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The number of paths in uniform cactus chains

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Abstract. A graph G is called a g-gonal cactus if G has two end blocks and every block of G is C_g, a cycle of g vertices. This paper aims to establish the generating function and the recurrence relation to count the total number of paths of all g-gonal cacti. Surprisingly, all g-gonal cacti (even the random structure) have the same total number of paths. By analyzing the Laurent series of the generating function, we derived the asymptotic formula for the total number of such paths as well. Furthermore, we constructed the formulae to calculate the number of paths of a given length of regular g-gonal cacti. The formulae are implemented in Python and provided in this paper.

1 Introduction and motivation

In this paper, we focus on simple graphs. For $v \in G$, we let $N_G(v)$ denote the *neighbor set* of v in G, which is the set of vertices adjacent to v. The *degree* of a vertex v in G is $|N_G(v)|$ and is denoted by $deg_G(v)$. A *component* is a maximal connected subgraph. If G is connected, then a vertex v is a *cut vertex* of G if the graph G is disconnected when v is removed. A *block* is a maximal connected subgraph that does not contain a cut vertex of itself. An *end block* is a block containing one cut vertex of the graph; otherwise, it is an *inner block*. For two blocks B and B', we say that B *joins* B' if $V(B) \cap V(B') \neq \varnothing$. A *cactus* is a graph in which any two cycle subgraphs have at most one vertex in common. Thus, a cactus is a graph whose all blocks are cycles or edges. A cactus is *g-uniform* if all blocks contain g vertices. Thus, if $g \geq 3$, then all the blocks are cycles C_g (or rings of C-gons), and we call a g-uniform cactus a *g-gonal cactus*. A *cactus chain* is a cactus in which all blocks contain at most two cut vertices of the

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graphs. Hence, for integers $g \geq 3$ and $n \geq 1$, a *g-gonal cactus chain* of n rings is a graph containing n blocks whose all of the blocks are C_g, a cycle of g vertices, and every block joins to at most two other blocks. Thus, a g-gonal cactus chain has exactly two end blocks. A g-gonal cactus chain is *regular* if the two cut vertices of each inner block are at the same distance for every inner block. In particular, a regular hexagonal cactus chain is said to be *ortho* (or *meta* or *para*) if the two cut vertices that belong to the same inner block are adjacent (or at distance two or at distance three, respectively).

In 1940, Mayer and Mayer [10] published the Theory of Condensation in their classical book of *Statistical Mechanics*, which was extended to the cluster and irreducible integrals by Husimi [9] in 1952. Interestingly, Husimi integrals were found, by Uhlenbeck [13], to link with graph structures in which every edge of these graphs is in at most one cycle. Such graphs were well-known by the name *Husimi trees* ever since and have attracted lots of attention, as evidenced by a number of publications. For instance, see [6, 8, 12]. In 1973, Harary and Palmer [7] published *Graphical Enumeration* containing results in Husimi trees, which were called cacti in the book, yielding that Husimi trees have become well-known in graph terminology as cacti. For more examples of the study in Husimi trees, or cacti, Došlić and Litz [1], Došlić and Måløy [3], and Došlić and Zubac [2] employed recurrence relations and generating functions to establish the number of independent sets and matchings in hexagonal cacti. In addition, by the concepts of meromorphic functions, see [14], the authors established the asymptotic behaviors of these sets when the number of blocks is large.

In this paper, the main purpose is to establish the generating function and recurrence relation of the total number of paths of all g-gonal cactus chains containing n of g-gons. Surprisingly, all g-gonal cactus chains have the same total number of paths. We obtain the asymptotic formula for this total number of paths using the behavior of the power series coefficients. Then, we establish the formulae to calculate the number of paths of a given length of the regular g-gonal cactus chains. Some computer programming codes were written for counting formulae, and we provide these at the end of the proofs. Finally, we establish exact formulae for the number of paths with a given length of para-hexagonal cactus chains.

2 Main results

This section lists all the results of this paper, while the proofs are given in the following sections. We present our results in three subsections.

2.1 The number of all paths of polygonal cactus chains

In this subsection, we establish the generating function and the recurrence relation of the total number of paths of all lengths in an arbitrary g-gonal cactus chain.

For integers $n \geq 0$ and $g \geq 3$, we let $G_g(n)$ be an arbitrary g-gonal cactus chain of n rings and let $D_g(n)$ be the total number of paths of all lengths in $G_g(n)$. Further, we have our theorems as follows.

Theorem 2.1. *For $g \geq 3$ and $n \geq 0$, we let $D_g(x)$ be the generating function of $D_g(n)$. That is, $D_g(x) = \sum_{n\geq 0} D_g(n)x^n$. Then*

$$D_g(x) = \frac{2x^3 + (2g^2 - 8g + 3)x^2 + g^2 x}{1 - 4x + 5x^2 - 2x^3}.$$

By Theorem 2.1, the recurrence relation of $D_g(n)$ is obtained as follows.

Theorem 2.2. *For $g \geq 3$, we obtain*

$$D_g(n) = 2D_g(n-3) - 5D_g(n-2) + 4D_g(n-1)$$

for all $n \geq 4$ where $D_g(1) = g^2$, $D_g(2) = 6g^2 - 8g + 3$, and $D_g(3) = 19g^2 - 32g + 14$.

By applying the idea of Laurent series and Cauchy's integral formula to the generating function in Theorem 2.1, we establish the asymptotic behavior of $D_g(n)$ as follows.

Theorem 2.3. *For $g \geq 3$ and $n \geq 0$, we obtain*

$$D_g(n) \approx 2^{n+2}(g-1)^2.$$

2.2 The number of paths of given length of regular polygonal cactus chains

In this part, we show the formulae to count the number of paths in regular polygonal cactus chains when the length is given.

For integers $g \geq 3$ and $n \geq 1$, let $G(n, g)$ be a regular g-gonal cactus chain of n rings. Since $G(n, g)$ is regular and all the blocks of $G(n, g)$ are C_g, every inner block of $G(n,g)$ has two cut vertices at the same distance, say q. By the minimality of q, we have that

$$q \leq g - q. \tag{1}$$

Hence, we can let $G(n,g,q)$ be a regular g-gonal cactus chain of n rings in which the two cut vertices of each inner block are at distance q. For an integer $\ell \geq 0$, we let $p^g_{\ell,q}(n)$ be the number of paths of length ℓ of $G(n,g,q)$. Further, we let

$$f(\ell,g) = \begin{cases} ng & \text{if } \ell \leq g-1, \\ 0 & \text{otherwise.} \end{cases}$$

Now, we are ready to establish formulae for counting $p^g_{\ell,q}(n)$ due to inequality (1).

Theorem 2.4. *If* $q < g - q$, *then*

$$p^g_{\ell,q}(n) = f(\ell,g) + 4\sum_{j=r}^{n}(n-j+1)\sum_{i=1}^{g-1}\sum_{t=1}^{g-1}F_1(\ell,t,i,j,q)$$

where $r = \max\left\{0,\ \left\lceil \frac{\ell-2g+2}{g-q} \right\rceil\right\} + 2$ *and*

$$F_1(\ell,t,i,j,q) = \begin{cases} \dbinom{j-2}{\frac{\ell-t-i-qj+2q}{g-2q}} & \text{if } \frac{\ell-t-i-qj+2q}{g-2q} \in \mathbb{N}\cup\{0\}, \\ 0 & \text{otherwise.} \end{cases}$$

Theorem 2.5. *If* $2q = g$, *then*

$$p^g_{\ell}(n) = f(\ell,g) + 4\sum_{j=r}^{n}(n-j+1)\sum_{i=1}^{g-1}\sum_{t=1}^{g-1}F_2(\ell,t,i,j,q)$$

where $r = \max\left\{0, \left\lceil \frac{\ell-2g+2}{g-q} \right\rceil\right\} + 2$ *and*

$$F_2(\ell,t,i,j,q) = \begin{cases} 2^{(\ell-t-i)/q} & \text{if } \frac{\ell-t-i}{q} = j-2, \\ 0 & \text{otherwise.} \end{cases}$$

2.3 Exact formulae of the number of paths of given length of para-hexagonal cactus chains

In this part, we establish the exact formulae for the number of paths of para-hexagonal cactus chains.

Lemma 2.6. *Let G be a para-hexagonal cactus chain of n hexagons and let $p_\ell(n)$ be the number of paths of length ℓ in G. Then,*

$$p_\ell(n) = \begin{cases} 5n+1 & \text{if } \ell = 0, \\ 6n & \text{if } \ell = 1, \\ 10n-4 & \text{if } \ell = 2, \\ 14n-8 & \text{if } \ell = 3, \\ 18n-12 & \text{if } \ell = 4. \end{cases}$$

Lemma 2.7. *If $p_5(n)$ is the number of paths of length five of a para-hexagonal cactus chain of n hexagons, then*

$$p_5(n) = \begin{cases} 6 & \text{if } n = 1, \\ 28 & \text{if } n = 2, \\ 30n-32 & \text{if } n \geq 3. \end{cases}$$

Lemma 2.8. *If $p_6(n)$ is the number of paths of length six of a para-hexagonal cactus chain of n hexagons, then*

$$p_6(n) = \begin{cases} 0 & \text{if } n = 1, \\ 20 & \text{if } n = 2, \\ 36n-52 & \text{if } n \geq 3. \end{cases}$$

Lemma 2.9. *If $p_7(n)$ is the number of paths of length seven of a para-hexagonal cactus chain of n hexagons, then*

$$p_7(n) = \begin{cases} 0 & \text{if } n = 1, \\ 16 & \text{if } n = 2, \\ 40n-64 & \text{if } n \geq 3. \end{cases}$$

Theorem 2.10. *For integers $\ell \geq 8$ and $n \geq \lfloor \frac{\ell-2}{3} \rfloor$, we let $p_\ell(n)$ be the number of paths of length ℓ of a para-hexagonal cactus chain of n hexagons.*

If $\ell = 3k$*, then*

$$p_\ell(n) = \begin{cases} 2^k & \text{if } n = k-1, \\ 7 \cdot 2^k & \text{if } n = k, \\ 20 \cdot (n-k-1) \cdot 2^{k-1} + 17 \cdot 2^k & \text{if } n \geq \lceil \frac{\ell+2}{3} \rceil. \end{cases}$$

Theorem 2.11. *For integers* $\ell \geq 8$ *and* $n \geq \lfloor \frac{\ell-2}{3} \rfloor$*, we let* $p_\ell(n)$ *be the number of paths of length* ℓ *of a para-hexagonal cactus chain of* n *hexagons. If* $\ell = 3k+1$*, then*

$$p_\ell(n) = \begin{cases} 2^{k-1} & \text{if } n = k-1, \\ 5 \cdot 2^k & \text{if } n = k, \\ 21 \cdot (n-k-1) \cdot 2^{k-1} + 31 \cdot 2^{k-1} & \text{if } n \geq \lceil \frac{\ell+2}{3} \rceil. \end{cases}$$

Theorem 2.12. *For integers* $\ell \geq 8$ *and* $n \geq \lfloor \frac{\ell-2}{3} \rfloor$*, we let* $p_\ell(n)$ *be the number of paths of length* ℓ *of a para-hexagonal cactus chain of* n *hexagons. If* $\ell = 3k+2$*, then*

$$p_\ell(n) = \begin{cases} 0 & \text{if } n = k-1, \\ 3 \cdot 2^k & \text{if } n = k, \\ 30 \cdot (n-k-1) \cdot 2^{k-1} + 14 \cdot 2^k & \text{if } n \geq \lceil \frac{\ell+2}{3} \rceil. \end{cases}$$

3 Proofs of Theorems 2.1, 2.2, and 2.3

We first establish the generating function and recurrence relation of the number of paths of any g-gonal cactus chain of n rings.

3.1 Proofs of Theorems 2.1 and 2.2

Recall that, for integers $n \geq 0$ and $g \geq 3$, we let $G_g(n)$ be a g-gonal cactus chain of n rings, and we let $D_g(n)$ be the total number of paths in $G_g(n)$. It is worth noting that, when $n = 0$, we let $D_g(0) = 0$ as there is no graph, resulting in no path of any length (a path of length 0 is considered a vertex). When it is clear from the context, we may name all the g-gons of $G_g(n)$ consecutively by the 1^{st} to the n^{th} rings. That is, the 1^{st} and n^{th} rings are the two end blocks of $G_g(n)$ while the $2^{\text{nd}}, \ldots, (n-1)^{\text{th}}$ rings are the inner blocks.

Further, we let $\overline{D}(n-1)$ denote the total number of paths of lengths at least one in $G_g(n)$ whose one end vertex is at the cut vertex of the n^{th} ring and the other end vertex is in the i^{th} ring for some $1 \leq i \leq n-1$.

Clearly, there are a total of g^2-1 paths of lengths 0 to $g-1$ in the n^{th} ring (excluding the common vertex between the $(n-1)^{\text{th}}$ ring and the n^{th} ring, which is already counted in $D_g(n-1)$), and there are $2(g-1)\overline{D}(n-1)$ paths crawling across the $(n-1)^{\text{th}}$ ring and the n^{th} ring. Thus, for $n \geq 2$, we have that

$$D_g(n) = g^2 - 1 + D_g(n-1) + 2(g-1)\overline{D}(n-1). \tag{2}$$

Next, we count $\overline{D}(n)$. It can be checked that there are $2(g-1)$ paths of length at least one that start from the common vertex, say x, of the n^{th} ring and the $(n+1)^{\text{th}}$ ring and are in only the n^{th} ring. For the paths starting from x and ending in the $1^{\text{st}}, \ldots, (n-1)^{\text{th}}$ rings, there are two possibilities to crawl across the n^{th} ring. Since $\overline{D}(1) = 2(g-1)$, we have that

$$\begin{aligned}
\overline{D}(n) &= 2(g-1) + 2\overline{D}(n-1) \\
&= 2(g-1)(1+2) + 2^2\overline{D}(n-2) \\
&= 2(g-1)(1+2+2^2) + 2^3\overline{D}(n-3) \\
&\ \ \vdots \\
&= 2(g-1)(1+2+2^2+\cdots+2^{n-2}) + 2^{n-1}\overline{D}(1) \\
&= 2(g-1)(2^n-1).
\end{aligned}$$

Thus,

$$\overline{D}(n-1) = 2(g-1)(2^{n-1}-1).$$

By (2), we have that

$$\begin{aligned}
D_g(n) &= g^2 - 1 + D_g(n-1) + 2(g-1)(2(g-1)(2^{n-1}-1)) \\
&= D_g(n-1) + (g-1)^2 2^{n+1} - (3g^2 - 8g + 5).
\end{aligned}$$

Let $b = (g-1)^2$ and $a = 3g^2 - 8g + 5$. Therefore,

$$D_g(n) = D_g(n-1) + b \cdot 2^{n+1} - a. \tag{3}$$

By repeated substitution, we obtain

$$D_g(n) = D_g(2) + b(2^{n+2} - 16) - (n-2)a.$$

Because $D_g(2) = 6g^2 - 8g + 3$, the exact formula of $D_g(n)$ for $n \geq 2$ is

$$D_g(n) = 6g^2 - 8g + 3 + b(2^{n+2} - 16) - (n-2)a.$$

In the following, we derive the generating function of $D_g(n)$ from (3), which we use to establish the asymptotic behavior of $D_g(n)$. Let $D_g(x)$ be the generating function of $D_g(n)$, that is, $D_g(x) = \sum_{n \geq 0} D_g(n)x^n$.

For $n \geq 2$, we multiply x^n to (3) and sum over all the values of n. We have that

$$\sum_{n\geq 2} D_g(n)x^n = \sum_{n\geq 2} D_g(n-1)x^n + 2b\sum_{n\geq 2} 2^n x^n - a\sum_{n\geq 2} x^n \tag{4}$$

We consider L.H.S. of (4). Thus,

$$\begin{aligned}\sum_{n\geq 2} D_g(n)x^n &= \sum_{n\geq 1} D_g(n)x^n - D_g(1)x^1 - D_g(0)x^0\\ &= \sum_{n\geq 0} D_g(n)x^n - g^2x - D_g(0)\\ &= D_g(x) - g^2x.\end{aligned}$$

We next consider R.H.S. of (4). Thus,

$$\sum_{n\geq 2} D_g(n-1)x^n = x\sum_{n\geq 1} D_g(n)x^n = xD_g(x),$$

$$2b\sum_{n\geq 2} 2^n x^n = 2b\left(\sum_{n\geq 0}(2x)^n - (2x)^1 - 1\right) = \frac{2b}{1-2x} - 4bx - 2b,$$

$$-a\sum_{n\geq 2} x^n = -a\left(\sum_{n\geq 0} x^n - x^1 - x^0\right) = \frac{-a}{1-x} + ax + a.$$

Plugging in (4), we have

$$D_g(x) - g^2x = xD_g(x) + \frac{2b}{1-2x} - 4bx - 2b + \frac{-a}{1-x} + ax + a,$$

which can be solved such that

$$\begin{aligned}D_g(x) &= \frac{(2g^2+2a-8b)x^3 + (8b-a-3g^2)x^2 + g^2x}{1-4x+5x^2-2x^3}\\ &= \frac{2x^3 + (2g^2-8g+3)x^2 + g^2x}{1-4x+5x^2-2x^3}.\end{aligned} \tag{5}$$

This proves Theorem 2.1.

It is worth noting that the generating function in (5) can be used to obtain the recurrence relation of $D_g(n)$ as

$$D_g(n) = 4D_g(n-1) - 5D_g(n-2) + 2D_g(n-3),$$

for all $n \geq 4$, where

$$D_g(1) = g^2, \qquad D_g(2) = 6g^2 - 8g + 3, \qquad D_g(3) = 19g^2 - 32g + 14,$$

establishing the proof of Theorem 2.2.

3.2 Proof of Theorem 2.3

We establish the asymptotic behavior of the number of all paths. From

$$D_g(x) = \frac{2x^3 + (2g^2 - 8g + 3)x^2 + g^2 x}{1 - 4x + 5x^2 - 2x^3},$$

the denominator gives the poles as $x_0 = 0.5$, $x_1 = 1$, $x_2 = 1$. Then consider the principal part of the Laurent series of $D_g(x)$ at $x_0 = 0.5$:

$$\sum_{n=1}^{\infty} a_{-n}(x - x_0)^{-n}$$

where $a_{-n} = \frac{1}{2\pi i}\int_c \frac{D_g(x)}{(x-x_0)^{-n+1}}\, dx;\ n = 1, 2, 3, \ldots$ with a simple closed curve c in a suitable region.

Computing the coefficients a_{-n} for $n = 1, 2, 3, \ldots$, we have

$$\begin{aligned} a_{-n} &= \frac{1}{2\pi i}\int_c \frac{2x^3 + (2g^2 - 8g + 3)x^2 + g^2 x}{-2(x - 0.5)^{-n+2}(x - 1)^2}\, dx \\ &= \frac{1}{2\pi i}\int_c \frac{\left(2x^3 + (2g^2 - 8g + 3)x^2 + g^2 x\right)(x - 0.5)^{n-2}}{-2(x - 1)^2}\, dx. \end{aligned}$$

For $n = 1$, by Cauchy's integral formula, one can compute that

$$\begin{aligned} a_{-1} &= \frac{1}{2\pi i}\int_c \frac{\left(2x^3 + (2g^2 - 8g + 3)x^2 + g^2 x\right)(x - 0.5)^{-1}}{-2(x - 1)^2}\, dx \\ &= \left(\frac{2(0.5^3) + (2g^2 - 8g + 3)0.5^2 + g^2(0.5)}{-2(0.5 - 1)^2}\right) \\ &= 2g^2 - 4g + 2. \end{aligned} \tag{6}$$

For $n \geq 2$, by Cauchy's integral formula, we obtain

$$a_{-n} = \frac{1}{2\pi i}\int_c \frac{\left(2x^3 + (2g^2 - 8g + 3)x^2 + g^2 x\right)(x - 0.5)^{n-2}}{-2(x - 1)^2}\, dx = 0. \tag{7}$$

Therefore, the principal part of the Laurent series of $D_g(x)$ is

$$\frac{-2(g - 1)^2}{x - 0.5}.$$

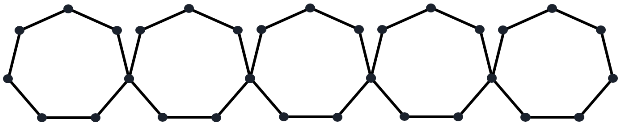

Figure 4.1: The regular g-gonal cactus chain $G(5, 7, 3)$.

Rewriting coefficients that approximate our number of all paths $D_g(n)$ as

$$\begin{aligned}\frac{-2(g-1)^2}{(x-(0.5))} &= \frac{2(g-1)^2}{(0.5)(1-(x/0.5))} \\ &= \sum_{n\geq 0}\left(\frac{2(g-1)^2}{0.5}\right)\frac{1}{0.5^n}x^n \\ &= \sum_{n\geq 0}\left(\frac{2(g-1)^2}{0.5^{n+1}}\right)x^n \\ &= \sum_{n\geq 0} 2^{n+2}(g-1)^2x^n.\end{aligned}$$

4 Proofs of Theorems 2.4 and 2.5

Recall that, for integers $g \geq 3$ and $n \geq 1$, $G(n, g)$ is a regular g-gonal cactus chain of n rings. Since $G(n, g)$ is regular and all the blocks of $G(n, q)$ are C_g, every inner block of $G(n, g)$ has two cut vertices at the same distance, say q. Therefore, we can let $G(n, g, q)$ be a regular g-gonal cactus chain of n rings in which the two cut vertices of each inner block are at distance q. See Figure 4.1 for an illustration with this notation. Further, for an integer $\ell \geq 0$, let $p^g_{\ell,q}(n)$ be the number of paths of length ℓ of $G(n, g, q)$.

Further, we let

$$f(\ell, g) = \begin{cases} ng & \text{if } \ell \leq g-1, \\ 0 & \text{otherwise.}\end{cases}$$

Now, we are ready to establish the formulae for counting $p^g_{\ell,q}(n)$ based on the inequality (1).

4.1 Proof of Theorem 2.4

Let $f(\ell, g)$ be the number of paths that crawl inside exactly one ring. When $\ell \geq g$, it is easy to see that $f(\ell, g) = 0$. When $\ell \leq g-1$, it is possible that

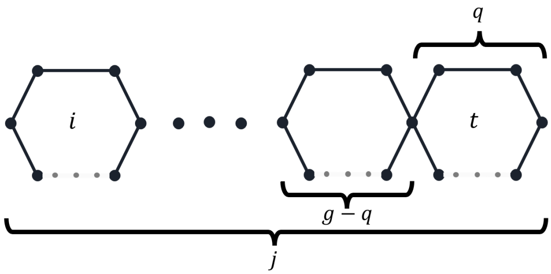

Figure 4.2: Regular g-gonal cactus chain.

a path of length ℓ crawls in one ring. There are g of such paths, resulting in ng additional paths in this case. Thus,

$$f(\ell, g) = \begin{cases} ng & \text{if } \ell \leq g-1, \\ 0 & \text{otherwise.} \end{cases}$$

When counting the number of paths that crawl in at least two rings, every path of length ℓ must crawl in at least

$$r = \max\left\{0, \left\lceil \frac{\ell - 2g + 2}{g - q} \right\rceil \right\} + 2$$

rings and crawl in at most n rings. For $r \leq j \leq n$, let j be the number of rings that a path of length ℓ lies on.

For convenience, we count when the path crawls in ring 1 to ring j. For integers i, t and a path P of length ℓ, we let i be the number of edges of P in ring 1 and t be the number of edges of P in ring j. Since P crawls in more than one ring, we have that $1 \leq t \leq g-1$ and $1 \leq i \leq g-1$. Further, let x_q be the number of rings $2, \ldots, j-1$ that P passes with q edges and x_{g-q} be the number of rings $2, \ldots, j-1$ that P passes with $g-q$ edges. Thus,

$$qx_q + (g-q)x_{g-q} = \ell - t - i$$
$$x_q + x_{g-q} = j - 2$$

which can be solved such that

$$x_{g-q} = \frac{\ell - t - i - qj + 2q}{g - 2q}.$$

Since x_{g-q} is the number of rings (which is always a non-negative integer), it follows that
$$\frac{\ell - t - i - qj + 2q}{g - 2q} \in \mathbb{N} \cup \{0\}.$$
There are $\binom{j-2}{\frac{\ell-t-i-qj+2q}{g-2q}}$ possibilities of selecting rings $2, \ldots, j-1$ so that the path P passes with q edges. Further, there are 2 possibilities for the head and 2 possibilities for the tail of P to lie on rings 1 and j, respectively. Thus, for each $r \leq j \leq n$, there are $4 \cdot \binom{j-2}{\frac{\ell-t-i-qj+2q}{g-2q}}$ paths of length ℓ that crawl across ring 1 to ring j. Since the path of length ℓ crawling across j rings can lie from rings 1 to j until from rings $n-j+1$ to n, it follows that the number of paths of length ℓ in $G(n, g, q)$ is
$$p^g_{\ell,q}(n) = f(\ell, g) + 4\sum_{j=r}^{n}(n-j+1)\sum_{i=1}^{g-1}\sum_{t=1}^{g-1}\binom{j-2}{\frac{\ell-t-i-qj+2q}{g-2q}}.$$
This proves Theorem 2.4.

4.2 Proof of Theorem 2.5

We can prove the result on $f(\ell, g)$, the number of paths that crawl inside exactly one ring, similarly to the proof of Theorem 2.4.

We then count the number of paths that crawl in at least two rings. Similarly, in this case, every path of length ℓ must crawl in at least
$$r = \max\left\{0, \left\lceil \frac{\ell - 2g + 2}{g - q} \right\rceil\right\} + 2$$
rings and crawl in at most n rings. For $r \leq j \leq n$, let j be the number of rings that a path of length ℓ lies on.

We first count when the path crawls in the ring 1 to ring j. Let i be the number of edges of P in ring 1 and t be the number of edges of P in ring j. Since P crawls in more than one ring, we have that $1 \leq t \leq g-1$ and $1 \leq i \leq g-1$. We also let x_q be the number of rings $2, \ldots, j-1$ that P passes with q edges. Thus,
$$qx_q = \ell - t - i$$
$$x_q = j - 2$$
which can be solved such that
$$j - 2 = \frac{\ell - t - i}{q}.$$

There are 2 possibilities when a path crawls across each of the rings $2, \dots,$ $j-1$, and there are 2 possibilities for the head and 2 possibilities for the tail of a path to crawl across rings 1 and j, respectively. Thus, for each $r \leq j \leq n$, there are $4 \cdot 2^{\frac{\ell-t-i}{q}}$ paths of length ℓ that crawl across ring 1 to ring j. Since the path of length ℓ crawling across j rings can lie from rings 1 to j until from rings $n-j+1$ to n, it follows that the number of paths of length ℓ in $G(n,g,q)$ is

$$p^g_{\ell,q}(n) = f(\ell,g) + 4\sum_{j=r}^{n}(n-j+1)\sum_{i=1}^{g-1}\sum_{t=1}^{g-1}2^{\frac{\ell-t-i}{q}}.$$

This proves Theorem 2.5.

We also coded in Python the formula to count the number of paths of given lengths of regular polygonal cactus chains. See [11] to obtain the python code.

5 Proofs of Lemmas 2.6–2.9

In this section, we prove the exact formulae for the number of paths of para-hexagonal cactus chains when the number of rings is at most 7. The following observation is routine and we omit the proof.

Observation 5.1. For $0 \leq \ell \leq 3n+4$ and $1 \leq k \leq n-1$ such that $k = \lfloor \frac{\ell}{3} \rfloor$, let G be a para-hexagonal cactus chain that contains n hexagons and let $\bar{p}_\ell(n)$ be the number of paths of length ℓ in G having one end vertex at the vertex at distance three from the cut vertex of the first hexagon. Then,

$$\bar{p}_\ell(n) = \begin{cases} 1 & \text{if } \ell = 0, \\ 2 & \text{if } \ell \in \{1,2\}, \\ 2^k & \text{if } \ell = 3k, \\ 3\cdot 2^k & \text{if } \ell \in \{3k+1, 3k+2\}, \\ 2^n & \text{if } \ell \in \{3n+2, 3n+1, 3n\}, \\ 0 & \text{if } \ell \in \{3n+3, 3n+4\}. \end{cases}$$

Next we establish the formulae of $p_\ell(n)$, the number of paths of length ℓ in para-hexagonal cactus chains.

5.1 Proof of Lemma 2.6

Clearly, when $\ell = 0$, then $p_0(n)$ is the number of vertices of G, which is $5n+1$. When $\ell = 1$, then $p_1(n)$ is the number of edges of G, which is $6n$. When $\ell = 2$, we count $p_2(n)$ via the combination of the neighbors of each vertex choosing two. There are $4n+2$ vertices of degree two and there are $n-1$ vertices of degree four. Thus, $p_2(n) = (4n+2)\binom{2}{2}+(n-1)\binom{4}{2} = 10n-4$. This completes the proof when $0 \leq \ell \leq 2$. We distinguish 3 cases according to the value of ℓ.

Case 1: $\ell = 3$.

When $\ell = 3$, there are six copies of P_3 that are completely in the n^{th} hexagon. Further, there are $2\bar{p}_2(n-1)$ of the paths P_3 that have one edge in the n^{th} hexagon, there are $2\bar{p}_1(n-1)$ of paths P_3 that have two edges in the n^{th} hexagon, and there are $p_3(n-1)$ that do not have any edges in the n^{th} hexagon. Thus

$$\begin{aligned} p_3(n) &= 6 + p_3(n-1) + 2\bar{p}_2(n-1) + 2\bar{p}_1(n-1) \\ &= 14 + p_3(n-1). \end{aligned}$$

By applying this equation $n-1$ times, we obtain

$$p_3(n) = 14(n-1) + p_3(1) = 14n - 8.$$

This proves case 1.

Case 2: $\ell = 4$.

When $\ell = 4$, there are six copies of P_4 that are completely in the n^{th} hexagon. Further, there are $2\bar{p}_3(n-1)$ of paths P_4 that have two edges in the n^{th} hexagon, there are $2\bar{p}_2(n-1)$ of paths P_4 that have two edges in the n^{th} hexagon, there are $2\bar{p}_1(n-1)$ of paths P_4 that have two edges in the n^{th} hexagon, and there are $p_4(n-1)$ that do not have any edges in the n^{th} hexagon. Thus

$$\begin{aligned} p_4(n) &= 6 + p_4(n-1) + 2\bar{p}_3(n-1) + 2\bar{p}_2(n-1) + 2\bar{p}_1(n-1) \\ &= 18 + p_4(n-1). \end{aligned}$$

By applying this equation $n-1$ times, we obtain

$$p_4(n) = 18(n-1) + p_4(1) = 18n - 12.$$

This proves case 2.

5.2 Proof of Lemma 2.7

There are six of P_5 that are completely in the n^{th} hexagon. Thus, $p_5(1) = 6$. It is routine to check that $p_5(2) = 28$ and $p_5(3) = 58$. Thus, we may assume that $n \geq 4$.

It can be observed that every path of length five has 0, 1, 2, 3, or 4 edges in the n^{th} hexagon. There are $p_5(n-1)$ paths of length five that have no edges in the n^{th} hexagon, there are $2\bar{p}_4(n-1)$ paths of length five that have one edge in the n^{th} hexagon, there are $2\bar{p}_3(n-1)$ paths of length five that have two edges in the n^{th} hexagon, there are $2\bar{p}_2(n-1)$ paths of length five that have three edges in the n^{th} hexagon, and there are $2\bar{p}_1(n-1)$ paths of length five that have four edges in the n^{th} hexagon. Thus,

$$p_5(n) = 6 + p_5(n-1) + 2(\bar{p}_4(n-1) + \bar{p}_3(n-1) + \bar{p}_2(n-1) + \bar{p}_1(n-1)).$$

By Observation 5.1, we have that

$$p_5(n) = 6 + p_5(n-1) + 2(6 + 2 + 2 + 2) = p_5(n-1) + 30.$$

By applying this equation $n-3$ times, we obtain

$$p_5(n) = 30(n-3) + p_5(3) = 30n - 32.$$

This completes the proof.

5.3 Proof of Lemma 2.8

There is no path of length six in a hexagon. Thus, $p_6(1) = 0$. It is routine to check that $p_6(2) = 20$ and $p_6(3) = 56$. Thus, we may assume that $n \geq 4$.

It can be observed that every path of length six has 0, 1, 2, 3, 4, or 5 edges in the n^{th} hexagon. There are $p_6(n-1)$ paths of length six that have no edges in the n^{th} hexagon, there are $2\bar{p}_5(n-1)$ paths of length six that have one edge in the n^{th} hexagon, there are $2\bar{p}_4(n-1)$ paths of length six that have two edges in the n^{th} hexagon, there are $2\bar{p}_3(n-1)$ paths of length six that have three edges in the n^{th} hexagon, there are $2\bar{p}_2(n-1)$ paths of length six that have four edges in the n^{th} hexagon, and there are $2\bar{p}_1(n-1)$ paths of length six that have five edges in the n^{th} hexagon. Thus,

$$\begin{aligned} p_6(n) = p_6(n-1) + 2\Big(&\bar{p}_5(n-1) + \bar{p}_4(n-1) \\ &+ \bar{p}_3(n-1) + \bar{p}_2(n-1) + \bar{p}_1(n-1)\Big). \end{aligned}$$

By Observation 5.1, we have that

$$\begin{aligned} p_6(n) &= p_6(n-1) + 2(6+6+2+2+2) \\ &= p_6(n-1) + 36. \end{aligned}$$

By applying this equation $n-3$ times, we obtain

$$p_6(n) = 36(n-3) + p_6(3) = 36n - 52.$$

This completes the proof.

5.4 Proof of Lemma 2.9

There is no path of length seven in a hexagon. Thus, $p_7(1) = 0$. It is routine to check that $p_7(2) = 16$ and $p_7(3) = 56$. Thus, we may assume that $n \geq 4$.

It can be observed that every path of length seven has 0, 1, 2, 3, 4, 5, or 6 edges in the n^{th} hexagon. There are $p_7(n-1)$ paths of length seven that have no edges in the n^{th} hexagon, there are $2\bar{p}_6(n-1)$ paths of length seven that have one edge in the n^{th} hexagon, there are $2\bar{p}_5(n-1)$ paths of length seven that have two edges in the n^{th} hexagon, there are $2\bar{p}_4(n-1)$ paths of length seven that have three edges in the n^{th} hexagon, there are $2\bar{p}_3(n-1)$ paths of length seven that have four edges in the n^{th} hexagon, and there are $2\bar{p}_2(n-1)$ paths of length seven that have five edges in the n^{th} hexagon. Thus,

$$\begin{aligned} p_7(n) = p_7(n-1) + 2\Big(&\bar{p}_6(n-1) + \bar{p}_5(n-1) \\ &+ \bar{p}_4(n-1) + \bar{p}_3(n-1) + \bar{p}_2(n-1)\Big). \end{aligned}$$

By Observation 5.1, we have that

$$\begin{aligned} p_7(n) &= p_7(n-1) + 2(4+6+6+2+2) \\ &= p_7(n-1) + 40. \end{aligned}$$

By applying this equation $n-3$ times, we obtain

$$p_7(n) = 40(n-3) + p_7(3) = 40n - 64.$$

This completes the proof.

6 Proofs of Theorems 2.10–2.12

Throughout the rest of this paper, for a given length $\ell \geq 8$ of a path, the smallest n such that a para-hexagonal cactus chain of n hexagons that can contain a P_ℓ is $\lfloor \frac{\ell-2}{3} \rfloor$ (which is not true when $\ell \leq 7$), and the smallest n such that we may count the number of P_ℓ in the general case is $\lceil \frac{\ell+2}{3} \rceil$. We are ready to establish the number of paths P_ℓ for all $\ell \geq 8$.

6.1 Proof of Theorem 2.10

First, we assume that $n = k-1$. Thus, there are only two possibilities: (i) the first hexagon contains 5 edges of a P_{3k} while the $(k-1)^{\text{th}}$ hexagon contains 4 edges of the P_{3k}, and (ii) the first hexagon contains 4 edges of a P_{3k} while the $(k-1)^{\text{th}}$ hexagon contains 5 edges of the P_{3k}. In each case, there are 2^{k-1} copies of P_{3k}. Thus, $p_{3k}(k-1) = 2^k$.

Now, we may assume that $n = k$. Thus, we arrive at the following possibilities:

(i) for all $1 \leq i \leq 5$, the first hexagon contains i edges of a P_{3k} while the k^{th} hexagon contains $6-i$ edges of the P_{3k};

(ii) the first hexagon does not contain any edges of the P_{3k}; and

(iii) the k^{th} hexagon does not contain any edges of the P_{3k}.

In each of the cases (ii) and (iii), there are $p_{3k}(k-1) = 2^k$ copies of P_{3k}. Furthermore, for the case (i), it can be checked that there are 2^k copies of P_{3k}. Thus, $p_{3k}(k) = 7 \cdot 2^k$.

To consider the case when $n \geq \lceil \frac{\ell+2}{3} \rceil$, we first assume that $n = k+1$. In this case, we have the following possibilities:

(i) for all $1 \leq i \leq 2$, the first hexagon contains i edges of a P_{3k} while the $(k+1)^{\text{th}}$ hexagon contains $3-i$ edges of the P_{3k};

(ii) the first hexagon does not contain any edges of the P_{3k}; and

(iii) the $(k+1)^{\text{th}}$ hexagon does not contain any edges of the P_{3k}.

In each of the cases (ii) and (iii), there are $p_{3k}(k) = 2^k$ copies of P_{3k}. However, it is possible for the cases (ii) and (iii) to occur simultaneously, which results in an overcount. Thus, there are

$$p_{3k}(k) + p_{3k}(k) - p_{3k}(k-1) = 7 \cdot 2^k + 7 \cdot 2^k - 2^k = 13 \cdot 2^k$$

copies of P_{3k} in cases (ii) and (iii). For each i of case (i), it can be checked that there are 2^{k+2} copies of P_{3k}. Thus,

$$p_{3k}(k+1) = 13 \cdot 2^k + 2^{k+2} = 17 \cdot 2^k.$$

Now, for the general case $n \geq \lceil \frac{\ell+2}{3} \rceil$, it can be observed that every path of length ℓ has 0, 1, 2, 3, 4, or 5 edges in the n^{th} hexagon. There are $p_\ell(n-1)$ paths of length ℓ that have no edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-1}(n-1)$ paths of length ℓ that have one edge in the n^{th} hexagon, there are $2\bar{p}_{\ell-2}(n-1)$ paths of length ℓ that have two edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-3}(n-1)$ paths of length ℓ that have three edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-4}(n-1)$ paths of length ℓ that have four edges in the n^{th} hexagon, and there are $2\bar{p}_{\ell-5}(n-1)$ paths of length ℓ that have five edges in the n^{th} hexagon. Thus,

$$\begin{aligned} p_\ell(n) = p_\ell(n-1) + 2\Big(&\bar{p}_{\ell-1}(n-1) + \bar{p}_{\ell-2}(n-1) + \bar{p}_{\ell-3}(n-1) \\ &+ \bar{p}_{\ell-4}(n-1) + \bar{p}_{\ell-5}(n-1)\Big). \end{aligned}$$

By Observation 5.1, we have that

$$p_\ell(n) = p_\ell(n-1) + 20 \cdot 2^{k-1}.$$

By applying this equation $n-k-1$ times, we obtain

$$\begin{aligned} p_\ell(n) &= 20(n-k-1) \cdot 2^{k-1} + p_\ell(k+1) \\ &= 20(n-k-1) \cdot 2^{k-1} + p_{3k}(k+1) \\ &= 20(n-k-1) \cdot 2^{k-1} + 17 \cdot 2^k. \end{aligned}$$

This completes the proof.

6.2 Proof of Theorem 2.11

First, we assume that $n = k-1$. Thus, there is only one possibility, which is the first hexagon and the $(k-1)^{\text{th}}$ hexagon contain 5 edges of a P_{3k+1}. There are 2^{k-1} copies of P_{3k+1}. Thus, $p_{3k+1}(k-1) = 2^{k-1}$.

Now, we assume that $n = k$. Thus, we arrive at the following possibilities:

(i) for all $2 \leq i \leq 5$, the first hexagon contains i edges of a P_{3k+1} while the k^{th} hexagon contains $7-i$ edges of the P_{3k+1};

(ii) the first hexagon does not contain any edges of the P_{3k+1}; and

(iii) the k^{th} hexagon does not contain any edges of the P_{3k+1}.

In each of the cases (ii) and (iii), there are $p_{3k+1}(k-1) = 2^{k-1}$ copies of P_{3k+1}. Further, for the case (i), it can be checked that there are 2^{k+2} copies of P_{3k+1}. Thus, $p_{3k+1}(k) = 2^{k+2} + 2^{k-1} + 2^{k-1} = 5 \cdot 2^k$.

To consider the case when $n \geq \lceil \frac{\ell+2}{3} \rceil$, we first assume that $n = k+1$. In this case, we have the following possibilities:

(i) for all $1 \leq i \leq 3$, the first hexagon contains i edges of a P_{3k+1} while the $(k+1)^{\text{th}}$ hexagon contains $4-i$ edges of the P_{3k+1};

(ii) the first hexagon does not contain any edge of the P_{3k+1}; and

(iii) the $(k+1)^{\text{th}}$ hexagon does not contain any edge of P_{3k+1}.

In each of the cases (ii) and (iii), there are $p_{3k+1}(k) = 2^k$ copies of P_{3k+1}. However, it is possible that the cases (ii) and (iii) occur at the same time, and this yields an overcount. Thus, there are

$$p_{3k+1}(k) + p_{3k+1}(k) - p_{3k+1}(k-1) = 5 \cdot 2^k + 5 \cdot 2^k - 2^{k-1} = 19 \cdot 2^{k-1}$$

copies of P_{3k+1} in cases (ii) and (iii). For each i of case (i), it can be checked that there are 2^{k+1} copies of P_{3k+1}. Thus,

$$p_{3k+1}(k+1) = 19 \cdot 2^{k-1} + 3 \cdot 2^{k+1} = 31 \cdot 2^{k-1}.$$

Now, for the general case $n \geq \lceil \frac{\ell+2}{3} \rceil$, it can be observed that every path of length ℓ has 0, 1, 2, 3, 4, or 5 edges in the n^{th} hexagon. There are $p_\ell(n-1)$ paths of length ℓ that have no edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-1}(n-1)$ paths of length ℓ that have one edge in the n^{th} hexagon, there are $2\bar{p}_{\ell-2}(n-1)$ paths of length ℓ that has two edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-3}(n-1)$ paths of length ℓ that have three edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-4}(n-1)$ paths of length ℓ that have four edges in the n^{th} hexagon, and there are $2\bar{p}_{\ell-5}(n-1)$ paths of length ℓ that have five edges in the n^{th} hexagon. Thus,

$$\begin{aligned} p_\ell(n) = p_\ell(n-1) + 2\Big(&\bar{p}_{\ell-1}(n-1) + \bar{p}_{\ell-2}(n-1) + \bar{p}_{\ell-3}(n-1) \\ &+ \bar{p}_{\ell-4}(n-1) + \bar{p}_{\ell-5}(n-1)\Big). \end{aligned}$$

By Observation 5.1, we have that

$$p_\ell(n) = p_\ell(n-1) + 21 \cdot 2^{k-1}.$$

By applying this equation $n-k-1$ times, we obtain

$$\begin{aligned} p_\ell(n) &= 21(n-k-1) \cdot 2^{k-1} + p_\ell(k+1) \\ &= 21(n-k-1) \cdot 2^{k-1} + p_{3k+1}(k+1) \\ &= 21(n-k-1) \cdot 2^{k-1} + 31 \cdot 2^{k-1}. \end{aligned}$$

This completes the proof.

6.3 Proof of Theorem 2.12

First, we assume that $n = k - 1$. Thus, there is only one possibility, which is the first hexagon and the $(k-1)^{\text{th}}$ hexagon contain 5 edges of a P_{3k+2}. There are 2^{k-1} copies of P_{3k+1}. Thus, $p_{3k+2}(k-1) = 0$.

Now, we may assume that $n = k$. Thus, we arrive at the following possibilities:

(i) for all $3 \leq i \leq 5$, the first hexagon contains i edges of a P_{3k+2} while the k^{th} hexagon contains $8 - i$ edges of the P_{3k+2};

(ii) the first hexagon does not contain any edges of the P_{3k+2}; and

(iii) the k^{th} hexagon does not contain any edges of the P_{3k+2}.

In each of the cases (ii) and (iii), there are $p_{3k+2}(k-1) = 0$ copies of P_{3k+2}. Further, for case (i), it can be checked that there are $3 \cdot 2^k$ copies of P_{3k+2}. Thus, $p_{3k+2}(k) = 3 \cdot 2^k + 0 + 0 = 3 \cdot 2^k$.

To consider the case when $n \geq \lceil \frac{\ell+2}{3} \rceil$, we first assume that $n = k + 1$. In this case, we have the following possibilities:

(i) for all $1 \leq i \leq 4$, the first hexagon contains i edges of a P_{3k+2} while the $(k+1)^{\text{th}}$ hexagon contains $5 - i$ edges of the P_{3k+2};

(ii) the first hexagon does not contain any edges of the P_{3k+2}; and

(iii) the $(k+1)^{\text{th}}$ hexagon does not contain any edges of the P_{3k+2}.

In each of the cases (ii) and (iii), there are $p_{3k+2}(k) = 0$ copies of P_{3k+2}. However, it is possible that cases (ii) and (iii) occur at the same time resulting in an overcount. Thus, there are

$$p_{3k+2}(k) + p_{3k+2}(k) - p_{3k+2}(k-1) = 3 \cdot 2^k + 3 \cdot 2^k - 0 = 6 \cdot 2^k$$

copies of P_{3k+2} in cases (ii) and (iii). For each i of case (i), it can be checked that there are 2^{k+3} copies of P_{3k+2}. Thus,

$$p_{3k+2}(k+1) = 6 \cdot 2^k + 2^{k+3} = 14 \cdot 2^k.$$

Now, for the general case $n \geq \lceil \frac{\ell+2}{3} \rceil$, it can be observed that every path of length ℓ has 0, 1, 2, 3, 4, or 5 edges in the n^{th} hexagon. There are $p_\ell(n-1)$ paths of length ℓ that have no edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-1}(n-1)$ paths of length ℓ that have one edge in the n^{th} hexagon, there are $2\bar{p}_{\ell-2}(n-1)$ paths of length ℓ that have two edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-3}(n-1)$ paths of length ℓ that have three edges in the n^{th} hexagon, there are $2\bar{p}_{\ell-4}(n-1)$ paths of length ℓ that have four edges in the n^{th} hexagon, and there are $2\bar{p}_{\ell-5}(n-1)$ paths of length ℓ that have five edges in the n^{th} hexagon. Thus,

$$p_\ell(n) = p_\ell(n-1) + 2\Big(\bar{p}_{\ell-1}(n-1) + \bar{p}_{\ell-2}(n-1) + \bar{p}_{\ell-3}(n-1) + \bar{p}_{\ell-4}(n-1) + \bar{p}_{\ell-5}(n-1)\Big).$$

By Observation 5.1, we have that

$$p_\ell(n) = p_\ell(n-1) + 30 \cdot 2^{k-1}.$$

By applying this equation $n-k-1$ times, we obtain

$$\begin{aligned} p_\ell(n) &= 30(n-k-1) \cdot 2^{k-1} + p_\ell(k+1) \\ &= 30(n-k-1) \cdot 2^{k-1} + p_{3k+1}(k+1) \\ &= 30(n-k-1) \cdot 2^{k-1} + 14 \cdot 2^k. \end{aligned}$$

This completes the proof.

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