On Wiener numbers of polygonal nets

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On Wiener Numbers of Polygonal Nets*

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Abstract

The Wiener number of a connected graph is equal to the sum of distances between all pairs of its vertices. In this paper, we shall generalize the elementary cuts method to homogeneous n-gonal nets and give a formula to calculate the Wiener numbers of irregular convex triangular hexagons.

Key words and phrases : Graph, distance, polygonal net, Wiener number.
AMS 2000 MSC : 05C12

1 Introduction

An important invariant of connected graphs is the *Wiener number* (or *Wiener index*) W, which is equal to the sum of distances between all pairs of vertices of the respective graph. American physico-chemist Harold Wiener first examined the quantity W in 1947 and 1948 [24–28]. He conceived this index in an attempt to formulate a mathematical model capable of describing molecular shapes. Wiener, and after him numerous researchers reported the existence of correlation between W and a variety of physico-chemical properties of alkanes. For recent reviews on this matter and references to previous work in this area, please see [7–10, 16]. The Wiener number was extensively studied also in the mathematical literature (see, for instance, [4–6, 13, 17–23, 29]). The generalization of the Wiener number, can be found in [3] and [11].

Despite large number of works on the theory of the Wiener number, some basic problems remain unsolved. For example, there is no known recursive method to calculate W of general graphs, especially for polycyclic graphs. In 1995, Shiu *et al.* ([18] published in 1997) introduced the "method of wall", which leads to recursive expression of the Wiener number of benzenoid hydrocarbons (i.e. hexagonal nets) [18–22]. In 1995, Klavzar, Gutman and Mohar [14] introduced the "elementary cuts method". It was demonstrated and exemplified how the method work in [12]. Proof of this method can be found in [14] or [23]. By using this method, the Wiener number of irregular hexagonal nets can be found efficiently [23].

Both the elementary cuts method and the method of wall cannot be applied to polycyclic graphs with odd-sided regular polygons, called *cells*. In this paper, we would like to generalize the elemen-

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tary cuts method to regular polygonal plane graphs with odd-sided cells.

2 Definitions and main results

In this paper, all undefined notations and terminologies are referred to the book [1]. In the following, a plane graph G is called a *homogeneous n-gonal net* or simply an *n-net* if each bounded face of G is a regular n-side polygon. We first define some homogeneous 3-gonal nets, which we call *triangular nets.*

Suppose $\{H_1, H_2, \ldots, H_h\}$, $\{R_1, R_2, \ldots, R_r\}$ and $\{L_1, L_2, \ldots, L_l\}$ are three sets of parallel lines lying on the same plane, where $h, r, l \geq 2$. Moreover the following conditions are satisfied:

(a) All H-lines run horizontally (East-West). All R-lines run towards North-East (or South-West) cutting an H-line at an angle of $2\pi/3$. All L-lines run towards North-West (or South-East) cutting an H-line at an angle of $2\pi/3$.

(b) Two successive lines in the same set have unit distance between them when measured along another sets of lines.

(c) Each line has at least one point which is the intersection of three lines (called *triple intersection point*).

From the sets of lines $\{H_1, H_2, \ldots, H_h\}$, $\{R_1, R_2, \ldots, R_r\}$ and $\{L_1, L_2, \ldots, L_l\}$, a graph is obtained by taking all triple intersection points as vertices and all unit line-segments joining two triple intersection points as edges. This graph is called a *convex triangulation mesh*, and is denoted by $\Delta_{h,r,l}$. Note that there are non-isomorphic convex triangulation meshes having the same parameters [15].

Let G be a plane graph. The *boundary of G*, denoted by ∂G, is the boundary of the unbounded face of G. A convex triangulation mesh $\Delta_{h,r,l}$ is called a *triangular trapezium* if its boundary forms a trapezium. In this case, $r = l$ and the length of the longer base and the height are $r-1$ and $h-1$ respectively. We denote this triangular trapezium by $T_{h-1,r-1}$. When $h = r$, $T_{h-1,r-1}$ becomes a *triangular triangle* which is simply denoted by T_{h-1} . For $n \geq 1$, $T_{1,n}$ is called a *$(2n-1)$-triangular chain* and is denoted by I_{2n-1}.

$\Delta_{h,r,l}$ is called a *triangular parallelogram* if its boundary forms a parallelogram. In this case, $|r-l| = h-1$ and $\Delta_{h,r,l}$ is isomorphic to $\Delta_{h,l,r}$. In the following, we shall always assume that $l > r$ and denote the triangular parallelogram $\Delta_{h,r,h+r-1}$ by $P_{h-1,r-1}$, which is sometimes called a $(h-1)\times(r-1)$- *triangular parallelogram.* For $n \geq 1$, $P_{1,n}$ is called a *$2n$-triangular chain*, denoted by I_{2n}.

Definition 2.1: A graph obtained by merging the longer base of $T_{p,n}$ and $T_{q,n}$ with two bases of $P_{m,n}$ forming a convex 6-sided polygon, is called an *irregular convex triangular hexagon* and denoted by $H_{q,p,m,n}$ (see Figure 1), where $0 \leq p, q \leq n$ and $m \geq 0$. By reflection it is easy to see that $H_{q,p,m,n} \cong H_{p,q,m,n}$. Therefore, we always assume that $q \geq p$.

Note that $H_{q,0,0,n} = T_{q,n} \cong T_{n,q}$; $H_{n,0,0,n} = T_n$; $H_{0,0,m,n} = P_{m,n} \cong P_{n,m}$; $H_{1,0,0,n} = I_{2n-1}$ and $H_{0,0,1,n} = I_{2n}$. Some triangular nets defined above can be seen in Figure 1.

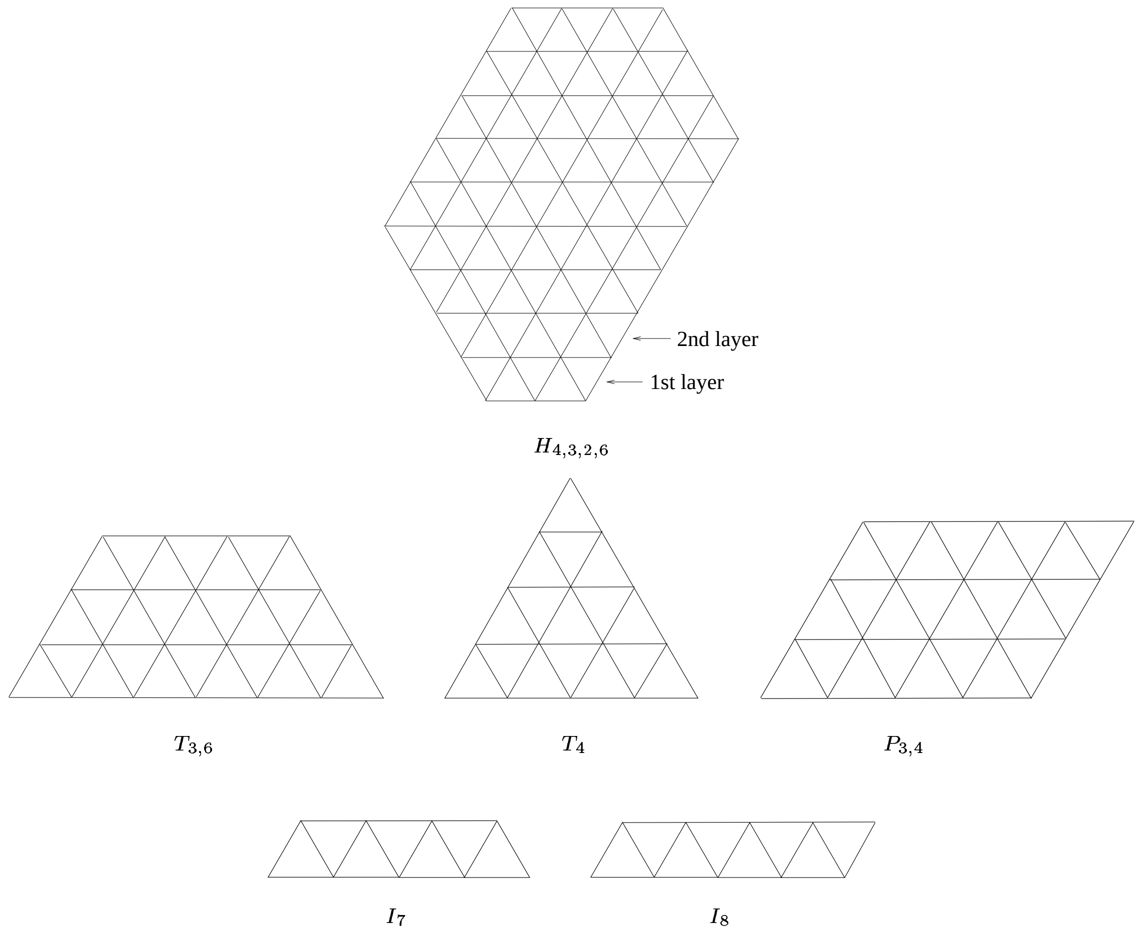

Figure 1: Some triangular nets.

We shall introduce the generalized elementary cut of a homogeneous polygonal net and use it to compute the Wiener numbers of irregular convex triangular hexagons.

Definition 2.2: Let H be an n-net and let e be an edge in a cell of H. We define the k^-*-edge of* e to be the k-th edge e' in the same cell counting in clockwise direction from e, whereas the k^+*-edge of* e to be the k-th edge e'' in the same cell counting in anti-clockwise direction from e.

Remark: Suppose that G is an n-net. If $e \in E(G) \setminus \partial G$, then e is incident with exactly two cells of G. If $e \in \partial G$, then e is incident with exactly one cell of G and the unbounded face.

Definition 2.3 [Generalized elementary cut]:

Let G be an n-net and $s = \lfloor \frac{n}{2} \rfloor$. For any $e \in \partial G$, we shall define two generalized elementary cuts $C^+(e)$ and $C^-(e)$. A *cutline* for $C^+(e)$ is obtained by joining a number of line segments. The first of such line segments, say L^+, links the mid-point M of e with the mid-point of e', where e' is the s^+-edge of e. If $e' \notin \partial G$, then e' belongs to another cell of G, say P. In P, draw a straight line segment L^- through the mid-point of e' and the mid-point of e'', where e'' is the s^--edge of e'. If $e'' \in \partial G$, then stop. Otherwise, continue the process with alternate orientations until it reaches the boundary (say at the point N).

The other generalized elementary cut, starting at the edge e with reverse the orientation, i.e. firstly, joining e to s^--edge of e and continue with alternate orientation.

Finally, let C be a polygonal path joined by M and N followed by the line segments defined above. Note that by elementary geometry it is easy to see that C is a straight line. Please see Appendix for details. C with endpoints M and N is called a *generalized elementary cut pertaining to* e. Identify the generalized elementary cut C with the set of edges of G which are crossed by C. The set of all generalized elementary cuts of G is denoted by $\mathcal{C}(G)$.

Remarks: Note that if n is even, then $L^+ = L^-$ and hence the generalized elementary cut is the same as elementary cut described in [12] or [23].

Let C be a generalized elementary cut of G. Then $G - C$ consists of two components denoted by $G'(C)$ and $G''(C)$ respectively. Let e_1, e_2 be edges cut by C. Let m_i be the intersection point of e_i and C, $i = 1, 2$. Define the *distance* between e_1, e_2, denoted by $\rho(e_1, e_2)$, to be the number of cells crossed by the line segment $m_1 m_2$. For example, if e_1 and e_2 lie in the same cell, then $\rho(e_1, e_2) = 1$.

Lemma 2.1 *Suppose G is an n-net. Let $C \in \mathcal{C}(G)$ and let $e_1 = u_1 v_1, e_2 = u_2 v_2$ be edges cut by C. Suppose u_1 and u_2 lie in $V(G'(C))$. Then there is a unique shortest (u_1, u_2)-path in G which lies in $G'(C)$. Moreover, this shortest path lies in the subgraph formed by the cells crossed by C.*

Proof: Proof by induction on $\rho(e_1, e_2)$. Suppose $\rho(e_1, e_2) = 1$. Let H be the cell that contains e_1 and e_2. It is clear that there is a (u_1, u_2)-path, say P, of length $s = \lfloor \frac{n}{2} \rfloor$ lying in $G'(C) \cap H$. Let Q be a shortest (u_1, u_2)-path, then either the boundary of the subgraph $H \cup Q$ or $P \cup Q$ forms a regular polygon of size at most n. But this polygon contains another regular n-side polygon H. It is impossible unless $P = Q$.

The inductive step is easy to see. □

We have the following corollary.

Corollary 2.1 *Suppose G is an n-net. Let $C \in \mathcal{C}(G)$ and let u, v be any two vertices of G. For any shortest (u,v)-path $P_{u,v}$, $|E(P_{u,v}) \cap C| = 0$, if u and v belong to the same component of $G - C$, otherwise, $|E(P_{u,v}) \cap C| = 1$.*

Theorem 2.1 *Let G be an n-net, where n is odd. Further assume that ∂G is connected. Then the Wiener number of G, $W(G)$ is*

$$\frac{1}{2} \sum_{C \in \mathcal{C}(G)} |G'(C)||G''(C)| = \frac{1}{2} \sum_{C \in \mathcal{C}(G)} |G'(C)|\{|G| - |G'(C)|\}$$

where $|H|$ denotes the order of H.

Proof: Each edge $e \in E(G)$ belongs to exactly two generalized elementary cuts, since there are exactly two distinct directions which passing through e.

For $u, v \in V(G)$, let $P_{u,v}$ be a shortest (u,v)-path in G. Since each edge of G belongs to exactly two generalized elementary cuts, it follows that

$$W(G) = \sum_{\{u,v\} \in S} |E(P_{u,v})| = \frac{1}{2} \sum_{C \in \mathcal{C}(G)} \sum_{\{u,v\} \in S} |E(P_{u,v}) \cap C|,$$

where S is the set of all unordered pairs of $V(G)$. By Corollary 2.1, we have

$$\sum_{\{u,v\} \in S} |E(P_{u,v}) \cap C| = |G'(C)||G''(C)|,$$

and hence we have our conclusion. □

We acknowledge that V. Chepoi *et al.* [2] obtained the result on Wiener number of L_1 graphs (namely, they are isometrically embeddable into hypercube). The case of polygonal nets are independently discovered by us with different consideration. The notion of generalized elementary cut corresponds to alternating cut.

3 Wiener numbers of convex triangular nets

Let $G = H_{q,p,m,n}$. Then the order of G is $(n+1)(m+q+p+1) - \frac{1}{2}[p(p+1) + q(q+1)]$. We partition $\mathcal{C}(G)$ into three subsets $\mathcal{C}_H(G)$, $\mathcal{C}_L(G)$, and $\mathcal{C}_R(G)$, which are the sets of generalized elementary cuts whose cutlines are parallel to the H-lines, L-lines and R-lines, respectively. Then

$$W(G) = \frac{1}{2}(f_H + f_L + f_R)$$

where

$$f_H = \sum_{C \in \mathcal{C}_H(G)} |G'(C)|(|G| - |G'(C)|) = f(q,p,m,n);$$

$$f_L = \sum_{C \in \mathcal{C}_L(G)} |G'(C)|(|G| - |G'(C)|);$$

$$f_R = \sum_{C \in \mathcal{C}_R(G)} |G'(C)|(|G| - |G'(C)|).$$

We shall first compute f_H. Let C_z be the generalized elementary cut of G which passes through the z-th layer of G (the bottom layer is the first layer). Let $G'(C_z)$ be the lower component of $G - C_z$. Then $|G'(C_z)|$ is equal to

$$\begin{cases} \sum_{i=0}^{z-1}(n-q+1+i) & \text{if } 1 \le z \le q, \\ \sum_{i=0}^{q-1}(n-q+1+i) + \sum_{j=q}^{z-1}(n+1) & \text{if } q \le z \le m+q, \\ \sum_{i=0}^{q-1}(n-q+1+i) + \sum_{j=q}^{m+q-1}(n+1) + \sum_{k=m+q}^{z-1}(n+1+m+q-k) & \text{if } m+q \le z \le m+q+p. \end{cases}$$

After simplifying we have

$$|G'(C_z)| = \begin{cases} \frac{1}{2}(1+2n-2q+z)z & \text{if } 1 \le z \le q, \\ \frac{1}{2}[2(n+1)z - q(q+1)] & \text{if } q \le z \le m+q, \\ \frac{1}{2}[(2n+2m+2q+3-z)z - 2q(m+q+1) - m(m+1)] & \text{if } m+q \le z \le m+q+p. \end{cases}$$

Let $f_1(q,p,m,n) = \sum_{z=1}^{q} |G'(C_z)|(|G| - |G'(C_z)|)$, $f_2(q,p,m,n) = \sum_{z=q+1}^{m+q} |G'(C_z)|(|G| - |G'(C_z)|)$ and $f_3(q,p,m,n) = \sum_{z=m+q+1}^{m+q+p} |G'(C_z)|(|G| - |G'(C_z)|)$. Then by symmetry, $f_3(q,p,m,n) = f_1(p,q,m,n)$. After computation we have

$$f_1(q,p,m,n) = \frac{1}{60}\{q(1+q)(18+20m+40n+50mn+20n^2+30mn^2+10p+35np+30n^2p-10p^2- 15np^2-13q-20mq-20mnq+10n^2q-10pq-20npq+10p^2q-7q^2-10nq^2+2q^3)\}.$$

$$f_2(q,p,m,n) = \frac{1}{12}\{m(4+6m+2m^2+8n+12mn+4m^2n+4n^2+6mn^2+2m^2n^2+3p+3mp+ 9np+9mnp+6n^2p+6mn^2p-3p^2-3mp^2-3np^2-3mnp^2+3q+3mq+9nq+ 9mnq+6n^2q+6mn^2q+3pq+12npq+12n^2pq-3p^2q-6np^2q-3q^2-3mq^2-3nq^2- 3mnq^2-3pq^2-6npq^2+3p^2q^2)\}.$$

Then

$$f(q,p,m,n) = \frac{1}{60}\{20m + 30m^2 + 10m^3 + 40mn + 60m^2n + 20m^3n + 20mn^2 + 30m^2n^2 + 10m^3n^2 + 18p + 35mp + 15m^2p + 40np + 95mnp + 45m^2np + 20n^2p + 60mn^2p + 30m^2n^2p + 5p^2 - 15mp^2 - 15m^2p^2 + 40np^2 + 15mnp^2 - 15m^2np^2 + 30n^2p^2 + 30mn^2p^2 - 20p^3 - 20mp^3 - 10np^3 - 20mnp^3 + 10n^2p^3 - 5p^4 - 10np^4 + 2p^5 + 18q + 35mq + 15m^2q + 40nq + 95mnq + 45m^2nq + 20n^2q + 60mn^2q + 30m^2n^2q + 20pq + 15mpq + 70npq + 60mnpq + 60n^2pq + 60mn^2pq - 10p^2q - 15mp^2q - 30mnp^2q + 30n^2p^2q - 10p^3q - 20np^3q + 5q^2 - 15mq^2 - 15m^2q^2 + 40nq^2 + 15mnq^2 - 15m^2nq^2 + 30n^2q^2 + 30mn^2q^2 - 10pq^2 - 15mpq^2 - 30mnpq^2 + 30n^2pq^2 + 15mp^2q^2 - 30np^2q^2 + 10p^3q^2 - 20q^3 - 20mq^3 - 10nq^3 - 20mnq^3 + 10n^2q^3 - 10pq^3 - 20npq^3 + 10p^2q^3 - 5q^4 - 10nq^4 + 2q^5\}.$$

Similar expression may be obtained for f_L and f_R after rotating G for $2\pi/3$ and $4\pi/3$ radians respectively. In fact,

$$f_L = \begin{cases} f(m+q, m+p, n-m-q-p, m+q+p) & \text{if } q+p \leq n-m, \\ f(n-p, n-q, m+q+p-n, n) & \text{if } q+p \geq n-m. \end{cases}$$

$$f_R = \begin{cases} f(q, p, n-q-p, m+q+p) & \text{if } q+p \leq n, \\ f(n-p, n-q, q+p-n, m+n) & \text{if } q+p \geq n. \end{cases}$$

After some computation, we obtain the following formula for the Wiener number of an irregular convex triangular hexagon $H_{q,p,m,n}$.

Theorem 3.1

1. *If $q+p \leq n-m$, then the Wiener number of $H_{q,p,m,n}$ is*
$$\frac{1}{120}\{36m + 60m^2 + 25m^3 - m^5 + 40n + 130mn + 125m^2n + 40m^3n + 5m^4n + 60n^2 + 140mn^2 + 90m^2n^2 + 10m^3n^2 + 20n^3 + 40mn^3 + 20m^2n^3 + 14p + 60mp + 45m^2p - 5m^4p + 70np + 150mnp + 90m^2np + 20m^3np + 110n^2p + 150mn^2p + 30m^2n^2p + 40n^3p + 40mn^3p + 5p^2 - 10mp^2 - 30m^2p^2 - 10m^3p^2 + 30n^2p^2 + 20n^3p^2 - 10p^3 - 30mp^3 - 10m^2p^3 - 20np^3 - 20n^2p^3 - 5p^4 - 10mp^4 + 10np^4 - 4p^5 + 14q + 60mq + 45m^2q - 5m^4q + 70nq + 150mnq + 90m^2nq + 20m^3nq + 110n^2q + 150mn^2q + 30m^2n^2q + 40n^3q + 40mn^3q + 40pq + 60mpq - 20m^3pq + 80npq + 120mnpq + 60m^2npq + 120n^2pq + 60mn^2pq + 40n^3pq + 10p^2q - 30mp^2q - 30m^2p^2q - 20p^3q - 20mp^3q - 10p^4q + 5q^2 - 10mq^2 - 30m^2q^2 - 10m^3q^2 + 30n^2q^2 + 20n^3q^2 + 10pq^2 - 30mpq^2 - 30m^2pq^2 - 10q^3 - 30mq^3 - 10m^2q^2 - 20nq^3 - 20n^2q^3 - 20pq^3 - 20mpq^3 - 5q^4 - 10mq^4 + 10nq^4 - 10pq^4 - 4q^5\}.$$

2. *If $n-m \leq q+p \leq n$, then the Wiener number of $H_{q,p,m,n}$ is*
$$\frac{1}{120}\{40m + 60m^2 + 20m^3 + 36n + 130mn + 140m^2n + 40m^3n + 60n^2 + 125mn^2 + 90m^2n^2 + 20m^3n^2 + 25n^3 + 40mn^3 + 10m^2n^3 + 5mn^4 - n^5 + 18p + 60mp + 30m^2p + 70np + 180mnp + 90m^2np + 95n^2p + 150mn^2p + 60m^2n^2p + 40n^3p + 20mn^3p + 5n^4p + 5p^2 - 25mp^2 - 30m^2p^2 + 15np^2 - 30m^2np^2 + 30n^2p^2 + 30mn^2p^2 + 10n^3p^2 - 15p^3 - 30mp^3 - 20np^3 - 20mnp^3 - 10n^2p^3 - 5p^4 - 5mp^4 + 5np^4 - 3p^5 + 18q + 60mq + 30m^2q + 70nq + 180mnq + 90m^2nq + 95n^2q + 150mn^2q + 60m^2n^2q + 40n^3q + 20mn^3q +$$

$5n^4q+40pq+30mpq+110npq+120mnpq+120n^2pq+120mn^2pq+20n^3pq-5p^2q-30mp^2q-60mnp^2q+30n^2p^2q-20p^3q-20np^3q-5p^4q+5q^2-25mq^2-30m^2q^2+15nq^2-30m^2nq^2+30n^2q^2+30mn^2q^2+10n^3q^2-5pq^2-30mpq^2-60mnpq^2+30n^2pq^2+30mp^2q^2-30np^2q^2+10p^3q^2-15q^3-30mq^3-20nq^3-20mnq^3-10n^2q^3-20pq^3-20npq^3+10p^2q^3-5q^4-5mq^4+5nq^4-5pq^4-3q^5\}$.

3. *If $n \le q+p$, then the Wiener number of $H_{q,p,m,n}$ is*
$\frac{1}{120}\{40m+60m^2+20m^3+32n+130mn+140m^2n+40m^3n+60n^2+125mn^2+90m^2n^2+20m^3n^2+30n^3+40mn^3+10m^2n^3+5mn^4-2n^5+22p+60mp+30m^2p+70np+180mnp+90m^2np+80n^2p+150mn^2p+60m^2n^2p+40n^3p+20mn^3p+10n^4p+5p^2-25mp^2-30m^2p^2+30np^2-30m^2np^2+30n^2p^2+30mn^2p^2-20p^3-30mp^3-20np^3-20mnp^3-5p^4-5mp^4-2p^5+22q+60mq+30m^2q+70nq+180mnq+90m^2nq+80n^2q+150mn^2q+60m^2n^2q+40n^3q+20mn^3q+10n^4q+40pq+30mpq+140npq+120mnpq+120n^2pq+120mn^2pq-20p^2q-30mp^2q-60mnp^2q+60n^2p^2q-20p^3q-40np^3q+5q^2-25mq^2-30m^2q^2+30nq^2-30m^2nq^2+30n^2q^2+30mn^2q^2-20pq^2-30mpq^2-60mnpq^2+60n^2pq^2+30mp^2q^2-60np^2q^2+20p^3q^2-20q^3-30mq^3-20nq^3-20mnq^3-20pq^3-40npq^3+20p^2q^3-5q^4-5mq^4-2q^5\}$.

By considering some special cases, we have the following theorems.

Theorem 3.2 *The Wiener number of I_n is*

$$\begin{cases} \frac{1}{24}(n+1)(n+3)(2n+7) & \text{for odd } n, \\ \frac{1}{24}(n+2)(n+4)(2n+3) & \text{for even } n. \end{cases}$$

Theorem 3.3 *The Wiener number of a triangular triangle T_m is*

$$\frac{1}{40}m(m+1)(m+2)(m+3)(2m+3).$$

Since the Wiener number is invariant under rotation and reflection, so we may simply assume that $m \le n$ for the triangular parallelogram $P_{m,n}$ and triangular trapezium $T_{m.n}$.

Theorem 3.4 *The Wiener number of $P_{m,n}$, where $m \le n$, is*

$$\tfrac{1}{120}(m+1)\{-m^4+(5n+1)m^3+(10n^2+35n+24)m^2+(20n^3+80n^2+90n+36)m+20n(n+1)(n+2)\}.$$

Theorem 3.5 *The Wiener number of $T_{m,n}$, where $m \le n$, is*

$$\tfrac{1}{120}(m+1)\{-4m^4+(10n-1)m^3-(20n^2+30n+9)m^2+(20n^3+50n^2+30n+14)m+20n(n+1)(n+2)\}.$$

Remarks: The method always works in the case of a plane graph formed by n-side regular polygons with ∂G is connected. If a plane graph consisting of n-gons that are not regular, then some elementary cuts may cross itself (see Figure 2). In general, no recursive method is known for calculating the Wiener number of general odd polycyclic graphs.

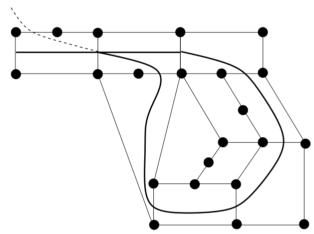

Figure 2

Appendix

Consider a homogeneous n-gonal net G, without loss of generality, we can regard G as a net consisting of two polygons P_1 and P_2 only.

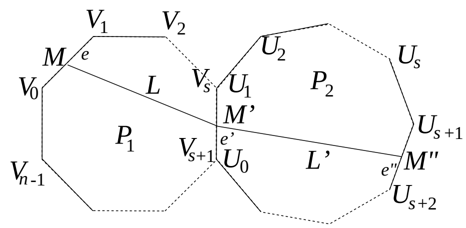

Figure 3

Starting with the edge $e \in P_1$ and counting with s^+-step, where $s = \lfloor \frac{n}{2} \rfloor$ (assume), let M and M' be the mid-point of $V_1V_0 = e$ and $V_sV_{s+1} = e'$ respectively and L be the line segment that joining M and M'. By symmetry, $\angle V_1MM' = \angle V_sM'M$. In the polygon P_2, relabeling the vertices V_{s+1} to U_0 and V_s to U_1 (see the diagram). Starting with the edge $e' \in P_2$ and counting with s^--step, let L' be the line segment joining M' and M'', where M'' is the mid-point of $U_{s+1}U_{s+2} = e''$. By symmetry, $\angle U_0M'M'' = \angle U_{s+2}M''M$. In addition, the polygon $MV_1V_2 \ldots V_sM'$ is congruent to the polygon $M'U_0U_{n-1} \ldots U_{s+2}M''$ and hence $\angle V_sM'M = \angle V_{s+1}M'M''$. In conclusion, $C = L \cup L'$ is a straight line. $\square$

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