A Crowning Moment for Wiener Indices

Bo-Yin Yang
Department of Mathematics
Tamkang University*, Tamsui,
Taipei County, Taiwan, R.O.C.

Yeong-Nan Yeh
Institute of Mathematics
Academia Sinica†, Nankang
Taipei, Taiwan, R.O.C.

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Abstract

The Wiener (Sum of All Distances) Index for three out of the four classes of *hexagonal models* or regular planar hex-patterns used to model graphite and similar structures have been known for a few years. In this paper we find the Wiener Index for the Crown or Beehive hexagonal model.

1 Wiener Indices and Chemical graphs

Chemists have worked extensively with graphs. To an organic chemist, the graph of a compound is a natural concept – take the (non-hydrogen) atoms as vertices and bonds as edges.

The Wiener vertex is a function defined on connected graphs. Often such a function, or "topological index" would have a good correlation with some measurable property of a chemical.

For a connected graph $G = (V, E)$, let $d_G(u, v)$ denote the shortest distance between the vertices u and v on the graph, then sum over all pairs of vertices $\{u, v\} \in \binom{V}{2}$ to get $\mathcal{W}(G) \equiv \sum_{\{u,v\}} \Delta_G(u, v)$.
We also write $\mathcal{W}(u|G) \equiv \sum_{v \in G} \Delta_G(u, v)$, so $\mathcal{W}(G) = \frac{1}{2} \sum_u \mathcal{W}(u|G)$.

There are many interesting applications for Wiener indices in physical chemistry and other branches of science. A discussion of these and their general usefulness in chemistry can be found in many chemical treatises such as [1, 10, 14]; general chemical interest can be found in the other

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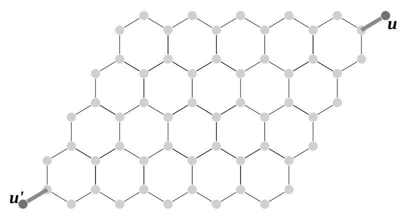
references. One specific usage is found in modeling some behaviors of carbon (in the allotrope of graphite).

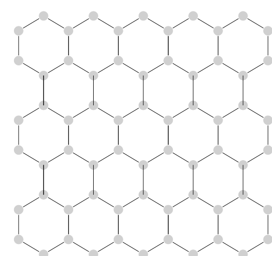
The authors has been involved with most of the previously known results about the Wiener Indices of graphs involving hexagons ([5, 6, 16, 17]). Most of the work has started here:

Lemma 1 (Shelling Lemma for Wiener Indices) *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), then we have*

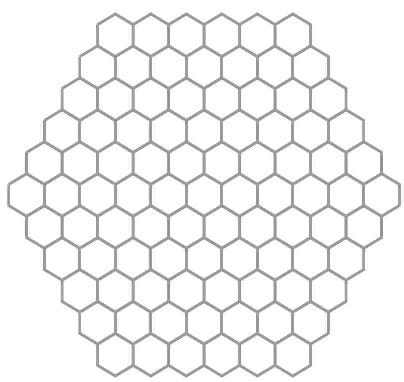
$$\mathcal{W}(G) = \mathcal{W}(G_0) + \sum_{j=1}^{K} \left[\sum_{u \in V_j} \mathcal{W}(u|\mathcal{G}_j) - \mathcal{W}(G_j) \right], \tag{1}$$



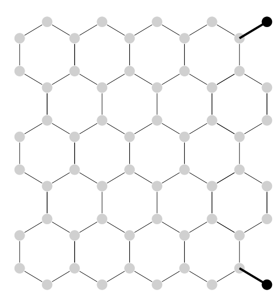
(a) Parallelogram Model



(b) Rectangular Model



(c) Crown Model



(d) Square Model

Figure 1: The Four classes of hexagonal carpets

In fact, straightforward approaches work for cases (a), (b), and (d) — see [5] for details, but not for the kind of graph as depicted in (c). We present a solution to this problem.

2 A Formula for Wiener Indices of Crowns

The hexagon "crown" or beehive model (see Fig. 1(c)) differs with the other three 'hexagonal models', as discussed in [5] in that one cannot modify, as in the Crown into a graph that has a Wiener Index that is easy to compute, and the "shelling" lemma (Eq. 1) used for the polygonal chains doesn't work, because the natural order of things would be to divide the graph into concentric tracks, and the distance in the Crown is not preserved by the this subdivision.

Theorem 1 (Wiener Index of Crowns)

$$\begin{aligned}\mathcal{W}(Z_j, Z_k|\mathrm{Cr}_n) &= (2m-1)\left[18(8k^2-8k+3)+40j(j-1)\right]\\ \mathcal{W}(\mathrm{Cr}_n) &= \sum_{k=1}^{n}\left\{\sum_{j=1}^{k-1}\mathcal{W}(Z_j, Z_k|\mathrm{Cr}_n)+\frac{1}{2}\mathcal{W}(Z_k, Z_k|\mathrm{Cr}_n)\right\}\\ &= \frac{1}{5}(164n^5-30n^3+n). \qquad (2)\end{aligned}$$

While the shelling lemma does not apply, we still divide the graph into the concentric hexagon tracks (the center hex will be Z_1 and the next track out Z_2, and so on). It is easy to see that (see Figure 2) the distances from antipodal pair of vertices in Z_k to one of the center vertices always add up to $4k-1$ for the "outer" part of Z_k and $4k-3$ for the "inner" part. So $\mathcal{W}(Z_1, Z_k|\mathrm{Cr}_n) \equiv \sum_{u\in Z_1, v\in Z_k} d(u,v)$ is equal to

$$6\times 3\times[k(4k-1)+(k-1)(4k-3)]$$

or $\mathcal{W}(Z_1, Z_k|\mathrm{Cr}_n) = 18(8n^2-8n+3)$.

To find $\mathcal{W}(Z_j, Z_k|\mathrm{Cr}_n)$, the sum of distances from Z_j to Z_k, we need a little trick (see Fig. 3).

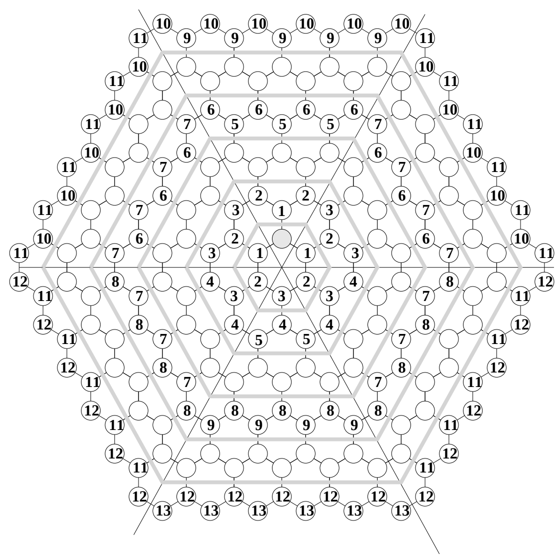


Figure 2: Distances between a center vertex to the rest of Cr_6 (the tracks Z_1, Z_2, Z_4, and Z_6 are shown).

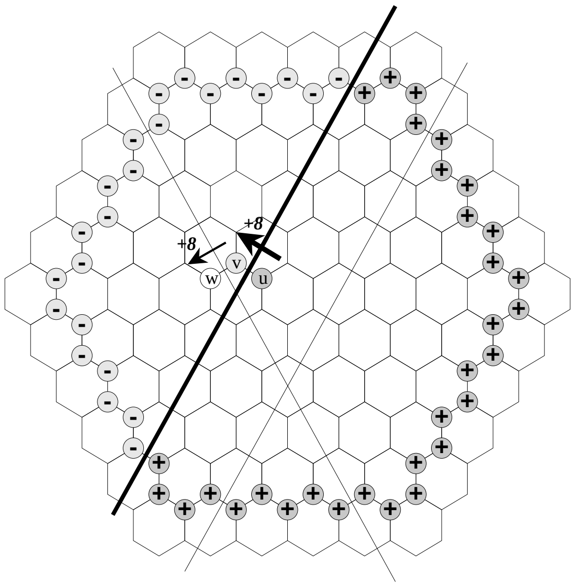


Figure 3: The difference in sum of distances.

Let u (a center vertex) and v (an “inner” vertex of Z_2) be as marked and take another vertex $x \in \mathrm{Cr}_n$. What is the difference $d(v,x) - d(u,x)$? Obviously, x is one further away from u than from v if x lies on v's side of the thick black line shown (marked “+”), and vice versa (marked “-”). So $d(v,x) - d(u,x)$ summed over any set S of vertices is difference between the number of vertices in S on the right side of the thick line and those on the left. For the track Z_5 (marked in shade), we see that this difference is 8.

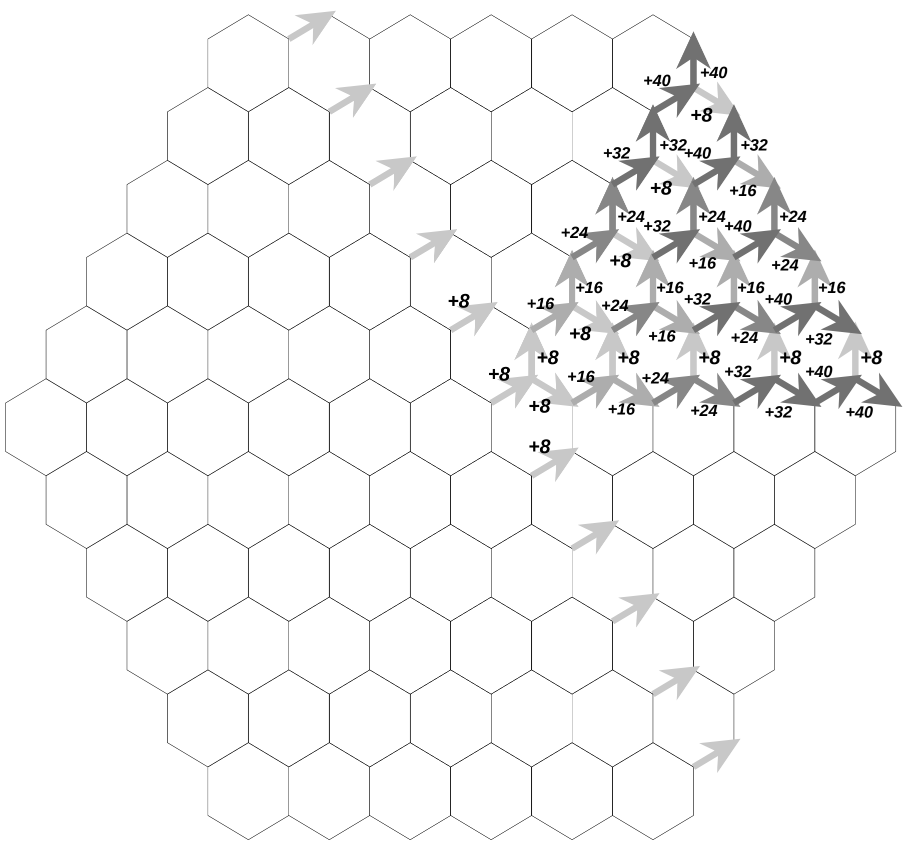


Figure 4: Differences in the sum of distances from a vertex to any outer track as we slide it around.

Indeed, since the parallel lines in Fig. 3 are symmetric to to each other with respect to the center of the graph, and there will always be 8 vertices, 4 on each side, on any track Z_k that lie between those two lines, we see that for any k,

$$\sum_{x \in Z_k} (d(v,x) - d(u,x)) = 8.$$

A similar comparison yields the difference between the sum of distances to an outer track from two adjacent vertices, for example for the vertex w (in the "outer" half of Z_2) in Fig. 3, we have

$$\sum_{x \in Z_k} (d(w,x) - d(u,x)) = 8 + \sum_{x \in Z_k} (d(w,x) - d(v,x)) = 16.$$

We exhibit $\mathcal{W}(v, Z_k|\mathrm{Cr}_n) - \mathcal{W}(u, Z_k|\mathrm{Cr}_n)$ for various v in Fig. 5. From this, we also have

$$\begin{aligned} \mathcal{W}(Z_2, Z_k|\mathrm{Cr}_n) &= 3 \times \mathcal{W}(Z_1, Z_k|\mathrm{Cr}_n) + 6 \times 8 + 12 \times 16 \\ &= 432k^2 - 432k + 402. \end{aligned}$$

It is by now clear that $\mathcal{W}(Z_j, Z_k|\mathrm{Cr}_n) = (2j-1)\mathcal{W}(Z_1, Z_k|\mathrm{Cr}_n) + p_j$ where p_j is a constant for $k > j$. All that remains is to find p_j and we shall have

$$\mathcal{W}(\mathrm{Cr}_n) = \sum_{1 \leq j < k \leq n} \mathcal{W}(Z_j, Z_k|\mathrm{Cr}_n) + \frac{1}{2}\sum_{j=1}^{n} \mathcal{W}(Z_j, Z_j|\mathrm{Cr}_n).$$

From the numbers in Fig. 4, we can now compute

$$\begin{aligned} p_2 &= 6 \times (8 + 2 \times 16) \\ &= 240 \\ p_3 &= 1200 \\ p_4 &= 3360 \\ p_5 &= 7200 \\ p_6 &= 8800 \\ \vdots & \;\vdots\; \vdots \end{aligned}$$

and inductively

$$p_j = 40m(m-1)(2m-1) \quad (3)$$

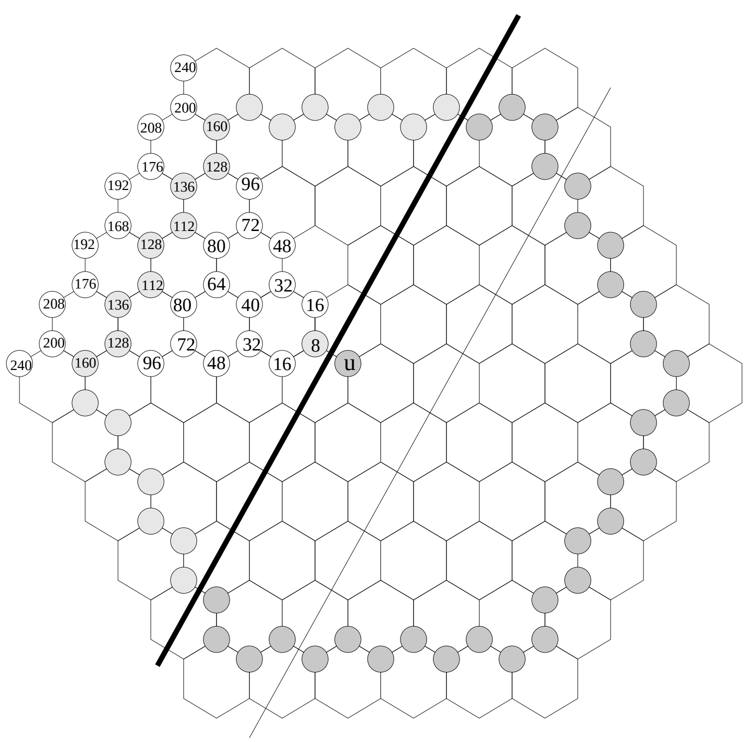


Figure 5: Difference in sum of distances to any outer track, as measured from that of the center vertex u.

Now all we need is to prove Eq. 3. Let the sum of numbers in the inner part of the j-th row be q_j and that of the outer part r_j. A look at Fig. 4 tells us that $r_1 = 8$ and each number in the "inner j-th row" is greater than the corresponding one in the previous "outer row" by $8(j-1)$, so

$$q_j = r_{j-1} + 8(j-1)^2.$$

Similarly, since we can see that the number on either end of the "outer j-th row" is $8j(j-1)$, we have

$$\begin{aligned} r_j &= q_j + 8\sum_{\ell=1}^{j-1} \ell + 8j(j-1) \\ &= q_j + 12j(j-1). \end{aligned}$$

So, we have with a little manipulation:

$$\begin{aligned} q_j + r_j &= q_{j-1} + r_{j-1} + 40(j-1)^2 \\ &= 20j(j-1)(2j-1)/3. \end{aligned}$$

Since $p_j = 6(q_j + r_j)$ we have proved Eq. 3. Finally we can sum the various terms and get Eq. 2

This is the last of the four "hexagonal models" for which Wiener numbers have been computed. One possible extension is to hex carpets that looks like a hexagon with three different edge-lengths.

We would also like to find, in some useful manner, the computation of the q-analog of Wiener Indices $\mathcal{W}(Cr_n, q) = \sum_{\{u,v\}} q^{d(u,v)}$. Unfortunately, while we can brute-force the computation of the Wiener polynomial for the Crown graph, it lends to no elegance whatever.

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