Wiener Polynomials of Some Chemically Interesting Graphs

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Received 25 March 2003; accepted 14 January 2004
Published online 28 April 2004 in Wiley InterScience (www.interscience.wiley.com).
DOI 10.1002/qua.20100

ABSTRACT: The chemist Harold Wiener found $\mathcal{W}(G)$, the sum of distances between all pairs of vertices in a connected graph G, to be useful as a predictor of certain physical and chemical properties. The q-analogue of $\mathcal{W}$, called the Wiener polynomial $\mathcal{W}(G; q)$, is also useful, but it has few existing useful formulas. We will evaluate $\mathcal{W}(G; q)$ for certain graphs G of chemical interest. Int J Quantum Chem 99: 80–91, 2004

Key words: Wiener polynomial; polygonal chains; hexagonal carpets; AMS Classification: combinatorics (05)

1. Introduction

A structural formula in organic chemistry corresponds naturally to a connected graph, each non-hydrogen atom to one vertex. The distance between vertices corresponds to the number of bonds between two atoms, which influences physical and chemical properties quantum mechanically. In 1947, Harold Wiener proposed a formula [1] for boiling points of alkanes, after some heuristic reasoning:

$$\text{b.p.} = \alpha\mathcal{W} + \beta w_3 + \gamma \tag{1}$$

where (we quote) "$\mathcal{W}$ is the sum of distances and w_3 the number of pairs of vertices three apart." As the correlation was surprisingly good, he published a few more papers on the same topic. $\mathcal{W}$ was rediscovered during the 1970s, and in time the mathematical properties were probed in some detail; the most notable result of this period was the Merris–McKay theorem relating Wiener numbers to eigenvalues of trees [2]. Descriptions of its applications have abound in the literature since, numbering hundreds of articles. "Topological indices"—the chemists' term for a function on a graph—in general, as well as their applications, are discussed in chemical texts (e.g., [3–5]), surveys on Wiener numbers and their applications, and so forth, can be

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Contract grant sponsor: National Science Council.
Contract grant number: NSC89-2115-M-001-024.

found in refs. [4, 6–8]; other treatments may be found in refs. [9–22].

We hasten to mention that whether the Wiener index is a good indicator for all compounds remains controversial. Some experts have suggested that the Wiener index is not suitable for prediction or, at least, that it can be improved. Ivan Gutman [23] proposed the Szeged (Sz) index as an extension of the Wiener index to cyclic structures, in which pairs of equidistant vertices in a cycle may have its contribution canceled out, to reflect certain quantum mechanical realities. This particular index attracted considerable attention, although, again, its value is a subject of dispute i.e., as recently as 2002, Randić [24] presented evidence pointing toward the use of a new index, which we might tentatively call the Randić index, which included halved contributions instead of full or canceled contributions. As these debated issues remain unresolved, we restrict our attention to the Wiener index, the "elder statesman" of indices.

It is natural to consider generating functions ("counting polynomials") when studying something in a combinatorial structure in aggregate; a direct extension of Wiener's idea was mentioned earlier by Haruo Hosoya, and formalized as well as investigated in some detail by Sagan and Yeh.

Definition 1 [15, 25]. Let $d_G : V \times V \to \mathbb{N}$ be the function representing the minimal distance between vertices of the connected graph $G = (V, E)$. We shall write $\mathbb{N}$ for the set of non-negative integers and $\mathbb{P}$ positive ones in this article; other notations for convenience we will use are u for the singleton set $\{u\}$, and d for d_G when confusion is unlikely. The counting polynomial of distances on G, the Wiener polynomial of G, is

$$\mathcal{W}(G; q) \equiv \sum_{\{u,v\} \in \binom{V}{2}} q^{d_G(u,v)};$$

we also define $\mathcal{W}(u|G; q) \equiv \sum_{v \in V} q^{d_G(u,v)}$ and $\mathcal{W}(S_1, S_2|G; q) \equiv \sum_{u \in S_1, v \in S_2} q^{d(u,v)}$. These are q-analogues of $\mathcal{W}(G)$, $\mathcal{W}(u|G)$, and $\mathcal{W}(S_1, S_2|G; q)$ [26]. Each quantity relate to its q-analogue in the usual manner, e.g., $\mathcal{W}(G) = (d/dq)\mathcal{W}(G; q)|_{q=1}$.

Like most generating functions, Wiener polynomials have some independent interest: an example [25] is its linking the absolute Poincaré polynomials of a Coxeter group and its induced graph. Knowing how to compute Wiener polynomials would also yield Wiener's "polarity number" w_3. Wiener number laid dormant for a decade and a half before being rediscovered at least partly, due to the scarcity of efficient formulas for w_3 in chemically interesting graphs. There are a few other practical situations in which points at a given distance need to be counted.

Wiener polynomials of simple graphs are well known:

$$\mathcal{W}(C_{2n}; q) = n\left[\frac{(q+1)(q^n-1)}{q-1} - 1\right]; \quad (2)$$

$$\mathcal{W}(C_{2n+1}; q) = (2n+1)q\,\frac{q^n-1}{q-1}; \quad (3)$$

$$\mathcal{W}(P_n; q) = \sum_{j=1}^{n-1} (n-j)q^j = \frac{q(q^n-1)}{(q-1)^2} - \frac{nq}{(q-1)}. \quad (4)$$

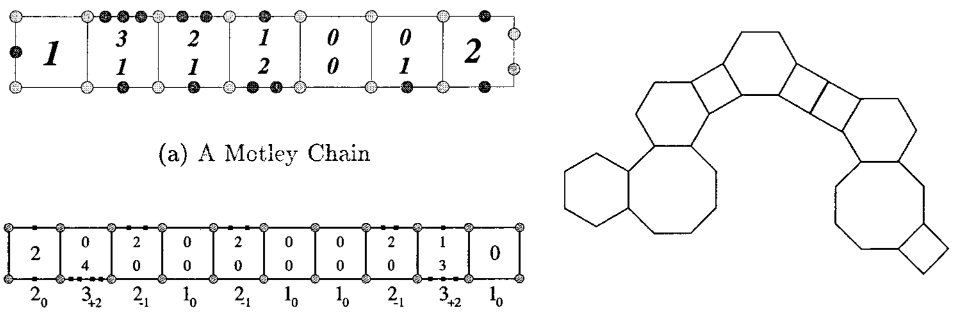
Sagan et al. [25] discussed certain relationships that allow us to construct Wiener polynomials of graphs formed by some binary operations from simpler graphs, such as paths P_n and cycles C_n. The most useful of these relations pertain to the Cartesian product:

$$\mathcal{W}(G \times H; q) = 2\mathcal{W}(G; q)\mathcal{W}(H; q) + |V(H)|\mathcal{W}(G; q) + |V(G)|\mathcal{W}(H; q).$$

In particular, for the $m \times n$ chessboard $Cb_{m,n} \equiv P_m \times P_n$:

$$\mathcal{W}(Cb_{m,n}; q) = \frac{[2q(q^m-1) - m(q^2-1)][2q(q^n-1) - n(q^2-1)]}{2(q-1)^4} - \frac{mn}{2}. \quad (5)$$

The authors [8, 26–28] have presented ways to compute Wiener numbers, and occasionally polynomials, for some chemically useful graphs. However, the computation of Wiener polynomials often presents taller obstacles than when dealing with Wiener numbers, where neat formulas often result by cancellation. When manipulating generating functions, this can become difficult to impossible.



(a) A Motley Chain

(b) An Even Motley Chain

(c) Another rendering of (b), depicting a real compound

FIGURE 1. Chains of motley gems.

For example, this elegant result is not easily generalizable, as shown by Proposition 1.

Proposition 1 (Merris [2]). Let $A(T)$ be the adjacency matrix of the tree T and $D(T)$ be the diagonal matrix of the same size with the degree as the entry corresponding to each vertex. The Laplacian matrix $L(T)$ is defined as $D(T) - A(T)$. Merris showed that

$$\mathscr{W}(T) = |V(T)| \sum \frac{1}{\lambda},$$

where λ ranges over all eigenvalues of $L(T)$.

In Section 2, we will treat the problem of how to compute Wiener polynomials of polygonal chains; these graphs ("motley chains") are the abstractions of aromatic compounds and their Wiener numbers and polynomials are of significant interest. In Section 3, we will deal with Wiener polynomials for some regular two-dimensional (2D) hexagonal patterns. These graphs ("hex carpets") depict slices of graphite.

2. Wiener Polynomials of Polygonal Chains

Definition 2 [29]. A motley chain is a graph of concatenated, or edge-sharing, polygons. Given n ordered pairs of non-negative integers $S = (a_1, b_1), \ldots, (a_n, b_n)$, we may create a graph as follows: take the graph $Cb_{2,n+1} = P_2 \times P_{n+1}$ and subdivide the upper and lower edges by inserting a_j and b_j extra vertices, respectively (see Fig. 1). The resulting graph is the motley chain associated with S. Because only $a_1 + b_1$ and $a_n + b_n$ matters, we will denote equivalence classes as:

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

When each cycle is of even order, as in Figure 1(b), we call it an even motley chain. Let integers k_i and j_i satisfy $|j_i| < k_i$, $i = 1 \cdots n$, then we write

$$E = k_0(k_1)_{j_1}(k_2)_{j_2} \cdots (k_n)_{j_n} k_{n+1}$$

as a representation for the even motley chain in which the ith polygon has $2(k_i + 1)$ vertices, of which $k_j + j_i + 1$ are along the lower edge, or $2j_i$ more than those along the upper edge. For obvious reasons, k_i is called the length of the ith cell. $\mathscr{K} \equiv \sum_{j=0}^{n+1} k_j$ is the total length of the chain.

It is useful to compare a "straight" $E_0 = k_0 k_1 \cdots k_{n+1}$ even motley chain (all the j_i's are 0) to $P_{\mathscr{K}+1} \times P_2$ (a chain of $\mathscr{K}$ squares). Noting that when any $2k + 2$-gon is cut into k squares (Figure 2), the distances between other vertices do not change, and using Eqs. (2) and (5), we obtain Proposition 2.

Proposition 2 [8]. The Wiener polynomial of the straight even motley chain E_0 to be (independent of the order of the polygons):

$$\mathscr{W}(E_0; q) = \mathscr{W}(Cb_{\mathscr{K}+1,2}) + \sum_j \frac{q+1}{q-1} \times \left[(k_j - 1)q \frac{q^{k_j+1} - 1}{q-1} - (k_j + 1)q^2 \frac{q^{k_j-1} - 1}{q-1} \right]. \quad (6)$$

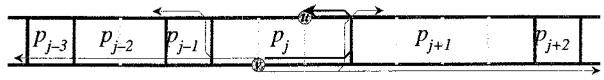


FIGURE 2. Evaluating Wiener polynomials of straight even motley chains.

The general idea will be to start with $E_0 = k_0 k_1 k_2 \cdots k_n k_{n+1}$, which is $E = k_0 (k_1)_{j_1} (k_2)_{j_2} \cdots (k_n)_{j_n} k_{n+1}$ with every kink straightened out, and to morph it into E, one rotation at a time, starting from the left: the lth step in the process is rotating the i_lth polygon from being "straight" into the "bent" position specified by $(k_{i_l})_{j_l l}$. But first we need the generally useful result shown in Proposition 3.

Proposition 3 (Shelling lemma [8]). Let $G = (V, E)$ be a connected graph, and partition its vertex set V into $V_0 \uplus V_1 \uplus V_2 \uplus \cdots \uplus V_k$ in such a way that the restriction of $d_G \equiv d$ to $G_j \equiv G|_{V_j}$ is the same as d_{G_j} (hence, each V_j is connected). Also let $\mathcal{G}_j$ be the subgraph induced by $\uplus_{i=1}^{j} V_j$, then

$$\mathcal{W}(G; q) = \sum_{j=0}^{k} \mathcal{W}(G_j; q) + \sum_{0 \le i < j \le K} \mathcal{W}(G_i, G_j; q)$$

$$= \mathcal{W}(G_0; q) + \sum_{j=1}^{k} \left[\sum_{u \in V_j} \mathcal{W}(u|\mathcal{G}_j; q) - \mathcal{W}(G_j; q) - |V_j| \right]. \quad (7)$$

The portion of the chain to the left of a bend will be the "residue" R, and the remaining straight portion on the right the "tail" T. Now introduce just one bend (nonzero j) into a straight chain, so that R is also straight.

Lemma 4. Let there be only the one bend $(k_i)_{j_i}$ (see Fig. 3), where $i = i_1$ is the only index corresponding to nonzero j_i. Then

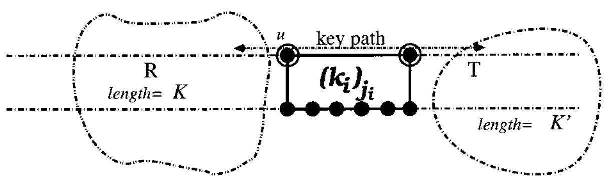


FIGURE 3. Changes after one rotation.

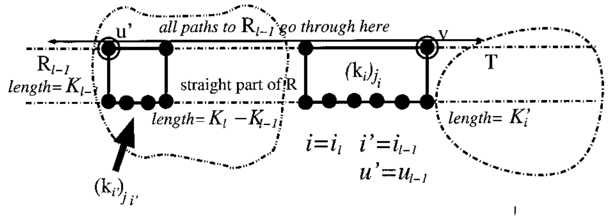


FIGURE 4. Two segments of *R*.

$$\mathcal{W}(E_0; q) - \mathcal{W}(E; q) = q^{k_i+2-|j_i|}(q+1) \times (2q^{|j_i|} - q - 1)\frac{q^{K'}-1}{q-1}\frac{q^K-1}{q-1},$$

where K and K' are the length of R and T, respectively.

Proof. Use Proposition 3 with R, the polygon of the bend, and T as the parts. When we rotate the ith polygon only the distances from R to T change. These distances originally contribute the following sum to the Wiener polynomial:

$$2(q+1)q^{k_i+2}\left(\frac{q^K-1}{q-1}\right)\left(\frac{q^{K'}-1}{q-1}\right),$$

which now becomes (all pertinent distances going through the marked path):

$$(q+1)^2 q^{k_i+2-|j_i|}\left(\frac{q^K-1}{q-1}\right)\left(\frac{q^{K'}-1}{q-1}\right).$$

Before we proceed, we need to tidy up some notations:

$$K_l \equiv \sum_{h=0}^{i_l-1} k_h, \qquad K_l' \equiv \sum_{h=i_l+1}^{n+1} k_h,$$

$$\hat{\jmath}_l \equiv \begin{cases} |j_{i_l}|, & \text{if } j_{i_l} j_{i_{l-1}} > 0, \\ |j_i| - 1, & \text{if } j_{i_l} j_{i_{l-1}} < 0 \\ 0 & \text{else.} \end{cases} \qquad L_l \equiv K_l - \sum_{h=0}^{l-1} (\hat{\jmath}_h)$$

As we shall see, K_l and K_l' are the sizes of leading and tail partial chains ($K_0 \equiv 0$). $\hat{\jmath}_l$ represent the "kink" at the i_lth polygon, and L_l is the "true" length of the leading partial chain. Now, to account for more than one bend or kink in a chain (see Fig. 4). For each bend $(k_{i_l})_{j_l l}$, let u_l be the top vertex between the $(i_l - 1)$th polygon (and the rest of the remaining chain R_l) to the i_l-th polygon if $j_l > 0$, and the bottom vertex if $j_l < 0$. Also let $\mathcal{X}_l(q) \equiv \mathcal{W}(u_l|R_l; q)$, which we will need later, in lemma 5.

Lemma 5.

$$\mathcal{W}(E_0; q) - \mathcal{W}(E; q) = \sum_l (q+1)\left(\frac{q^{K_l'}-1}{q-1}\right) \times \left\{\left(\frac{q^{K_l-K_{l-1}}-1}{q-1}\right)q^{k_{i_l}+2-|j_{i_l}|}(2q^{|j_{i_l}|}-q-1) + (q^{K_l-K_{l-1}} - q^{K_l-K_{l-1}-\hat{j}_{i_l}})\frac{\mathcal{X}_{l-1}(q)}{q}\right\}. \quad (8)$$

Proof. In general, the residue R_l bends, but comprises one straight segment (effectively two paths of length $K_l - K_{l-1}$) attached to the lth bend, and a remainder $R_l - 1$ beyond it. Use the Shelling lemma with the polygons at the kinks and the straight segments in between as the parts. So the lth rotation decrease the Wiener polynomial by

$$q^{k_{i_l}+2-|j_{i_l}|}(q+1)(2q^{|j_{i_l}|}-q-1)\frac{q^{K_l'}-1}{q-1}\frac{q^{K_l-K_{l-1}}-1}{q-1} + \quad (\text{contribution from } R_{l-1}).$$

The term involving R_{l-1} can be deduced thus: any shortest path from T into R_{l-1} must traverse the path $\overline{uv}$. So the partial Wiener sum starts out as (again, using the Shelling lemma)

$$\mathcal{W}(u_{l-1}|R_{l-1}; q)\cdot q^{K_l-K_{l-1}-|j_{i_{l-1}}|+k_{i_l}+1}\cdot(q+1)\frac{q^{K_l'}-1}{q-1},$$

and is scaled down by a factor of $q^{\hat{j}_i l}$, where $\hat{j}$ is the kink defined earlier.

Now we are ready for the finale, shown in Theorem 6.

Theorem 6. Let $E = k_0(k_1)_{j_1}(k_2)_{j_2}\cdots(k_n)_{j_n}k_{n+1}$ be an even motley chain, with exactly $j_{i_1}, j_{i_2}, \ldots, j_{i_m}$ nonzero among all the j_i. With notations as above, the Wiener polynomial of E is given by:

$$\mathcal{W}(E; q) = \mathcal{W}(Cb_{\mathcal{K}+1,2}; q) + \sum_j \frac{q+1}{q-1} \times \left[(k_j-1)q\frac{q^{k_j+1}-1}{q-1} - (k_j+1)q^2\frac{q^{k_j-1}-1}{q-1}\right]$$

$$-\sum_l (q+1)\left(\frac{q^{K_l'}-1}{q-1}\right)\left\{\left(\frac{q^{K_l-K_{l-1}}-1}{q-1}\right)q^{k_{i_l}+2-|j_{i_l}|} \times (2q^{|j_{i_l}|}-q-1) + (q+1)(q^{K_l-K_{l-1}}-q^{K_l-K_{l-1}-\hat{j}_l}) \times \left[\frac{q^{L_{l-1}}-1}{q-1} + \sum_{h=1}^{l-2} q^{L_{l-1}-L_h}\left(\frac{q^{\hat{j}_h}-1}{q-1}\right)\right]\right\}. \quad (9)$$

From Eq. (9), we can deduce all previous results about Wiener numbers and polynomials of an even motley chain; actually, Eq. (8) suffices when we note that there are $2K_l$ vertices in R_l and hence that many terms in $\mathcal{X}_l(q)$.

Proof. We still need to find $\mathcal{X}_i(q)$. First, we look at a few diagrams. As for hex chains, it is easy to see that

$$\mathcal{X}_i^*(q) = q(q+1)\left(\frac{q^{K_i}-1}{q-1}\right).$$

When the chain develops a kink, the chain effectively became shorter. Note that the upper and lower edges differ, due to the starting location u (which is on top or bottom when j_i is positive or negative, respectively). $\mathcal{X}$ becomes

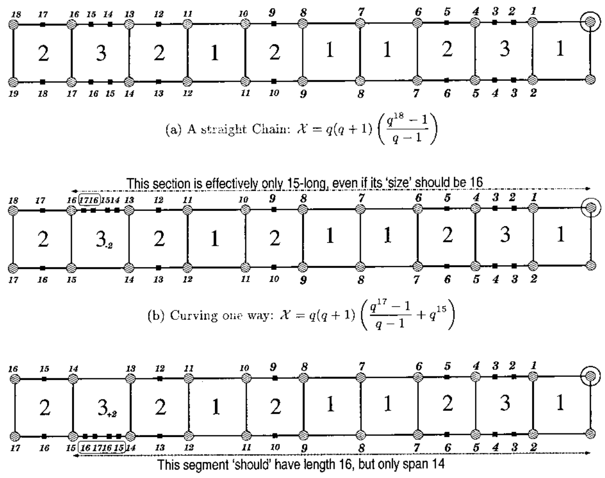
$$q(q+1)\left(\frac{q^{K_i-\hat{j}}-1}{q-1} + q^p\frac{q^{\hat{j}}-1}{q-1}\right)$$

after one kink is introduced (Figure 5), where p is the 'effective length' between the kink and the endpoint u, and $\hat{j}$ is the amount of the kink, i.e., $|j|$ when it is the first curve of two in the same direction, and $|j|-1$ otherwise. Figure 6 shows what kind of terms appears as the polygons are rotated one by one to create our motley chain. We can now verify the important relation:

$$\mathcal{X}_l(q) = q(q+1)\left[\frac{q^{L_l}-1}{q-1} + \sum_{h=1}^{l-1} q^{L_l-L_h}\left(\frac{q^{\hat{j}_{i_h}}-1}{q-1}\right)\right]. \quad (10)$$

Now sum up the terms in straightforward fashion to get Eq. (9).

We sketch with some examples how to obtain the Wiener polynomials of polygonal chains involving odd cycles. Following [29], we term a motley chain zigzagging or straight (Fig. 7) if for at least one representation $S = (a_1, b_1), \ldots, (a_n, b_n)$, we have



(a) A straight Chain: $\mathcal{X} = q(q+1)\left(\frac{q^{18}-1}{q-1}\right)$

(b) Curving one way: $\mathcal{X} = q(q+1)\left(\frac{q^{17}-1}{q-1}+q^{15}\right)$

(c) Curving the other way: $\mathcal{X} = q(q+1)\left(\frac{q^{16}-1}{q-1}+q^{14}\frac{q^{2}-1}{q-1}\right)$

FIGURE 5. Partial Wiener polynomials for almost-straight even chains.

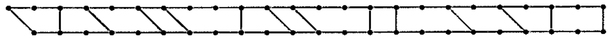


FIGURE 7. "Straight" motley chain.

$$\left\{\sum_{i=1}^{j}(a_i - b_j) \middle| 1 \le j \le n\right\} \subset \{0, 1\} \text{ or } \{0, -1\}.$$

We aim to work out the Wiener polynomials of motley chains, starting with straight ones and working our way down the line, adding terms for each bend or twist in a similar way to the above.

Lemma 7 (subdivision of even cycle). A polygonal chain of one $(2m+1)$ cycle, one $2(k+1)$ cycle, and one $(2n+1)$ cycle has its Wiener polynomial given by

$$\mathcal{W}\left(\left\langle (2m-3)\begin{matrix}k-1\\k-1\end{matrix}(2n-3)\right\rangle; q\right) = (2n+1)q\frac{q^n-1}{q-1} + (k+1)\left[\frac{(q+1)(q^n-1)}{q-1} - 1\right] + (2m+1)q\frac{q^m-1}{q-1} - 2q + \frac{q^{n+1+m+k}+4q^{n+m+k}-q^{n+m+k-1}-2q^{2+k}-2q^{1+k}-4q^{2+m}+4q^3+4q^2-4q^{n+2}}{(q-1)^2}.$$

In particular, the Wiener polynomial of fused $(2n+1)$ and $(2m+1)$ cycles, or $\mathcal{W}(\langle(2m-3), (2n-3)\rangle; q)$ is given by

$$\mathcal{W}(C_{2n+1}; q) + \mathcal{W}(C_{2m+1}; q) - q + \frac{q^{m+n}(q^2-1) + 4q^3(q^{m-1}-1)(q^{n-1}-1) - 2q^3 + 2q^2}{(q-1)^2}.$$

Denote a straight chain of n repetitions of fused cycles of $n_1, n_2, \ldots, n_k$ sides in that order to be $\mathcal{L}_{n_1,n_2,\ldots,n_k}(n)$. So a straight motley chain composed of n pairs of alternating pentagons and septagons would be $\mathcal{L}_{5,7}(n)$. Since the chain fragment consisting of one pentagon and one septagon can be created from partitioning a decagon (which has length 4), and the difference between its Wiener polynomial and four fused squares is $\mathcal{W}(\langle 1, 3\rangle; q) - \mathcal{W}(Cb_{5,2}; q) = -q^5 + 3q^3 - 2q$, one would expect $\mathcal{W}(\mathcal{L}_{5,7}(n); q)$ to be given by $\mathcal{W}(Cb_{10n+1,2}; q) - nq(q^2-1)(q^2-2)$, but this is not so. As we subdivide one of the decagons we have the four blobbed vertices marked in Figure 8 above, each getting closer to each of the circled ones by 1.

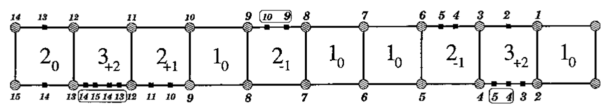


FIGURE 6. Chain with many turns: $\mathcal{X} = q(q+1)[(q^{14} - 1/q - 1) + q^{12}(q^2 - 1/q - 1) + q^8 + q^3]$.

So, to get $\mathcal{W}(\mathcal{L}_{2k+1,2m+1}(n); q)$, we have to add in addition to the differences between the fragments, which is $n[\mathcal{W}(\langle 2k-3, 2m-3\rangle; q) - \mathcal{W}(Cb_{k+m,2}; q)]$, the term

$$\sum_{j=1}^{n-1}\left[\frac{q^k-1}{q-1}\,\frac{q^{(k+m-1)j}-1}{q-1} + \frac{q^{m-1}-1}{q-1}\,\frac{q^{(k+m-1)j-k+1}-1}{q-1}\right],$$

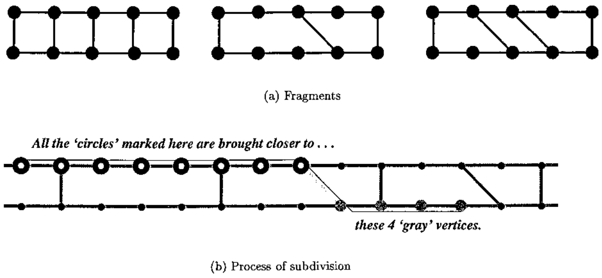
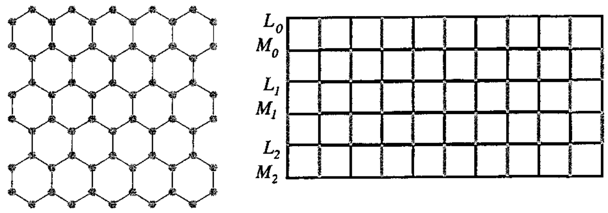


FIGURE 8. Septagon–pentagon chains.



(a) **Rectangular** carpet $R_{5,3}$ (b) $R^{\square}_{5,3}$

FIGURE 9. Rectangular carpet.

which ends in this lemma, which we can use to obtain the Wiener polynomial of all generic motley chains inductively.

Lemma 8 (one zigzagging straight chain).

$$\begin{aligned}\mathcal{W}[\mathcal{Z}_{2k+1,2m+1}(n); q] &= \mathcal{W}[Cb_{n(k+m-1)+1,2}; q] \\ &+ n[\mathcal{W}(\langle 2k-3, 2m-3\rangle; q) - \mathcal{W}(Cb_{k+m,2}; q)] \\ &- \frac{n-1}{(q-1)^2}(q^{m-1} + q^k - 2) \\ &+ \frac{(q^k-1)q^{k+m-1} + (q^{m-1}-1)q^m}{(q-1)^3}[q^{(k+m-1)(n-1)} - 1].\end{aligned}$$

3. Two-Dimensional Patterns

Mathematical chemists long ago posed the question of computing the Wiener numbers of graphs with 2D hexagonal patterns (called hexagonal animals or hex carpets; they resemble a hexagon tiling of the floor). Eventually, a solution was found via this idea:

Definition 3 (squaring). A graph $G = (V, E)$ representing a given hexagonal animal is said to be embedded in the set of lattice points $\mathbb{Z}^2$ if $V \subset \mathbb{Z}^2$,

$$E \subset \mathcal{L} \equiv (\{[(i, j), (i+1, j)] | i, j \in \mathbb{Z}\} \cup \{[(i, j), (i, j+1)] | i, j \in \mathbb{Z}\})$$

(i.e., and all edges in E can be drawn as line segments of length 1).

A graph G embedded in the lattice points is said to be partitioned into row-paths R_j if $V = \uplus R_j$ such that each R_j contains all vertices with ordinate j and is isomorphic to a path. It is easy to see that any lattice embedding of a hex carpet with a partition into row paths will show each 6-cycle (hex) as the boundary of a domino (horizontal 2×1 rectangle). Let $G = (V, E)$ be a hexagonal animal lattice-embedded; then the subgraph of the lattice grid induced by V

$$G^{\square} \equiv \left(V, \binom{V}{2} \cap \mathcal{L}\right) = (\mathbb{Z}^2, \mathcal{L})|_V,$$

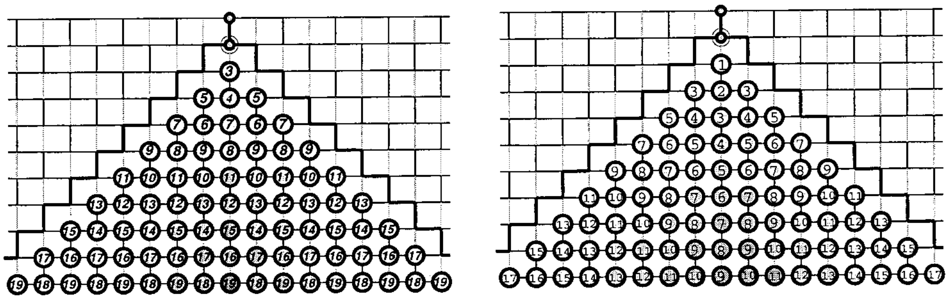
is defined as the squaring of G.

In the remainder of this section, we will demonstrate how to compute the Wiener polynomial for one case of the hex carpets.

One basic family of hex carpets is shown in Figure 9 with its squaring.

Lemma 9 (change of distance induced by squaring). If $u = (0, 0) \in R_0$ and $v = (i, j) \in R_j$ are two vertices j (>0) rows apart in a lattice embedding of $G = (V, E)$ and the row path partition $V = R_0 \uplus R_1 \uplus \cdots \uplus R_k$, then $d_{G^{\square}}(u, v) = |i| + j$; and

$$d|_G(u, v) = \begin{cases} |i| + j & j \le |i|; \\ |i| + j + 2\left\lfloor \dfrac{j - |i| + 1}{2} \right\rfloor & j > |i|, \{(0, 0), (0, 1)\} \notin E; \\ |i| + j + 2\left\lfloor \dfrac{j - |i|}{2} \right\rfloor & j > |i|, \{(0, 0), (0, 1)\} \in E. \end{cases} \quad (11)$$



(a) Before (b) After

FIGURE 10. Effects of squaring on distances in carpets.

We present Figure 10 instead of a formal proof.

Wiener polynomials of chessboards are easy. The following will show that careful manipulations of the changes induced by during squaring will yield the Wiener polynomial of any hex carpet in each of the three major families (see ref. [27]), using similar techniques to that for Wiener numbers. As an example, we compute the Wiener polynomial of the carpet $R_{n,k}$. Taking the squaring of $R_{n,k}$, we get the chessboard $Cb_{2n+1,2k}$, whose Wiener polynomial $\mathcal{W}(Cb_{2n+1,2k}; q)$ is given by

$$\frac{[2q(q^{2n+1}-1)-(2n+1)(q^2-1)][2q(q^{2k}-1)-2k(q^2-1)]}{2(q-1)^4} - k(2n+1).$$

However, we hit a snag. Instead of differences as when dealing with Wiener numbers, we must find the actual terms of the respective Wiener polynomials. Cancellation becomes difficult and patterns can be hard to locate.

Lemma 10. The difference terms in the Wiener polynomial induced between the marked vertex p and the next l rows of vertices (as shown in Fig. 10) is given by:

$$\begin{aligned}\Delta_p^+(l; q) &= q^3\left[\frac{1-q^{2l}}{(1-q^2)^2} - \frac{lq^{2l}}{1-q^2}\right] \\ &\quad + q^4\left[\frac{1-q^{2l-2}}{(1-q^2)^2} - \frac{(l-1)q^{2l-2})}{1-q^2}\right] \text{ (``before'')} \\ &\quad - q\left[\left(\frac{1-q^l}{1-q}\right)^2 - \frac{1-q^l}{1-q} + \frac{1-q^{2l}}{1-q^2}\right] \text{ (``after'')} \\ &= -\frac{lq^{2l+2}}{1-q} - \frac{q^{2l+2}(q+2)}{(1+q)(1-q)^2} \\ &\quad + \frac{q^{l+1}(1+q)}{(1-q)^2} - \frac{q}{(1+q)(1-q)^2}. \quad (12)\end{aligned}$$

Proof. By direct summation of the patterns in Figure 10.

The above formula works when the vertex in question is on the "far" side of a hexagon. If we move it up one row (or look the other way), we get $\Delta_p^-(l; q)$, which is equal to $q\Delta_p^+(l-1; q)$.

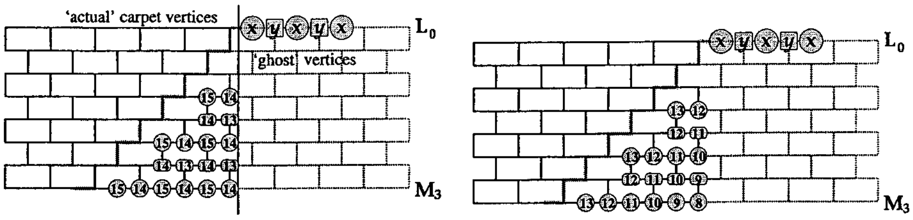
If we now sum over the whole of $\hat{R}_{n,k}$, always taking the pyramids of numbers (powers of t) upward, we get a differential of

$$\sum_{l=1}^{2k-1}\left\{\left[n+\frac{1+(-1)^l}{2}\right]\Delta_p^+(l; q) + \left[n+\frac{1-(-1)^l}{2}\right]\Delta_p^-(l; q)\right\},$$

which is rather hard to work with, and we do better this (equivalent) way:

$$\sum_{l=1}^{2k-1} n[\Delta_p^+(l; q) + \Delta_p^-(l; q)] + \sum_{l=1}^{k-1}[\Delta_p^+(2l; q)(1+q)].$$

Now we evaluate the sums in l, using Eq. (12) and get Lemma 11.



(a) Before: X

(b) After: X

FIGURE 11. "Edge effects" as seen before and after the squaring.

Lemma 11. The total difference in Wiener polynomials induced between the hex carpet $R_{n,k}$ and the row paths, which contain it is given by

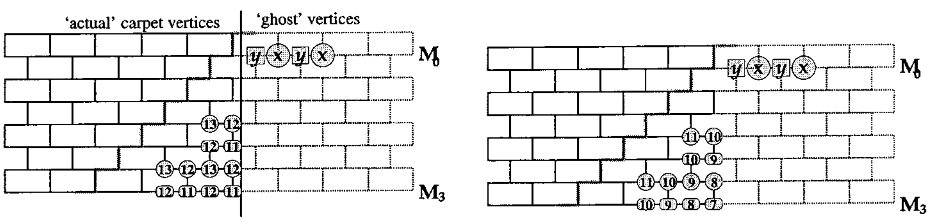
$$\Delta^*\mathcal{W}(R_{n,k}) = \frac{nq}{(1-q)^3}\left[(1-q^{2k})^2(1+q) - 2k(1-q)(1-q^{4k})\right] + \frac{2q^{4k+2}}{(1-q)^2(1-q^2)} - \frac{kq}{(1-q)^2} - \frac{q^{2k+1}(q+1)}{(1-q)^3} + \frac{q^{4k+2}(2q^4+q^3+2q^2+q+2)+(q+2q^3+2q^4+2q^5+q^7)}{(1+q)(1-q)^3(1+q^2)^2}. \quad (13)$$

The above formula sums up all the pyramid patterns of difference terms, assuming them to be complete throughout, which is not, unfortunately, since the hex carpets have finite width. Therefore, we must adjust for the incompleteness of these pyramid around the edges. As in [27], we would take two rows, and consider exactly which terms in these patterns "disappear over the edges." Let's call the row paths in $R_{n,k}$ (in order) L_0, M_0, L_1, $M_1, \ldots,$ L_{k-1}, M_{k-1}. We look at just one end of the rows L_0 and M_m (see Fig. 11), and call the difference terms X_m as in [27].

$$X_m(q) = \left[\binom{m+1}{2}q^{4m+2} + \binom{m}{2}q^{4m+1}\right](q+1) - (q+1)\left\{q^{2m+2}\left[\frac{1-q^{2m}}{(1-q^2)^2} - \frac{mq^{2m}}{1-q^2}\right] + q^{2m+3}\left[\frac{1-q^{2m-2}}{(1-q^2)^2} - \frac{(m-1)q^{2m-2}}{1-q^2}\right]\right\};$$

but this is insufficient—we need to do four kinds of boundary effects. On one side of M_0 and M_m (see Fig. 12) would be

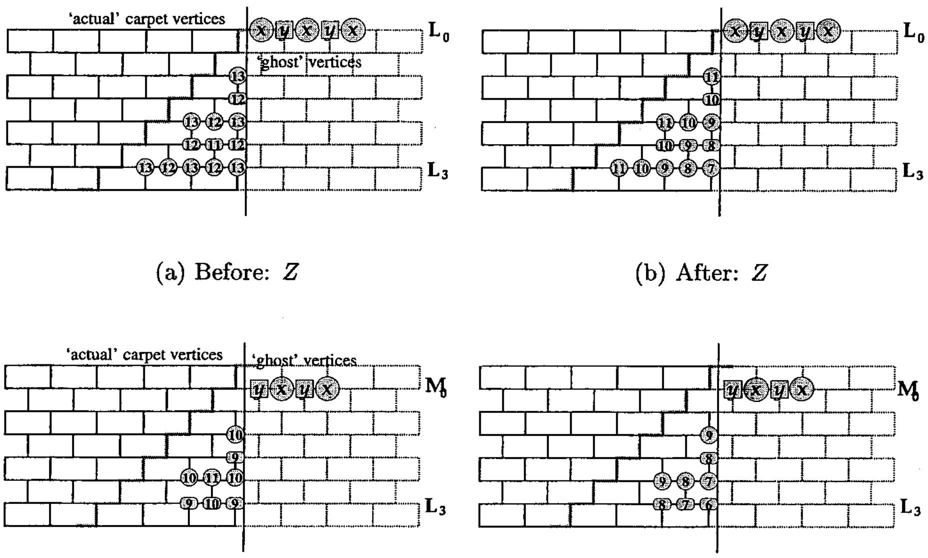
$$Y_m(q) = (q+1)^2\left\{\binom{m}{2}q^{4m-1} - q^{2m+1}\left[\frac{1-q^{2m-2}}{(1-q^2)^2} - \frac{(m-1)q^{2m-2}}{1-q^2}\right]\right\}.$$



(a) Before: Y

(b) After: Y

FIGURE 12. Different "edge effect," as shown before and after the squaring.



(a) Before: Z (b) After: Z

(c) Before: U (d) After: U

FIGURE 13. The two other "edge effects," before and after squaring.

Similarly (Fig. 13), for $Z_m(q)$ (from L_0 to L_m) and $U_m(q)$ (between M_0 and L_m):

$$Z_m(q) = \binom{m+1}{2} q^{4m+1} + m(m-1)q^{4m} + \binom{m}{2} q^{4m-1} - q^{2m+1}\left[\frac{1-q^{2m-1}}{(1-q)^2} - \frac{(2m-1)q^{2m-1}}{1-q}\right]$$

$$U_m(q) = \binom{m}{2} q^{4m-1} + (m-1)^2 q^{4m-2} + \binom{m}{2} q^{4m-3} - q^{2m}\left[\frac{1-q^{2m-2}}{(1-q)^2} - \frac{(2m-2)q^{2m-2}}{1-q}\right].$$

Finally, we can finish the computation for $\mathcal{W}(R_{n,k})$, when $n > k$:

$$\mathcal{W}(R_{n,k}; q) = \mathcal{W}(Cb_{2n+1,2k}; q) + \Delta^*\mathcal{W}(R_{n,k}) - 2\left\{\sum_{l=1}^{k-1} (k-l)[X_l(q) + Y_l(q) + Z_l(q) + U_l(q)]\right\}.$$

The last pair of braces can be evaluated by expanding the summand in l, then sum over $l = 1 \cdots k - 1$ to get:

$$\sum_{l=1}^{k-1} [X_l(q) + Y_l(q) + Z_l(q) + U_l(q)] = \sum_{l=1}^{k-1} \left\{ l^2 q^{4l}\left[\frac{(1+q)^2(1+q^2)^2}{2q^3}\right] - lq^{4l}\left[\frac{(1+q)(1+q^2)(1-2q-2q^2-2q^3+q^4)}{2q^3(1-q)}\right] + q^{4l}\left[\frac{(1+q)^2}{(1-q)^2}\right] - q^{2l}\left[\frac{(1+q)^2}{(1-q)^2}\right]\right\}$$

$$= \frac{k^2 q^{4k+1}}{2(1-q)^2} + \frac{k(q^{4k+5} + 2q^{4k+4} + 2q^{4k+3} + 2q^{4k+2} + q^{4k+1} - 2q^3)}{2(1-q)^2(1-q^4)} - \frac{q^2(1-q^{2k})[q^{2k}(q^6+q^5+2q^4+3q^3+2q^2+q+1) - (q^5+q^4+q^3+q^2+q)]}{(1-q)^2(1-q^4)^2}.$$

We have arrived at the Wiener polynomial of one of the hex carpets, as shown in Theorem 12.

Theorem 12. When $n > k$, we have

$$\begin{aligned}\mathcal{W}(R_{n,k}; q) = {} & \frac{[2q(q^{2n+1}-1) - (2n+1)(q^2-1)][2q(q^{2k}-1) - 2k(q^2-1)]}{2(q-1)^4} - k(2n+1) \\ & - \frac{nq}{(1-q)^3}[(1-q^{2k})^2(1+q) - 2k(1-q)(1-q^{4k})] - \frac{2q^{4k+2}}{(1-q)^2(1-q^2)} + \frac{kq}{(1-q)^2} \\ & + \frac{q^{2k+1}(q+1)}{(1-q)^3} + \frac{q^{4k+2}(2q^4+q^3+2q^2+q+2) - (q+2q^3+2q^4+2q^5+q^7)}{(1+q)(1-q)^3(1+q^2)^2} \\ & + \frac{k^2q^{4k+1}}{2(1-q)^2} + \frac{k(q^{4k+5}+2q^{4k+4}+2q^{4k+3}+2q^{4k+2}+q^{4k+1}-2q^3)}{2(1-q)^2(1-q^4)} \\ & - \frac{q^2(1-q^{2k})[q^{2k}(q^6+q^5+2q^4+3q^3+2q^2+q+1) - (q^5+q^4+q^3+q^2+q)]}{(1-q)^2(1-q^4)^2}.\end{aligned}$$

There is an "explicit formula" for each of the hex carpets—finding Wiener polynomials of $S_{n,k}$ and $P_{n,k}$, as defined in [27], and their variants is a similar process, except for fiddling with extra vertices to bring the squaring up to a more symmetric grid. Each result will take up half a page, however.

4. Summary and Discussion

Even in the new millennium, Wiener numbers and polynomials remain a topic for which interesting problems abound.

1. Wiener polynomials for branched or fused polycyclic chains, and for that matter polycyclic rings, do not have currently known nonrecursive derivation. Wiener numbers of a few other chemically interesting families of graphs with structure in more than one dimension have not been determined other than the regular hex carpets, as defined in [27].
2. It is also desirable to extend formulas for Wiener numbers to Wiener polynomials, but many results cannot be easily generalized. Several nice propositions do not yet have q-analogues, such as the elegant Eq. (14) and similar results on trees.
3. A formula for the Wiener number of a hex crown (Fig. 14, see [27]) was proved by the present authors [30], but computing the Wiener polynomial is not easy because of the same problem that precluded Eq. (14) from having a nice q-analogue, despite the high degree of symmetry.

The problems mentioned above in extending results from Wiener numbers to polynomials are exemplified by the following two propositions, aside from the aforementioned Merris–McKay result.

Proposition 13. The following holds for a tree T

1. For each vertex $x \in T$ that has degree at least three (a "branch point"), let $F(x)$ be the set of components of the forest $T \backslash \{x\}$. Then Gutman showed that
$$\mathcal{W}(T) = \binom{|T|+1}{3} - \sum_{\substack{x \in V(T) \\ \deg(x) \geq 3}} \sum_{\{T_1, T_2, T_3\} \in \binom{F(x)}{3}} |T_1||T_2||T_3|. \quad (14)$$

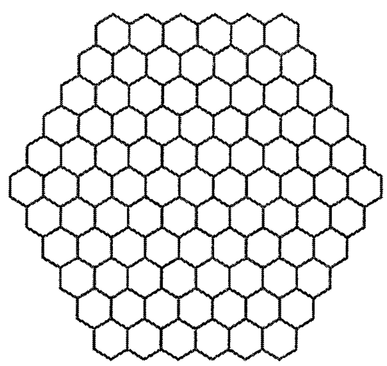


FIGURE 14. Crown of order 6.

2. It was shown by Wiener himself that if for each edge e we call $n_1(e)$ and $n_2(e)$ the number of vertices to either side of the edge e, then

$$\mathcal{W}(T) = \sum_{e \in T} n_1(e) n_2(e).$$

Equation (14) has a very good combinatorial interpretation and useful applications. Most recently [31], it was used to identify the high alkane isomer with the smallest Wiener index, but no analogous formula for Eq. (14) or either of the two other elegant results in Wiener polynomials exist so far. Many proofs of Wiener numbers depend on a counting argument that may simply be absent present when handling generating functions. This explains why formulas about Wiener numbers just do not generalize very easily at all to Wiener polynomials. In short, interesting work remains to be done.

ACKNOWLEDGMENTS

This work is dedicated to the memory of the late Professor Gian-Carlo Rota, to whose kind encouragement we owe much in this work.

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