.$$

Within Σ^* we have for each n the class of the strings of length n formed by the Cartesian product,

$$\Sigma^n = \overbrace{\Sigma \times \Sigma \times \cdots \times \Sigma}^{n},$$

and $\Sigma^0 \equiv \{\varepsilon\}$ containing only one element, the *empty string* ε. As an abbreviation we will write $S = s_1 s_2 \cdots s_n$, instead of $S = (s_1, s_2, \ldots, s_n) \in \Sigma^n$, and $S(j)$ as the jth character in S.

Concatenation on Σ^*, denoted by juxtaposition, is defined naturally via

$$(s_1 s_2 \cdots s_n)(s'_1 s'_2 \cdots s'_m) \equiv s_1 s_2 \cdots s_{n-1} s_n s'_1 s'_2 \cdots s'_m \in \Sigma^{n+m}$$

with both m and n non-zero and with the empty string as the unit element. Similarly, we define the *length*, *truncation*, and *last element* operations; i.e., for $S = s_1 s_2 \cdots s_n$ we have $|S| \equiv n$, $\tau(S) \equiv s_1 s_2 \cdots s_{n-1}$, $\lambda(S) \equiv s_n$. We will also write S^n instead of $\overbrace{SS \cdots S}^{n \text{ copies}}$ for short.

Hereafter we will be using the character set $\Sigma = \{0, 1\}$ or $\hat{\Sigma} = \{t, c\}$ ("trans" and "cis"). We augment to Σ^* an element ε' defined as of *length* -1 and get $\Sigma^\star$, the set of *extended strings* over Σ. Similarly, we augment $\hat{\Sigma}^*$ by $\mathscr{E}'$ and $\mathscr{E}''$, of length -1 and -2, to get $\hat{\Sigma}^\star$.

Definition 3 (Encryption of pentachains as strings). Given any string $S \in \Sigma^\star$ of length n, we associate with it a pentachain—a graph $P(S)$ of $(n + 2)$ concatenated pentagons in which no vertex is shared by three

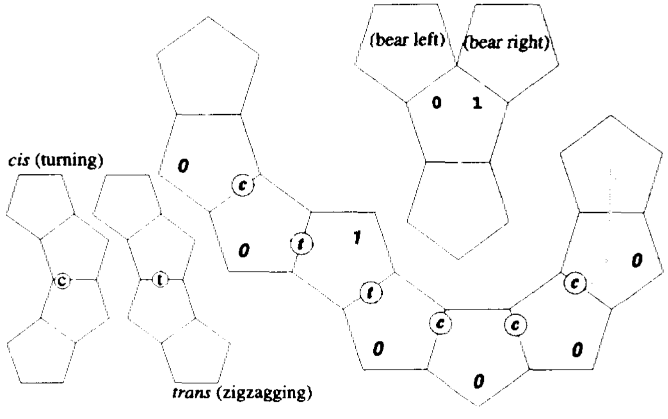

FIG. 1. Showing two encryptions of pentachains as strings.

pentagons—such that at every pentagon (see Fig. 1), except those at both ends, the direction of the "centerline" rotates 36° to the left (resp. right) if the corresponding character in the string is a 0 (resp. 1). Obviously $|P(S)| = 3|S| + 8$; i.e., a string of length n corresponds to a graph of $3n + 8$ vertices. In a similar fashion, each string $R \in \hat{\Sigma}^n$ is associated with a pentachain $\hat{P}(R)$ of $(n + 3)$ pentagons as follows: Orient the first three pentagons in any way and, starting from the *fourth* pentagon, each t (resp. c) in the string corresponds to an attachment to the existing chain segment in such a fashion that the centerline zigzags back to the *same* direction after two turns (resp. turns 72° to one side). Obviously $|\hat{P}(R)| = 3|R| + 11$.

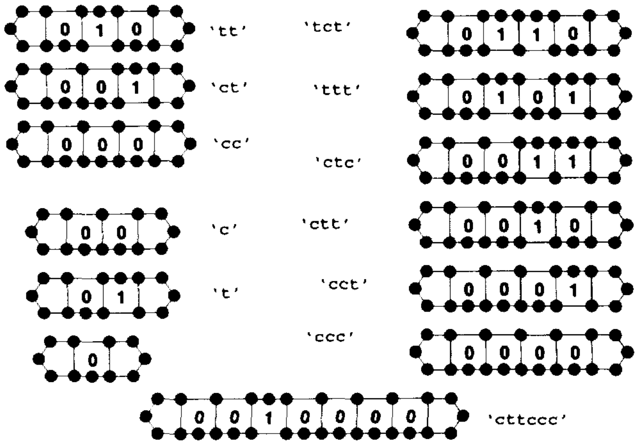

FIG. 2. Alternative way to draw pentachains.

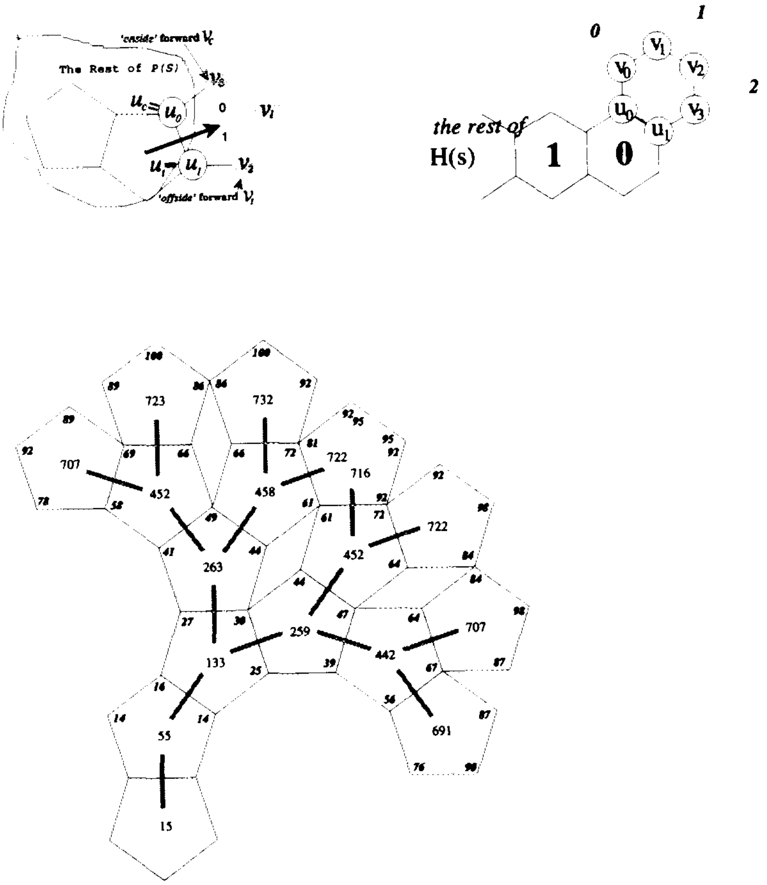

FIG. 3. Labeling of "forward" vertices and the analogy to hexchains. Also examples of the Wiener indices and partial Wiener indices for pentagonal chains of length up to 6.

Thus each string in Σ^* or $\hat{\Sigma}^*$ corresponds to a unique graph, although it is not necessary nor, in some cases, advisable, to insist on regular pentagons (which are hard to draw, among other things). Any isomorphic graph would do and an alternate depiction is given in Fig. 2.

Some properties of the encryptions defined above should by now be readily evident, especially after seeing the figures above:

1. Not all strings in Σ^* and $\hat{\Sigma}^*$ correspond to non-isomorphic graphs under the encryptions, in particular reading a string (either on Σ^* or $\hat{\Sigma}^*$) from back to front (we will term this the "reverse" string) does not change the pentachain as obtained above.

2. It may seem that $\hat{P}$ on $\hat{\Sigma}^*$ provides the more efficient representation. This is indeed correct! For each string $S = s_1 s_2 \cdots s_n \in \Sigma^n$, we can build the string $\hat{S} \in \Sigma^{n-1} \equiv r_1 r_2 \cdots r_{n-1} \in \hat{\Sigma}^{n-1}$, with r_j being c if $s_j = s_{j+1}$ and t if $s_j \neq s_{j+1}$. Obviously $P(S)$ and $\hat{P}(\hat{S})$ correspond to the same graph. If we define the "reflection" $\bar{s}$ to be 1 when s is 0 and vice versa, then the corresponding induced "reflection" on Σ^* materially changes neither the pentachain nor the corresponding string in $\hat{\Sigma}^*$.

3. That we could "save one bit" by counting the turns and zigzags, instead of right and left rotations, is a feature peculiar to pentachains and results directly from the small number of available choices. This makes calculations based on the zigs and zags hard, if not downright impossible, to generalize to other polygonal chains.

Following [14], for each $S \in \Sigma^*$ (and similarly for strings in $\hat{\Sigma}^*$; see Fig. 3) we label the *forward vertices* $v_i(S)$ and $u_i(S)$ of the graph $P(S)$ as indicated, from which notation we omit the string reference when context permits. Likewise v_- and v_+ means the "offside" and "onside," or rather the "*inside*" and "*outside*," forward vertices when necessary. For each i we denote the partial Wiener index $\mathscr{W}(v_i|P(S))$ by $\mathscr{X}_i(S)$, and the (total) Wiener index of the pentachain $P(S)$ simply as $\mathscr{W}(S)$.

Now we have the framework in which to carry out the work, and we start with a very useful fact about Wiener numbers in general.

LEMMA 1. *For any graph $G = (V, E)$ and $V' \subset V$ s.t. the distance functions on the induced subgraphs $G' = G|_{V'}$ and $G'' = G|_{V \setminus V'}$ satisfy*

$$d_{G'} = d_{G|G'}, \qquad d_{G''} = d_{G|G''}$$

(i.e., it is possible to find a shortest route between two points in either part (G' or G'') of G, without having to venture into "the other" part;) we have

$$\mathscr{W}(G) = \mathscr{W}(G') + \sum_{v \in V \setminus V'} \mathscr{W}(v|G) - \mathscr{W}(G''). \tag{1}$$

Proof.

$$\mathscr{W}(G) \equiv \sum_{\{u,v\} \subset V} d(u,v) = \left[\sum_{\{u,v\} \subset V'} + \sum_{\{u,v\} \subset V \setminus V'} + \sum_{u \in V \setminus V', v \in V'}\right] d(u,v)$$

$$= \left\{\sum_{\{u,v\} \subset V'} + \left[\sum_{u,v \in V \setminus V'} - \sum_{\{u,v\} \subset V \setminus V'}\right] + \sum_{u \in V \setminus V', v \in V'}\right\} d(u,v)$$

$$= \left[\sum_{\{u,v\} \subset V'} + \sum_{u \in V, v \in V'} - \sum_{\{u,v\} \subset V \setminus V'}\right] d(u,v)$$

$=$ R.H.S. of Eq. (1). □

LEMMA 2. *For any string $S \in \Sigma^*$ (and similarly for any string in $\hat{\Sigma}^*$) we have*

$$\mathscr{W}(S) = \mathscr{W}(\tau(S)) + \mathscr{X}_0(S) + \mathscr{X}_1(S) + \mathscr{X}_2(S) - 4. \qquad (2)$$

Proof. Take V' in this case to be all of $P(\tau(S))$, i.e., $P(S)$ minus the three points v_i, and the condition can easily be checked. Equation (2) trivially follows. □

Now we are ready to start on our main task. Obviously, if we can calculate $\mathscr{X}_i(S)$ for each i and S we can easily derive $\mathscr{W}$; we define some further notations, viz.,

$$g_0(S) = g_2(S) \equiv 3|S| + 8,$$
$$g_1(S) \equiv 6|S| + 10,$$
$$\Delta g(n) \equiv 3n + 2 = g_1(S) - g_0(S), \qquad \forall S \in \Sigma^n$$

and recursively, for $|S| = n$:

$$\phi_0(S,i) \equiv i$$
$$\phi(S,0) \equiv \lambda(S)$$
$$\phi(S,1) \equiv 2\lambda(S)$$
$$\phi(S,2) \equiv \lambda(S) + 1$$
$$\phi_{j+1}(S,i) \equiv \phi_j(\tau(S), \phi(S,i)).$$

Obviously for each (S, i) we can construct a reduction sequence (of sorts),

$$(S,i) \to (\tau(S), \phi(S,i)) \to (\tau^2(S), \phi_2(S,i))$$
$$\to \cdots \to (\varepsilon', \phi_{|S|+1}(S,i)),$$

and as we shall see, the *descent set* of (S, i), the set of the indices $j \in [n+1]$ for which $\phi_j(S, i) = 1$ will play an important role in the proceedings.

LEMMA 3(A). $\forall S \in \Sigma^n$, $a \in \Sigma$, $i = 0 \ldots 2$, *we have*

$$\mathscr{X}_i(S) = \mathscr{X}_{\phi(\lambda(S),i)}(\tau(S)) + g_i(S). \qquad (3)$$

Proof. See Fig. 4. All paths from v_0 to any point x in $P(\tau(S))$ must pass through either u_0 or u_1, but since it is shorter to get to u_1 via $v_0 \to u_0 \to u_1$ than $v_0 \to v_1 \to v_2 \to u_1$, any of the shortest routes from v_0

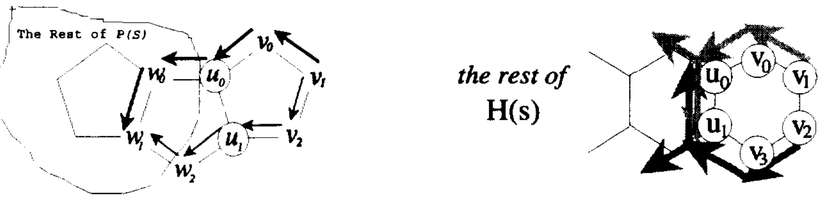

FIG. 4. Shortest paths from v_i and the analog to the hexchain case.

to x must consist of the move $v_0 \to u_0$ and a minimum-distance route to x. Thus we have

$$d(v_0, x) = d(u_0, x) + 1.$$

Similarly, we have

$$d(v_2, x) = d(u_1, x) + 1.$$

This is the *easy* part—v_1 is the hard part. Without loss of generality let us assume that $\lambda(S) = 0$ (as shown in Fig. 4); then obviously the routes $v_1 \to v_2 \to u_1 \to w_2 \to w_1$ and $v_1 \to v_0 \to u_1 \to w_0 \to w_1$ are equidistant and both are shortest routes. However, any path from v_1 into the rest of $P(S)$, i.e., $P(\tau^2(S))$, will obviously go through w_0 or w_1, which means that **for all vertices in $P(\tau(S))$ except w_2 and u_1, one shortest path proceeds via u_0.** *An identical analysis will show that if $\lambda(S) = 1$ then all points in* $P(\tau(S))$ except w_0 and u_0 have a shortest route to v_1 through u_1. What is more, for the two exceptions in each case the route through the "preferred side" is exactly one longer than is necessary. Taking into account that the number of vertices in $P(\tau(S))$ is $3|S| + 5$, we get

$$\begin{aligned}
\mathscr{X}_0(S) &= \sum_{x \in P(S)} d(x, v_0) \\
&= \sum_{x \in P(\tau(S))} (d(x, u_0) + 1) + d(v_1, v_0) + d(v_2, v_0) \\
&= \mathscr{W}(u_0(S)|P(\tau(S))) + 3|S| + 8, \\
\mathscr{X}_2(S) &= \mathscr{W}(u_1(S)|P(\tau(S))) + 3|S| + 8, \\
\mathscr{X}_1(S) &= \mathscr{W}\big(u_{\lambda(S)}(S)|P(\tau(S))\big) + 6|S| + 10,
\end{aligned}$$

Why the last equation? There are $3|S| + 5$ points in $P(\tau(S))$; all are *two* farther away from v_1 than from $u_{\lambda(S)}$, except *either* u_0 and w_0 *or* u_1 and w_2 (which are one farther away), and then there are v_0 and v_2, each of which is one away from v_1. This adds up to $2(3|S| + 5) - 2 + 2 =$

$6|S| + 10$. We then need to check that Eq. (3) does give the right answers, but we need only observe that $u_i(Sa) = v_{a+i}(S)$, and $u_{\lambda(S)}(S) = v_{2\lambda(S)}(\tau(S))$ which is quite apparent from Fig. 4 (and Fig. 3). □

Simply restated, a conspicuous difference between the pentachain case and the hexchain case is that in one, as shown on the right side of Fig. 4, v_0 and v_1 are known to be closer to u_0 and v_2 and v_3 to u_1 than the other u; in the other this is *not* true and we need to know what $\lambda(S)$ is before we know through which one of u_0 and u_1 the (majority of) paths from v_1 must go. However, despite this, we are still able to write recursion formulas that are not fundamentally different—to calculate the $\mathscr{X}$'s for each string one reduces the string by just *one* character. Furthermore, similarly to the above, we can find nice recursion formulas in the "zigzagging" form which are easily checked from the above lemma and figures.

LEMMA 3 (B). *For* $R \in \hat{\Sigma}^*$, $y \in \{t, c, 1\}$:

$$\begin{aligned} \mathscr{X}_t(R) &= \mathscr{X}_{\lambda(R)}(\tau(R)) + 3|R| + 11 \\ \mathscr{X}_c(R) &= \mathscr{X}_1(\tau(R)) + 3|R| + 11 \\ \mathscr{X}_1(R) &= \mathscr{X}_t(R) + 3|R| + 5 \\ &= \mathscr{X}_{\lambda(R)}(\tau(R)) + 6|R| + 16 \end{aligned} \tag{4}$$

and

$$\mathscr{X}_y(R) = \mathscr{X}_{\phi(\lambda(R), y)}(\tau(S)) + g_y(S), \tag{5}$$

where

$$g_c(R) = g_t(R) \equiv 3|R| + 11,$$
$$g_1(R) \equiv 6|R| + 16,$$

and, recursively,

$$\phi_0(R, y) \equiv y;$$
$$\phi(R, y) \equiv \begin{cases} \lambda(R), & \text{if } y = c \text{ or } 1; \\ 1, & \text{if } y = t. \end{cases}$$
$$\phi_{j+1}(R, y) \equiv \phi_j(\tau(R), \phi(R, y)).$$

We observe that with the recursion formulas Eqs. (2) and (3) or (4), we can (in principle) calculate whatever results we need about the Wiener indices of pentagonal chains!

3 Expected Wiener Index of Random Pentachain

Now we put the fundamental recursion formulas to some use by evaluating the expected value of the Wiener index over "random chains." Immediately, we face an interesting question. In [7] a "random" hex chain was suppose to have a fixed probability of having, at each position, an independent choice of 0, 1, and 2 (see again Fig. 3), and we *can* do the same here, having strings from Σ^n take 0 on each position (independent of other positions) with probability p and 1 with probability $q = 1 - p$. Under this assumption, if we denote the expectation $\mathscr{P}(\mathscr{X}_j(S)|(|S| = n))$ by $x_j(n)$, and $\mathscr{P}(\mathscr{W}(S)|(|S| = n))$ by $w(n)$, we then have

$$\begin{aligned} x_0(n+1) &= px_0(n) + qx_1(n) + 3n + 11 \\ x_1(n+1) &= px_0(n) + qx_2(n) + 6n + 16 \\ x_2(n+1) &= px_1(n) + qx_2(n) + 3n + 11 \\ w(n) &= w(n-1) + x_0(n) + x_1(n) + x_2(n) - 4. \end{aligned} \tag{6}$$

We can solve these difference equations in several ways. One is to use generating functions (setting $\xi_j(t) = \Sigma_n x_j(n)t^n$ then solving the resulting equations), but here we can solve the equation by straightforward decomposition thus:

$$\begin{aligned} y_0 &= p^2x_0 + pqx_1 + q^2x_2 \\ y_1 &= -\sqrt{p}\,x_0 + \left(\sqrt{p} + \sqrt{q}\right)x_1 - \sqrt{q}\,x_2 \\ y_2 &= \sqrt{p}\,x_0 + \left(-\sqrt{p} + \sqrt{q}\right)x_1 - \sqrt{q}\,x_2. \end{aligned}$$

Then, after using the initial conditions $\mathscr{X}_0(\varepsilon) = \mathscr{X}_2(\varepsilon) = 14$, $\chi_1(\varepsilon) = 16$,

$$\begin{aligned} y_0(n+1) - y_0(n) &= 3n + 11 - 6pq, \\ y_0(0) &= 14 - 12pq; \\ y_1(n+1) + \sqrt{pq}\,y_1(n) &= (3n+5)\left(\sqrt{p} + \sqrt{q}\right), \\ y_1(0) &= 2\left(\sqrt{p} + \sqrt{q}\right); \\ y_2(n+1) - \sqrt{pq}\,y_2(n) &= (3n+5)\left(-\sqrt{p} + \sqrt{q}\right), \\ y_2(0) &= 2\left(-\sqrt{p} + \sqrt{q}\right). \end{aligned} \tag{7}$$

$$y_0 = \frac{3n(n-1)}{2} + (11 - 6pq)n + (14 - 12pq)$$

$$y_1 = \left(\sqrt{p} + \sqrt{q}\right) \times \left[\left(-\sqrt{pq}\right)^{n+1} \frac{1 - 2\sqrt{pq}}{\left(1 + \sqrt{pq}\right)^2} + \frac{3n}{1 + \sqrt{pq}} + \frac{2 + 5\sqrt{pq}}{\left(1 + \sqrt{pq}\right)^2}\right]$$

$$y_2 = \left(-\sqrt{p} + \sqrt{q}\right) \times \left[\left(\sqrt{pq}\right)^{n+1} \frac{1 + 2\sqrt{pq}}{\left(1 - \sqrt{pq}\right)^2} + \frac{3n}{1 - \sqrt{pq}} + \frac{2 - 5\sqrt{pq}}{\left(1 - \sqrt{pq}\right)^2}\right].$$

And now, we can substitute back, given

$$x_0 + x_1 + x_2 = \frac{3y_0}{1 - pq} + \frac{-\left(\left(-\sqrt{p} + \sqrt{q}\right)^2\left(\sqrt{p} + \sqrt{q}\right)\right)y_1}{2\sqrt{pq}\left(1 + \sqrt{pq}\right)} + \frac{\left(-\sqrt{p} + \sqrt{q}\right)\left(\sqrt{p} + \sqrt{q}\right)^2 y_2}{2\sqrt{pq}\left(1 - \sqrt{pq}\right)}.$$

Hence,

$$\begin{aligned} w(n) - w(n-1) &= \frac{9}{2(1 - pq)}\binom{n}{2} + \left[\frac{3(11 - 6pq)}{1 - pq} + \frac{6(p - q)^2}{(1 - pq)^2}\right]n \\ &\quad + \left[\frac{3(14 - 12pq)}{1 - pq} - 4 + \frac{(1 - 13pq)(p - q)^2}{(1 - pq)^3}\right] \\ &\quad + \frac{(p - q)^2}{2(1 - pq)^3}\Big[\left(1 + \sqrt{pq}\right)^3\left(1 + 2\sqrt{pq}\right)\left(\sqrt{pq}\right)^n \\ &\qquad + \left(1 - \sqrt{pq}\right)^3\left(1 - 2\sqrt{pq}\right)\left(-\sqrt{pq}\right)^n\Big]. \end{aligned} \tag{8}$$

By carrying out a straightforward sum, we have the following.

THEOREM 1(A). *The expected Wiener index of a pentachain with random right–left turns is*

$$w(n) = 55 + \left[\frac{39 - 123pq + 128p^2q^2 - 32p^3q^3}{(1-pq)^3}\right]n$$
$$+ \left[\frac{3(11 - 21pq + 39p^2q^2)}{(1-pq)^2}\right]\binom{n+1}{2} + \frac{9}{2(1-pq)}\binom{n+1}{3}$$
$$+ \frac{(p-q)^2}{2(1-pq)^4}\Big\{\left(1+\sqrt{pq}\right)^4\left(1+2\sqrt{pq}\right)\left[1-\left(\sqrt{pq}\right)^{1+n}\right]$$
$$+\left(1-\sqrt{pq}\right)^4\left(1-2\sqrt{pq}\right)\left[1-\left(-\sqrt{pq}\right)^{1+n}\right]\Big\}. \quad (9)$$

This is somewhat easier than random hexchains! However, we *do* have another natural choice unavailable there, which is to treat a random pentachain as having a series of independent choices between *trans* (zigzag) and *cis* (turn). We consider this more meaningful, not just because the result is neater, but because the previous calculations seem to make little chemical sense, while a rough sort of *cis* and *trans* isomerism seems elegantly suited to the situation. In any case, we just show the calculations —noting, however, that we are using the *same n* as above, that is n is the number of pentagons *minus two*:

$$\begin{aligned} x_c(n+1) &= px_c(n) + qx_t(n) + 3n + 11, \\ x_t(n+1) &= x_c(n) + 6n + 13, \\ x_1(n) &= x_c(n) + 3n + 2, \\ w(n+1) &= w(n) + 2x_c(n+1) + x_t(n+1) + 3n + 1. \end{aligned} \quad (10)$$

Proceeding as before, we have (using the initial conditions)

$$x_t(n+1) - x_c(n+1) = -q\left(x_t(n) - x_c(n)\right) + 3n + 2,$$
$$\Rightarrow x_t(n) - x_c(n) = \frac{3n}{1+q} + \frac{-1+2q}{(1+q)^2}\left[1-(-q)^n\right];$$
$$qx_c(n+1) + x_t(n+1) = qx_c(n) + x_t(n) + (6q+3)n + (13q+11),$$
$$\Rightarrow qx_c(n) + x_t(n) = 3(1+2q)\binom{n}{2}$$
$$+ (11+13q)n + 14(1+q);$$

Ergo:

$$w(n) - w(n-1) = \frac{9(1+2q)}{2(1+q)}\binom{n}{2} + \left(\frac{31+40q+5q^2-13q^3}{(1+q)^2}\right)n + \left(43 - \frac{(1-2q)(2-q)}{(1+q)^3}\right) + \frac{(1-2q)(2-q)}{(1+q)^3}(-q)^n.$$

THEOREM 1(B). *The expected Wiener index of a pentachain with each stage randomly and independently chosen to be a zigzag or a turn is given by*

$$\Rightarrow w(n) = \frac{9(1+2q)}{2(1+q)}\binom{n+1}{3} + \left(\frac{31+40q+5q^2-13q^3}{(1+q)^2}\right)\binom{n+1}{2} + \left(43 - \frac{(1-2q)(2-q)}{(1+q)^3}\right)n + \frac{(1-2q)(2-q)}{(1+q)^4}\left[1+(-q)^n\right] + 55. \tag{11}$$

4. EXPLICIT EVALUATION OF WIENER INDEX OF *Any* PENTACHAIN

Now we try to find explicitly the Wiener index of a pentachain corresponding to any string in Σ^* or $\hat{\Sigma}^*$. First we find a "default" value against which we can evaluate the deviations.

THEOREM 2 (Wiener index and partial Wiener index of "coiled" pentachain).

$$\begin{aligned} \mathscr{X}_n^* \equiv \mathscr{X}_0(0^n) &= X_c(c^{n-1}) = \tfrac{1}{2}(3n^2 + 19n + 28), \\ \mathscr{X}_1(0^n) &= X_1(c^{n-1}) = \tfrac{1}{2}(3n^2 + 25n + 32), \\ \mathscr{X}_2(0^n) &= X_t(c^{n-1}) = \tfrac{1}{2}(3n^2 + 25n + 26), \end{aligned} \tag{12}$$

$$\mathscr{W}_n^* \equiv \mathscr{W}(0^n) = \mathscr{W}(c^{n-1}) = 55 + 78n + 48\binom{n}{2} + 9\binom{n}{3}. \tag{13}$$

The latter is the Wiener index of the "curly" pentagon-chain graph corresponding to the string 0^n (or 2^n), or a "coil" of just $n-1$ consecutive c's or "turns."

Proof. Directly from Eq. (3) we get

$$\mathscr{X}_0(0^n) = \mathscr{X}_0(\varepsilon') + \sum_{l=0}^{n} (3l + 8) = \tfrac{1}{2}(3n^2 + 19n + 28),$$

since $X_0(\varepsilon') = 6$. That and Lemma 3 yield Eqs. (12). Now we use Eq. (2) to get

$$\begin{aligned} \mathscr{W}(0^n) &= \mathscr{W}(0^{n-1}) + \mathscr{X}_0(0^n) + \mathscr{X}_1(0^n) + \mathscr{X}_2(0^n) + \mathscr{X}_3(0^n) - 4 \\ &= \mathscr{W}(0^{n-1}) + \tfrac{1}{2}(9n^2 + 69n + 78) \\ &= \cdots \\ &= \mathscr{W}(\varepsilon) + \frac{1}{2}\sum_{j=1}^{n} (9n^2 + 69n + 78) \end{aligned}$$

which sums out to be RHS of Eq. (13), after substituting $\mathscr{W}(\varepsilon) = 55$. □

For the rest of the section, we will assume that $S = s_1 s_2 \cdots s_n \in \Sigma^n$, $j \in [n]$, and $R \equiv \hat{S} = r_1 r_2 \cdots r_{n-1}$ and define (omitting references to strings unless the context is ambiguous):

$$B(R) \equiv B(S) \equiv \{j | r_j = c\} = \{j \in [n-1] | s_j = s_{j+1}\}.$$

$$\bar{j}(R) \equiv \bar{j}(S) \equiv \begin{cases} \min B(S) \setminus [j], & \text{if set nonempty;} \\ n, & \text{otherwise.} \end{cases}$$

$$C(R) \equiv C(S) \equiv \{j \in [n-1] | j \not\equiv \bar{j}(S) \pmod 2\}.$$

$$D_i(S) \equiv \begin{cases} C(s) \cup \{n+1\}, & \text{if } i = 1; \\ C\left(s\frac{i}{2}\right), & \text{otherwise.} \end{cases}$$

$$D_r(R) \equiv C(Rr) \qquad \text{if } r = t \text{ or } c, \text{ else } C(R) \cup \{n+1\}.$$

We note that $B(S)$ contains the same amount of information as $R = \hat{S}$—it is precisely the set of c positions in R. So obviously B determines S up to the reflection that switches the 0's with the 1's.

EXAMPLE 1. In Fig. 5 we illustrate the new concepts for the example $S = 010110$, $i = 2$, or $R = tttct$, $y = t$. As an imaginary traveller traverses the "path of reduction" $v_{\phi_l(S,i)}(\tau^l(S))$ (or $v_{\phi_l(R,i)}(\tau^l(R))$), corresponding to each stage of the recursion, we can simply draw the "reduction path" on

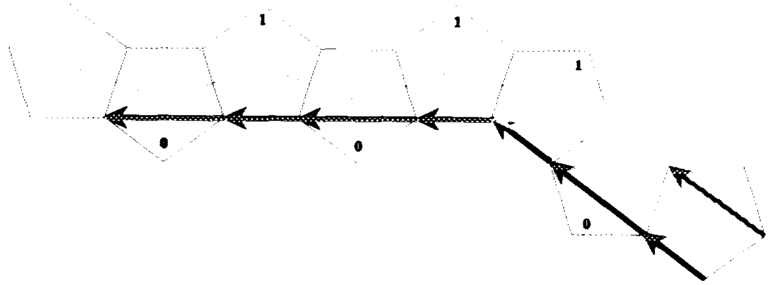

FIG. 5. The "descent set" in calculating $\mathscr{X}_2(010110)$ or $\mathscr{X}_i(tttct)$. The reduction sequence runs up the chain toward the beginning, with each "long jump" being an extra term in the final sum. The different toned arrows show the different reduction sequence starting with other values of i, and the details can be seen in Table I.

one side of the centerline (which is *never* crossed); a "long" step is taken when the next step is taken from v_1 of part of the chain. The initial location is determined by i (as shown by the two different sets of arrows). Table I sums up the illustration; with the brackets we denote things dealing with the augmentated version of S used in $D_i(S)$. The last row shows the differences (all of the form $3k - 1$) added to $\mathscr{X}^*(6)$ to get $\mathscr{X}_i(S)$.

EXAMPLE 2. We show an exaggerated example in order to give the reader some insight as to the rules of the reduction. As can be seen from the figure, when the chain is turning (coiling), all the steps are short; while it is zigzagging, the steps alternate between long and short, starting with a long one right after the last turning (c).

TABLE I
Various Concepts Illustrated by Fig. 5

j	1	2	3	4	5	6	7
S	0	1	0	1	1	0	[1]
$R = \hat{S}$	t	t	t	c	t	[t]	
$B(S)$	•	•	•		•		
$\bar{j}$	4	4	4	4	6[7]	6[7]	[7]
$C(S)$	•		•		•		
$D_i(S)$	[•]		[•]			[•]	
descent of (S, i)	•		•			•	
Δ	2		8			17	

LEMMA 4(A). *For* $S \in \Sigma^n$, $i \in \{0, 1, 2\}$ *we define* $\Delta\mathscr{X} = \Delta\mathscr{X}_i(S)$ *as* $\mathscr{X}_i(S) - \mathscr{X}_n^*$. *Then*

$$\Delta\mathscr{X} = \sum_{\substack{\phi_j(S,i)=1 \\ j=0\ldots n}} [3(n-j)+2] \tag{14}$$

$$= \sum_{j \in D_i(S)} (3j-1). \tag{15}$$

Proof. Recursively apply Eq. (3) to get

$$\begin{aligned}
\mathscr{X}_i(S) &= g_i(S) + \mathscr{X}_{\phi(S,i)}(\tau(S)) \\
&= g_i(S) + g_{\phi(S,i)}(\tau(S)) + \mathscr{X}_{\phi(\tau(S),\phi(S,i))}(\tau^2(S)) \\
&= g_{\phi_0(S,i)}(S) + g_{\phi_1(S,i)}(\tau(S)) + \mathscr{X}_{\phi_2(S,i)}(\tau^2(S)) \\
&= g_{\phi_0(S,i)}(S) + g_{\phi_1(S,i)}(\tau(S)) \\
&\quad + g_{\phi_2(S,i)}(\tau^2(S)) + \mathscr{X}_{\phi_3(S,i)}(\tau^3(S)) \\
&= \cdots \\
&= \sum_{l=0}^{n} g_{\phi_l(S,i)}(S,i) + \mathscr{X}_{\phi_{n+1}(S,i)}(\varepsilon').
\end{aligned}$$

Subtracting from the above the corresponding expansion for $\mathscr{X}_n^* = \mathscr{X}_1(1^n)$ (taking into account $X_i(\varepsilon') = 6$ irrespective of i), we get

$$\Delta\mathscr{X}_i(S) = \sum_{\substack{\phi_j(S,i)=1 \\ j=0\ldots n}} \Delta g(n-j),$$

which reduces to Eq. (14).

To get to Eq. (15), we need to know the *descent set* (please refer back to Figs. 5 and 6). From the "transition rules" of Eq. (3) (and Eq. (5)) we can see that if $j \in D$, $\phi_{n-j+1}(S, i)$ (which corresponds to the next vertex in the reduction path) will be equal to $2s_{j+1}$, and the same more or less happens at the very beginning if the start is not at v_1. Thereafter the reduction path, in the form of the value of ϕ, alternates between 1 and either 2 or 0 (always the one that corresponds to v_i) with each "zigzag" until the next element in D_i is encountered. All this, after some counting, equates to a term of $(3j + 2)$ in $\Delta\mathscr{X}_i(S)$ for each $j + 1$ in $D_i(S)$, or more precisely for each $j \in D_i$. □

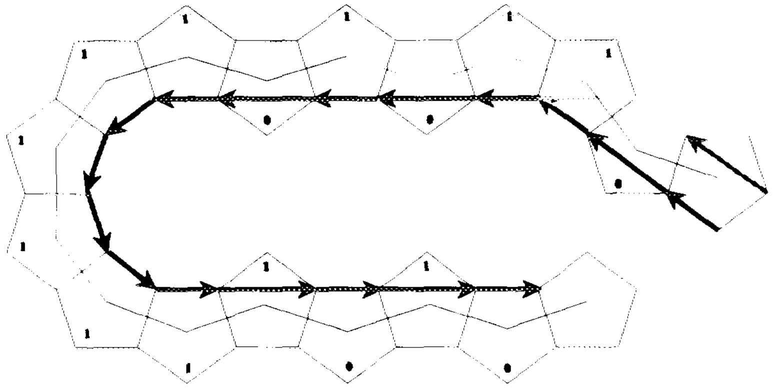

FIG. 6. "Reduction path" of $\mathscr{X}_2(0101111111010110)$, or $\mathscr{X}_t(ttccccccttttct)$.

LEMMA 4(B). *For any $R \in \hat{\Sigma}^{n-1}$ and $y \in \{t, c, 1\}$, we have via the same arguments*:

$$\Delta\mathscr{X} \equiv \Delta\mathscr{X}_y(R) = \sum_{\substack{\phi_j(R,y)=1 \\ j=0\dots n}} [3(n-j)+2] = \sum_{j\in D_y(R)} (3j-1). \quad (16)$$

EXAMPLE 3. $\Delta\mathscr{X}_2(010110)$ is seen from Table I to be $\frac{1}{2}(3\cdot 6^2 + 19\cdot 6 + 28) + 2 + 8 + 17 = 152$.

EXAMPLE 4. We tabulate the calculation of $\Delta\mathscr{X}_2(10010) = \Delta\mathscr{X}_t(tctt)$. From Table II it is easily seen to be $\frac{1}{2}(3\cdot 5^2 + 19\cdot 5 + 28) + 2 + 8 + 14 = 123$.

It remains to present our main theorem.

TABLE II

j	1	2	3	4	5	6
S	1	0	0	1	0	[1]
$R = \hat{S}$	t	c	t	t	[t]	
$B(S)$		•				
$\bar{j}$	2	2	[6]	[6]	[6]	[6]
$D_t(S)$	[•]		[•]		[•]	
Δ	2		8		14	

THEOREM 3. *Given $S \in \Sigma^n$ or $R = \hat{S} \in \hat{\Sigma}^{n-1}$ and $B, C, \bar{j}$ defined as before, we have*

$$\Delta\mathscr{W}(S) \equiv (\mathscr{W}(S) - \mathscr{W}_n^\star) = \Bigg[3 \sum_{j \in [n-1] \setminus C} (3j-1)\frac{\bar{j}-j}{2} + \sum_{j \in C} (3j-1)\left(2 + 3\left(n - \frac{j+\bar{j}+1}{2}\right)\right)\Bigg]. \quad (17)$$

Proof. From Eqs. (3) and (15) we again proceed recursively:

$$\begin{aligned}
\mathscr{W}(S) - \mathscr{W}(0^n) &= \mathscr{W}(R) - \mathscr{W}(c^{n-1}) \\
&= [\mathscr{W}(\tau(R)) + (\mathscr{X}_c(S) + \mathscr{X}_1(S) + \mathscr{X}_t(S)) - 4] \\
&\quad -[\mathscr{W}(c^{n-2}) + (\mathscr{X}_c(c^{n-1}) \\
&\qquad + \mathscr{X}_1(c^{n-1}) + \mathscr{X}_t(c^{n-1}) - 4] \\
&= \cdots \\
&= \sum_{l=0}^{n-1} [\mathscr{X}_c(\tau^l(R)) - \mathscr{X}_c(c^{n-l-1}) + \mathscr{X}_1(\tau^l(R)) \\
&\qquad - \mathscr{X}_1(c^{n-l-1}) + \mathscr{X}_t(\tau^l(R)) - \mathscr{X}_t(c^{n-l-1})] \\
&= \sum_{l=1}^{n} \Bigg\{2 \sum_{j \in C(s_1 s_2 \ldots s_l)} (3j-1) \\
&\qquad + \sum_{j \in C(s_1 s_2 \ldots s_{l-1})} (3j-1)\Bigg\}.
\end{aligned}$$

The last equality need some explanation. It is clear that

$$\begin{aligned}
\mathscr{X}_{\bar{s}_n}(S) - \mathscr{X}_2(0^n) &= \mathscr{X}_t(R) - \mathscr{X}_t(c^{n-1}) \\
&= \sum_{j \in C(\tau(R))} (3j-1) \\
&= \sum_{j \in C(\tau(S))} (3j-1),
\end{aligned}$$

since $\Delta\mathscr{X}_t(R)$ is just $\Delta\mathscr{X}_c(\tau(R)) + (3n-1)$ and $\Delta\mathscr{X}_t(c^{n-1})$ is just $3n-1$.

The coefficient of $3j-1$ in $\Delta\mathscr{W}(S)$, where $j \in [n-1]$, can thus be determined by a simple counting argument. It is easy to see that for $j \in [n-1] \setminus C(S)$ exactly half the terms with $j < l \leq \bar{j}$ would contain $(3j-1)$, and hence the first term on the right of Eq. (17). Similarly, for $j \in C$ we would have the factor $3(n - (j + \bar{j}(S) - 1)/2$, except for the

TABLE III

j	1	2	3	4	5	6
S	0	1	0	1	1	0
R	t	t	t	c	t	
$B(S)$				•		
$\bar{j}$	4	4	4	4	6	6
$C(S)$	•		•		•	
Δ	11×2	3×5	8×8		2×14	

fact that one term of $3j - 1$ is cancelled; hence we have the second term on the RHS of Eq. (17). □

EXAMPLE 5. We demonstrate how to calculate $\mathscr{W}(010110) = \mathscr{W}(tttct)$. As shown by Table III it is indeed $\mathscr{W}_6^* + (2 \times 14 + 8 \times 8 + 3 \times 5 + 11 \times 2) = 1552$.

COROLLARY 1. $\mathscr{W}(S) \equiv 1 + |C(S)| \pmod 3$.

Proof. Noting that $\mathscr{W}^* \equiv 1 \pmod 3$ and that each element in C corresponds to a term that is also $\equiv 1 \pmod 3$, this is quite clear. □

5. DISCUSSION

THEOREM 4 (Monotonicity of Wiener indices). *If $R, R' \in \hat{\Sigma}^{n-1}$ are identical except at the jth position, where the former has c and the latter has t, then $\mathscr{W}(R) \leq \mathscr{W}(R')$. If in R' the "run" of t's around the jth position starts from the hth to the $(k-1)$th positions, then*

$$\mathscr{W}(R') - \mathscr{W}(R) = \begin{cases} 3\left(\dfrac{j-h+1}{2}\right)\left[2 + 3\left(n - \dfrac{j+k+1}{2}\right)\right], & j-h \text{ odd}, k-j \text{ odd}; \\ \left(3\dfrac{j+h}{2} - 1\right)\left[2 + 3\left(n - \dfrac{j+k+1}{2}\right)\right], & j-h \text{ even}, k-j \text{ odd}; \\ 9\left(\dfrac{k-j}{2}\right)\left(\dfrac{j-h+1}{2}\right), & j-h \text{ odd}, k-j \text{ even}; \\ 3\left(3\dfrac{j+h}{2} - 1\right)\left(\dfrac{k-j}{2}\right), & j-h \text{ even}, k-j \text{ even}; \end{cases} \tag{18}$$

An easy-to-remember way to think of the above is that each side of the cutpoint j corresponds to a factor which is either half again as much the distance between the cutpoint and the nearest c, if that distance is even, or two plus half again as much the distance between the endpoint and the midpoint of the cutpoint and the nearest c, if not.

Proof. We consider the expansions of $\Delta\mathscr{W}(R)$ and $\Delta\mathscr{W}(R')$ according to Eq. (17). First we assume $k - j$ to be odd, which means that $C(R')$ contains $j, j-2, j-4, \ldots$ down to h and $C(R)$ contains $j-1, j-3, \ldots$. Then Eq. (17) gives

$$\mathscr{W}(R') - \mathscr{W}(R) = \Delta\mathscr{W}(R') - \Delta\mathscr{W}(R) = \sum_{i=h}^{j} (a_i - b_i),$$

where

$$a_i = \begin{cases} \left[2 + 3\left(n - \dfrac{k+i+1}{2}\right)\right](3i-1), & j-i \text{ even}, \\ 3\left(\dfrac{k-i}{2}\right)(3i-1), & j-i \text{ odd}; \end{cases}$$

$$b_i = \begin{cases} 3\left(\dfrac{j-i}{2}\right)(3i-1), & j-i \text{ even}, \\ \left[2 + 3\left(n - \dfrac{j+i+1}{2}\right)\right](3i-1), & j-i \text{ odd}; \end{cases}$$

$$a_i - b_i = (-1)^{j-i}\left[2 + 3\left(n - \frac{k+j+1}{2}\right)\right](3i-1).$$

Since each positive term and the following negative term adds up to $3[2 + 3(n - (k+i+1)/2)]$, the result follows in a straightforward fashion by cancellation.

If $k - j$ is even, we can see that $C(R) = C(R')$; only the j's change so we have unchanged b_i, and

$$a_i = \begin{cases} 3\left(\dfrac{k-i}{2}\right)(3i-1), & j-i \text{ even}, \\ \left[2 + 3\left(n - \dfrac{k+i+1}{2}\right)\right](3i-1), & j-i \text{ odd}; \end{cases}$$

$$a_i - b_i = (-1)^{j-i} \cdot 3\left(\frac{k-j}{2}\right)(3i-1);$$

and the same cancellations follow. Note the symmetry if one changes j to

$n-j$, k to $n-h+1$, h to $n-k+1$, which is to be expected from the intrinsic symmetry of the encryption with respect to order-reversals of strings. □

With the above we can obtain in short order the following theorem about the extrema of Wiener indices with a given, fixed length.

THEOREM 5 (Extremum Wiener indices with fixed-length chains). $\min\{\mathscr{W}(S): |S| = n\} = \mathscr{W}_n^*$; *the minimum occurs at* $S = 0^n$ *or* 1^n (*i.e.*, $\hat{S} = c^{n-1}$). *The second minimum is* $\mathscr{W}_n^* - 2(3n-4) = 55 + 78n + 48\binom{n}{2} + 9\binom{n}{3}$ *and occurs at* $\hat{S} = c^{n-2}t$ *or* $= tc^{n-2}$ (*i.e.*, $S = 01^{n-1}$ *or similar*). *The maximum Wiener index for the same fixed length* $(n+2)$ *occurs only at* $S = 0101\ldots$ *or* $S = 1010\ldots$ (*i.e.*, $\hat{S} = t^{n-1}$), *and*

$$\max\{\mathscr{W}(S): |S| = n\} = \begin{cases} 55 + 208l + 261\binom{l}{2} + 108\binom{l}{3}, & n = 2l; \\ 133 + 325l + 315\binom{l}{2} + 108\binom{l}{3}, & n = 2l+1. \end{cases} \tag{19}$$

The second maximum of $\{\mathscr{W}(S): |S| = n\}$ *equals*

$$\begin{matrix} 57 + 202l + 261\binom{l}{2} + 108\binom{l}{3}, & n = 2l; \\ 133 + 319l + 315\binom{l}{2} + 108\binom{l}{3}, & n = 2l+1; \end{matrix} \tag{20}$$

and it occurs at $\hat{S} = t^{n-2}c$ *or* $= ct^{n-2}$ (*i.e.*, $S = 001010\ldots$, *or similar*).

Proof. Since $\hat{S} = c^{n-1}$ corresponds to $\Delta\mathscr{W} = 0$ and anything else corresponds to a positive $\Delta\mathscr{W}$, the first part should be obvious, and since the second minimum cannot occur at a string with more than one t in it a little work confirms that part. Since the maximum $\mathscr{W}$ corresponds to the maximum $\Delta\mathscr{W}$, we need not do anything more to prove the third statement. The last can be obtained by a comparison of all the strings with exactly one c and finding the largest; the formula is the result. □

If one refers to the formulas in [14] one can see that the situation for pentachains is different from that of hexchains, indeed, any chain of even- or odd-sided polygons, because five is the smallest number of edges for which alternatives in formation are possible.

In fact, one can see that Eq. (18) above refers to changing a pentachain by reversing one segment of the chain entirely, flipping it to the other side.

To obtain a formula for *rotating* one part left-to-right or vice versa is harder and must be done via two flips—this corresponds to the fact that if S and S' in Σ^* differ by exactly one internal character (not at either end) then $\hat{S}$ and $\hat{S}'$ differ by *two* characters.

The other use for which one could conceivably employ Eq. (17) is, of course, repetitive patterns in chains, just as we did in [14]. However, we will not bother carrying out the calculations here. The cases where the repetition is taken in terms of strings in Σ^* and $\hat{\Sigma}^*$ must be treated differently, and a lot of specific adjustments for the correction effects at the two ends is simply too untidy for us to go into. However, the tools presented so far should enable easy calculation for each specific case should any repetitive patterns be encountered.

We would like to bring the reader's attention to one more thing: in theory all chains involving odd-sided polygons, not necessarily all the same, can be treated with the same algorithm as detailed in Section 2. In short, it is only the details that will be different (and much more complex and untidy).

Finally, as a further extension of the material covered here, we wish to point out that the Wiener polynomials of arbitrary polygonal chains may be obtained by the same principle used in Sections 2 and 3, and it is just possible that we will eventually be able to deduce a similarly compact formula.

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