On the number of hexagonal polyominoes

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Abstract

A combination of the refined finite lattice method and transfer matrices allows a radical increase in the computer enumeration of polyominoes on the hexagonal lattice, (equivalently, site clusters on the triangular lattice), p_n with n hexagons. We obtain p_n for $n \leq 35$. We prove that $p_n = \tau^{n+o(n)}$, obtain the bounds $4.8049 \leq \tau \leq 5.9047$, and estimate that $\tau = 5.1831478(17)$. Finally, we provide compelling numerical evidence that the generating function $\sum p_n z^n \approx A(z)\log(1-\tau z)$, for $z \to (1/\tau)^-$ with $A(z)$ holomorphic in a cut plane, estimate $A(1/\tau)$ and predict the sub-leading asymptotic behaviour, identifying a non-analytic correction-to-scaling term with exponent $\Delta = 3/2$. On the basis of universality and previous numerical work we argue that the mean-square radius of gyration $\langle R_g^2 \rangle_n$ of polyominoes of size n grows as $n^{2\nu}$, with $\nu = 0.64115(5)$.

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Polyominoes, hexagonal latice, enumeration, triangular lattice, site clusters

1 Introduction

While there is an extensive literature on lattice animals, otherwise known as polyominoes, on the square lattice [7], the available data on triangular or hexagonal lattices is much sparser. On the hexagonal lattice one can define a polyomino as a connected set of lattice cells. A self-avoiding polygon on the hexagonal lattice can be defined as the boundary of a simply connected (that is, hole free) polyomino on the hexagonal lattice. Alternatively a self-avoiding

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polygon can be defined as a self-avoiding walk that ends at a site adjacent to its starting point, with the addition of a single bond joining the end-points. For a more general discussion of polyominoes see [7]. The sparseness of the literature on hexagonal polyominoes is perhaps surprising as hexagonal lattice polyominoes are of considerable interest in computational chemistry, where they model a generalised *coronoid system.* Coronoid systems are defined as *benzenoid systems* with holes, where a *benzenoid* or *planar polyhex* is a special type of hydrocarbon molecule. Its hexagonal system is obtained by deleting all carbon-hydrogen bonds, leaving clusters of hexagons joined at an edge (a carbon-carbon bond.) They thus appear as connected geometric figures, being clusters of identical hexagons in the plane, joined at an edge. All internal regions of the cluster are filled with hexagons, that is to say, there are no internal holes. Clearly these are just hexagonal self-avoiding polygons enumerated by area. These have recently been counted up to area 35 for both *fixed* and *free* embeddings [25]. If one or more internal carbon-carbon bonds is missing, the polygon has an internal hole. Clearly such a hole must be of area at least two, as one cannot visually distinguish between the presence or absence of a single cell. However, any internal cluster of cells of area greater than one involves missing bonds, and so is visually distinct from a polygon. In the chemical literature therefore, coronoid systems differ from polyominoes by having internal holes of area at least two. Another feature of the definition of coronoid systems, which seems to us artificial, is that coronoid systems can have only a single hole (but of arbitrary size), whereas polyominoes can have any number of disjoint internal holes. There appears no *a priori* reason why a coronoid system with multiple holes could not be synthesised.

In this paper we will solely be discussing the number of fixed polyominoes counted by area. These are of course fully equivalent to the number of connected site clusters on the triangular lattice. A distinction is often made between *fixed* embeddings, and *free* embeddings. In the former, polyominoes are considered distinct up to a translation, that is to say, fixed polyominoes means "an equivalence class of polyominoes under translation" while free polyominoes are considered equivalent under translations, rotations and reflections. More precisely, free polyominoes refers to "an equivalence class of polyominoes under translation, rotation and reflection". In Figure 1 a simple example is shown of a hexagonal cluster which has a count of 1 as a free polyomino, and a count of 12 as a fixed polyomino. In the chemistry literature the number of free embeddings [8] of structures has been universally considered. In [25] a proof is given that the number of free embeddings of polygons is, asymptotically, given by 12 times the number of fixed embeddings. The corrections to this asymptotic result are exponentially small, that is to say, are of order $\exp(-cn)$ where n is the area of the polyomino and c is a positive constant. This proof holds *mutatis mutandis* for hexagonal polyominoes.

The monograph by Gutman and Cyvin [8] provides a comprehensive review of all aspects of hexagonal polygon and polyomino enumeration prior to 1990, with a more up-to-date review in ref. [2]. Progress has been slow, but incremental, as all previous calculations have been based on direct counting of polyominoes. As the number of these grow as 5.18^n for polyominoes of size n, it is clear that, to obtain one further term, one needs more than 5 times the computer power than one previously had—or 5 times as many computers if one is performing calculations in parallel. Up to 1972, the number of polyominoes to $n = 12$ was known [16]. Twenty years later, this had been improved to $n = 22$ [19]. Thus one extra term each two years has been found on average, reflecting a steady 2.6-fold increase per annum achieved by a combination of computer speed and resources.

In this paper, we present an improved algorithm that enables us to obtain p_n for $n \leq 35$. This represents an improvement of $5.18^{13} \approx 2 \times 10^9$ over pre-existing calculations. (Or a jump of about twenty-two years in terms of the traditional algorithms). The algorithm is in fact exponentially faster than direct counting, with both time and memory growing approximately as 1.65^n. Its drawbacks are that it is much more memory intensive than direct counting, for which memory requirements are negligible, as well as being much more difficult to implement.

We first prove some results about p_n. We then describe the algorithm, and give the number of fixed polyominoes up to size 35. We then apply a range of numerical techniques to the data, and thus provide compelling evidence that the generating function

$$P(z) = \sum_{n \geq 1} p_n z^n \approx A(z) \log(1 - \tau z), \text{ as } z \to (1/\tau)^-, \tag{1}$$

where $A(z)$ is holomorphic in a plane cut from $1/\tau$ to ∞ and, further, that

$$p_n \approx \tau^n/n[a_1 + a_2/n + a_3/n^{3/2} + a_4/n^2 + a_5/n^{5/2} + O(1/n^3)].$$

The symbol $\approx$ indicates that this is the singular part of the quantity appearing on the left hand side, but that an equality cannot be used as the right-hand side may have neglected, for example, additive analytic functions that do not contribute to the singular behaviour. We then establish rigorous upper and lower bounds on τ, and give a precise (but non-rigorous) estimate of τ.

Another interesting property of polyominoes is their average size. Many possible measures exist, such as radius of gyration, mean-span, mean distance of a site from another site, and most of these are equivalent in the sense that their asymptotic behaviour is characterised by the same exponential growth. A common measure is the *mean-square radius of gyration*, $\langle R_g^2 \rangle_n$, which is just the second moment about the centre of mass, of polyominoes of size n. Solely by reference to earlier work on polygons [12], and an appeal to universality, we provide compelling numerical arguments (though not a proof) that this grows as $n^{2\nu}$, with $\nu = 0.64115(5)$.

2 Rigorous results

We first prove (or outline proofs) of some rigorous results on the number of polyominoes. Let p_n denote the number of *fixed* configurations of n hexagons. Then,

Theorem 1 *There is a* growth constant τ *with* $1 < \tau < \infty$, *for fixed hexagonal polyominoes, such that*

$$\lim_{n\to\infty} p_n^{1/n} = \tau = \sup_{n\geq 1} p_n^{1/n}. \tag{2}$$

This follows from the observation that if one takes any two (fixed) polyominoes, one of size n_1 and one of size n_2, one can identify the rightmost, topmost cell of the first polyomino, and join it to the leftmost, bottommost cell of the second (so that they share an edge of a hexagon), as shown in Figure 2. In this way one produces a *unique* polyomino of size $n_1 + n_2$. However, not all polyominoes of size $n_1 + n_2$ can be produced in this way. Thus we arrive at the supermultiplicative inequality,

$$p_{n_1}p_{n_2} \leq p_{n_1+n_2} \text{ for } n_1, n_2 \geq 1. \tag{3}$$

Taking the logarithm and multiplying by -1 yields a sub-additive inequality. The final requirement to complete the proof is to show that the sequence $\{p_n^{1/n}\}$ is bounded above. A crude bound, $p_n^{1/n} \leq 2^4$ follows *mutatis mutandis* from the corresponding argument for square lattice bond animals given in ref. [28]. We give more details of a much tighter bound below.

A stronger result has recently been proved by Madras [18], who established that

Theorem 2 *If* p_n *denotes the number of polyominoes of area* n, *then*

$$\lim_{n\to\infty} p_n/p_{n-1} = \tau. \tag{4}$$

The proof relies on a pattern theorem for lattice animals. It requires three conditions to be satisfied. Two of these, translational invariance and a property on weights are trivially satisfied, while the third, which requires certain pattern translates to hold, was also proved by Madras [18]. Note that the proof does not hold for polygons enumerated by area. For polygons enumerated by perimeter, a similar result has been proved by Kesten [14]. Kesten considered, among other problems, the number u_{2n} of fixed polygons of *perimeter* $2n$. (Recall that $u_{2n+1} = 0$). For this problem, Kesten proved that

$$\lim_{n\to\infty} u_{2n}/u_{2n-2} = \mu^2, \tag{5}$$

where μ is the relevant growth constant when considering enumeration by perimeter. In fact it is generally accepted that $\mu^2 = 2 + \sqrt{2}$, [20], though this has not been proved.

It is widely believed, for polyominoes as well as for a very large class of related lattice objects, including lattice trees, self-avoiding walks, percolation clusters, and self-avoiding polyominoes, to name but a few, that the asymptotic behaviour is in fact

$$p_n \sim A\tau^n n^\theta \text{ as } n \to \infty.$$

Note that Theorem 1 implies that $p_n \sim A\tau^{n+o(n)}$, so this conjecture says something about the sub-dominant asymptotic behaviour, which is contained in the term n^θ. The conjectured logarithmic singularity of the generating function (1), which we justify below implies that $\theta = -1$. For most two-dimensional problems the existence of the sub-dominant term n^θ has not been proved, but for many problems, especially those that are conformally invariant [10], not only is it widely (indeed, universally) believed to be true, but it is equally widely held that the exact value of θ is known. For polyominoes, it is believed that $\theta = -1$. Furthermore, θ, unlike τ displays *universality.* That is to say, τ changes as one changes from the hexagonal lattice to say, the square or triangular lattice, but θ is expected to remain constant. (For three-dimensional polyominoes, θ is believed to take the value $-3/2$).

An additional universal property of such systems is the exponent characterising the *linear size* or an equivalent metric property, such as the *mean span.* This is just the average width (or, equivalently, height) of objects of size n, (polyominoes, in this case), averaged over all the objects of size n. We expect the mean span $\langle MS\rangle_n$ to be asymptotically proportional to n^ν, where ν is another universal critical exponent. An equivalent metric is the *mean-square radius of gyration*, discussed above, which is expected to grow like $n^{2\nu}$. In ref. [17] Madras proves an exponent inequality relating ν and θ, viz.

Theorem 3 *Provided that the critical exponents ν and θ exist, the inequality*

$$\nu \le -\theta$$

holds.

(Note that this result is rather weak in two dimensions, where $\theta = -1$). We outline the proof below. Of course it depends on the existence of the exponents

θ and ν. In this paper we do not estimate ν, but on the grounds of universality we expect it to be the same as for square-lattice polyominoes, which we have previously estimated [12] to be $\nu = 0.64115(5)$. The theorem is thus not "tight" as substituting the numerical estimates of the exponents we have $0.64115 \leq 1$.

Before giving the proof, we remark that for polyominoes there is a compelling argument [21] that θ for a d-dimensional system, is given by the Yang-Lee edge singularity exponent in $d-2$ dimensions. As this exponent is known in dimensions 0 and 1 it follows that $\theta = -1, -3/2$ for two- and three-dimensional polyominoes respectively. As our analysis below shows, this prediction is well borne out by the numerical data. The strongest rigorous result to date is due to Madras [17] who has proved

Theorem 4 *Assuming that the exponent θ exists for d-dimensional animals it satisfies $\theta \leq (1-d)/d$.*

For simplicity, we give the proof for the two-dimensional case, for which the theorem gives $\theta \leq -1/2$, which is consistent with the believed exact value $\theta = -1$. The proof requires the following lemma:

Lemma 1 *Let λ be a positive number and let $b_1, b_2, \cdots$, be a positive sequence such that $\lim_{n\to\infty} b_n^{1/n} = \lambda$. Also assume that there are numbers $C > 0$ and $s \geq 0$, and integer $k \geq 0$, such that*

$$b_{2n+k} \geq C n^s b_n^2 \text{ for every } n \geq 1.$$

Then

$$b_n \leq \frac{1}{C 2^s n^s} \lambda^{n+k} \text{ for every } n \geq 1.$$

This lemma is given and proved in ref. [17]. First, observe that any polyomino of n-cells has, by definition, area n, if we take a cell as the unit of area. As a space-filling object, it follows that one linear dimension must be at least $\sqrt{n}$. Orient two polyominoes, labelled l (for *left*) and r (for *right*), both of size n, so that their vertical dimension is at least $\sqrt{n}$. (This can be done by a rotation, if necessary.) We will consider joining two polyominoes together to form a polyomino system of size $2n+1$, in a manner similar to that discussed and illustrated above in the proof of Theorem 1. Move r to the right of l, and translate it vertically so that a horizontal line exists which intersects l and r. There are at least $2\sqrt{n}$ choices for this translation. Now translate r to the left until it is just one cell to the right of l. Insert this cell (shown shaded in Figure 3), which joins l and r. This produces a $2n+1$ cell system, which may be produced more than once (because of the permitted rotations). Each polyomino may be rotated through $2\pi/3$ radians, allowing up to 3 possible rotations. Thus up to $3^2 = 9$ possible realisations of this polyomino can occur. However not all such $2n+1$ cell systems can be produced in this way. Thus we obtain $9p_{2n+1} \geq 2\sqrt{n}p_n^2$, where the factor $2\sqrt{n}$ arises from the number of possible overlaps, and the factor of 9 arises from the rotational possibilities just discussed.

Then from the above lemma and Theorem 1, it follows that

$$p_n \leq \frac{9\tau^{n+1}}{2\sqrt{2n}}.$$

Thus $\theta \leq -1/2$ as claimed.

The proof that $\nu \leq -\theta$ follows from certain properties of the *projection* of the polyomino onto one of the lattice axes. Roughly speaking, the x-projection is the width of the polyomino (being its projection onto the x-axis), and the y-projection is its height. There exists a positive constant K such that for *each* polyomino of area n

$$\frac{1}{2}(x\text{-projection} + y\text{-projection}) \geq K \times \text{mean span}.$$

Then from the above concatenation argument leading to the proof of the bound on θ, we arrive at

$$p_{2n} \geq 2Kp_n^2\langle MS\rangle_n.$$

Next, from the scaling assumption $\langle MS\rangle_n \sim Bn^\nu$ as $n \to \infty$, (where B is a constant), we obtain

$$p_{2n} \geq 2KBp_n^2 n^\nu.$$

From the same lemma used above, we then obtain $p_n \leq \frac{\tau^n}{2BKn^\nu}$. The assumption $p_n \sim \text{const.}\tau^n n^\theta$, when substituted into the preceding expression, yields the required inequality.

3 Finite Lattice Method algorithm

The method used to enumerate polyominoes on the hexagonal lattice is a generalisation of the method devised by Enting [4] in his pioneering work on the enumeration of square lattice polygons by perimeter and the subsequent extension of this approach to hexagonal lattice polygons [6]. We also included the significant enhancements developed by Jensen and employed in previous work [11] on square lattice polygon perimeter enumeration. While all of these papers are concerned with enumeration by *perimeter*, the general method, described in detail in these papers, is the same when enumerating by *area* and for this reason we shall be brief and only give essential information.

As pointed out by Enting [5], there are three conditions that have to be fulfilled to make the FLM a successful technique for a specific problem:

- The coefficients of the generating function must be expressible in terms of the number of embeddings of a well-defined class of connected graphs.
- Weights for combining contributions from finite lattices have to be known or calculated.
- Efficient ways of constructing the finite lattice sums must exist. In practice, this means transfer matrix (TM) techniques.

In the following we shall outline how these conditions are realised in the calculation for (fixed) polyominoes on the hexagonal lattice.

We embed the hexagonal lattice in the square lattice as the brick-work lattice, as shown in Figure 4. Note that a brick consists of two cells of the square lattice but counts as being of area one when we enumerate polyominoes. There are two types of vertices on the hexagonal lattice, type 0 and 1, as shown in Figure 5 with corresponding vertices on the brick-work lattice.

In the case of polyominoes, the series expansion *is* the series of polyominoes enumerated by area on the hexagonal lattice itself. Since polyominoes are connected, this is, trivially, the required connected graph expansion. This addresses the first condition of the FLM.

To address the second condition above, consider the rectangles $Z^i_{m,n}$ with length m, and height n where the bottom left-hand corner is a vertex of type $i \in \{0,1\}$. Let $p^i_{m,n}(z) = \sum_k p^i_{m,n,k} z^k$ be the area generating function for polyominoes that fit inside the rectangle $Z^i_{m,n}$ and touch all its sides. $Z^i_{m,n}$ is called the bounding rectangle of such a polyomino. The bounding rectangle is unique. As a result $P(z)$, the generating function for fixed polyominoes, can be expressed as a sum over the generating functions of polyominoes on the finite lattices, $P(z) = \sum_{m,n,i,k} p^i_{m,n,k} z^k = \sum_{m,n,i} p^i_{m,n}(z)$. The $p^i_{m,n}(z)$ are polynomials. The minimal degree of $p^i_{m,n}(z)$ increases with m and n. It is at least $n + \max\{0, \lceil (m-n-1)/2 \rceil\}$. If one wants to calculate $P(z)$ up to order $N_{\max}$, only the $p^i_{m,n}(z)$ which have a minimal degree of $N_{\max}$ or less have to be calculated. Hence the generating function can be written as

$$P(z) = \sum_{\substack{1 \le n \le N_{\max} \\ 1 \le m \le 2N_{\max}-n+1 \\ i \in \{0,1\}}} p^i_{m,n}(z) + O(z^{N_{\max}+1}). \qquad (6)$$

For this we have to consider the finite lattices $Z^i_{m,n}$ with $1 \le n \le N_{\max}$, $1 \le m \le 2N_{\max} - n + 1$ and $i \in \{0,1\}$. Hence the weights are one for these lattices and zero otherwise.

To address the third point in Enting's list of conditions, we briefly discuss the TM method which we used to calculate the generating functions on the finite lattices. Enting [4] enumerated polygons on the square lattice by perimeter and outlined the principles of the TM method for enumerating polygons on a lattice in general. Enting and Guttmann [6] used the FLM/TM technique to enumerate polygons on the hexagonal lattice by perimeter. To apply the TM method we define the polyominoes by their perimeter, which includes the holes. That is to say, the total perimeter is the sum of the internal perimeter and the external perimeter. Note that while the perimeter is an essential part of the TM algorithm which we used, we still enumerate the polyominoes by area.

Polyominoes on the square lattice, unlike polygons, can have configurations with vertices of degree four. However this is impossible on a hexagonal lattice (which has coordination number three), and so the only topological feature that distinguishes a hexagonal lattice polyomino from a polygon is that in the former case isolated (disjoint) internal polygons are permitted. (On the square lattice one can define a model, called *polygonal polyominoes* that interpolates between polygons and polyominoes, by only allowing isolated polygons, and hence excluding polyomino configurations which include vertices of degree four. This model has been studied in [13].)

Terms in the the polyomino generating function $P(z) = \sum p_n z^n$ can be calculated using TM techniques to count the number of polyominoes in rectangles of height m and length n. The TM technique involves drawing a boundary line, which passes through the mid-points of the edges perpendicular to it, through the rectangle intersecting a set of $m+1$ edges. Each edge is either empty or occupied by part of the perimeter of a partially completed polyomino. (The boundary of an internal hole is considered part of the perimeter of a polyomino).

Cutting the polyomino with a line leads to a set of arcs to the left of that line. Each occupied edge is connected, via an arc to the left of the boundary line, to exactly one other occupied edge intersecting the boundary. We choose to encode the state σ_i of an edge as $\sigma_i = 0$ if the edge at position i is empty, $\sigma_i = 1$ if the edge is occupied *and* is the lower edge of an arc, and $\sigma_i = 2$ if the edge is the upper edge of an arc. Due to the self-avoidance condition and the two-dimensional nature of the problem this encoding uniquely specifies the connectivity of the edges.

For each configuration of occupied or empty edges along the boundary, we maintain a generating function for partially completed polyominoes. The generating function is a (truncated) polynomial $p_s(z)$, where $s = \{\sigma_i\}$ is the state vector specifying the configuration. Polyominoes in a given rectangle are enumerated by moving the boundary so as to add one unit cell at a time. When the boundary line is moved, a given state vector s is transformed into two new state vectors s_1 and s_2 and $z^{k_1} p_s(z)$ is added to $p_{s_1}(z)$ and $z^{k_2} p_s(z)$ is added to $p_{s_2}(z)$, where k_1 and k_2 count the additional unit cells added to the polyomino.

In the case of enumeration by area, k_1 and k_2 depend on the state vector, that is on whether the added cell is part of the polyomino or not. It is quite simple to determine whether a newly added unit cell of the hexagonal lattice belongs to a polyomino or not. Moving through a configuration we note that as we reach the first occupied edge we pass from the outside to the inside of a polyomino, the next occupied edge takes us to the outside again, and so on. In this fashion all unit cells intersected by the boundary line are uniquely assigned to the interior or exterior of a polyomino.

The rules for updating the partial generating functions are described in ref. [6] in the case of enumeration by perimeter. The generalisation to enumeration by area is quite simple since the encoding and transformations of the configurations are identical. The only change is that the weights assigned to a configuration count the area that has been already inserted. Furthermore, in the TM algorithm we have implemented, we move the intersection line over two vertices in one step instead over one vertex as in ref. [6]. The updating rules for *polygons* by area are given in [25]. The updating rules for polyominoes are given in Table 1. There is only one change from the rules in [25], to include the rule that permits the formation of holes. At the upper and lower boundary of the finite lattice the TMs are appropriately modified. The boundary line is drawn either vertically or horizontally through the rectangle. One follows the orientation in which the line intersects fewer edges. In the case of a horizontal boundary the TMs are appropriately modified at both the left and right boundary of the finite lattice.

If one wants to calculate the coefficients p_n up to $N_{\max}$, the maximal number of edges which the boundary line intersects in any of the required finite lattices grows as $2N_{\max}/3$. (This grows as $N_{\max}/2$ in the case of square lattice polyominoes). Every finite lattice falls into one of two cases, $m \geq 2n$ or $m < 2n$. In the first case a vertical boundary is used. In the second case, parenthesised below, a horizontal boundary is used. It is not necessary to calculate every $p^i_{m,n}(z)$ separately. One can consider all the finite lattices $Z^i_{m,n}$ with n fixed, i fixed and $m \geq 2n$ (m fixed, i fixed and $n > m/2$) together. That is to say, we can calculate the $p^i_{m,n}(z)$ of all these finite lattices in one sweep by aligning the left (lower) sides of the finite lattices. The boundary is moved from left to right (bottom to top). When a polyomino is closed it counts towards the $p^i_{m,n}(z)$ which is determined by its bounding rectangle.

In ref. [11] improvements of the FLM/TM were discussed which we have applied to the enumeration of polyominoes on the hexagonal lattice. The major improvement comes from the calculation of the polyominoes that span the finite lattices in length and width and not only in length as in previous work. This increases the number of state vectors required to describe all configurations by a factor of almost four, since one has to store a parameter that keeps track of whether the polyomino has touched the lower boundary of the rectangle and whether it has touched the upper boundary. This enables one to calculate how many cells are needed to close the polyomino (or find a lower bound) such that the resultant polyomino touches both the upper and the lower boundaries, stretches to the right boundary and finally that the resulting configuration is connected. If in addition we store the minimal area to the left of the intersection line we can calculate the minimal area (or a lower bound on the area) which every polyomino with the particular configuration on the intersection will have. If this is larger than $N_{\max}$ the configuration is discarded. This leads to an exponential reduction in the number of configurations that have to be stored. In the original approach all possible configurations were kept.

From the foregoing discussion of the encoding of the state vectors, it is clear that since every occupied edge is uniquely matched, any configuration is just an example of perfectly matched parenthesis with gaps. These are well-known in the combinatorics literature, (see [23], sequence M1184), and are called Motzkin numbers. For our purpose all we need to know is that the number of Motzkin numbers of length m grows like 3^m. This exponential growth obviously determines the computational complexity of the original approach. The maximal number of bonds intersected by the boundary line grows as $2N_{\max}/3$. This implies that the complexity of enumerating polyominoes of size n grows as $3^{2n/3} \approx 2.08^n$, multiplied by some polynomial in n. Thus this approach already provides a dramatic improvement over pre-existing direct enumeration algorithms, which have complexity 5.18^n. With the further improvements we have described, it is not possible to give a theoretical analysis of the computational complexity of the improved algorithm, but an empirical analysis suggests that the improvements reduce the complexity to λ^n with $\lambda \approx 1.65$.

In this way we have obtained the coefficients p_n for $p \leq 35$. The calculation took about 10 weeks on a single processor Compaq AlphaServer ES40, and utilised up to 5GB of memory. To minimise memory requirements, all calculations were done using 16 bit integers, *modulo* a prime. This was repeated five times, using five different primes, and the final result reconstructed using the Chinese Remainder theorem. Using 32 bit integers would have required only three runs, but would have doubled the memory requirements. With more memory still, only one run would be needed, and thus the time taken would be approximately two weeks. The results are shown in Table 2.

4 Series Analysis

From the coefficients p_n given in Table 2, we have the first 35 terms in the generating function for polyominoes, defined by $P(z) = \sum_{n\geq 1} p_n z^n$.

Given the expected asymptotic behaviour $p_n \sim C\tau^n n^\theta$, it follows that the expected generating function behaviour is $P(z) = \sum_n p_n z^n \approx A(z)(1-\tau z)^{-\theta-1}$. Here $C = A(1/\tau)/\Gamma(\theta+1)$, and the radius of convergence of the generating function is given by $1/\tau$. As we alluded to above, we find below that $\theta = -1$, so that the exponent $-\theta-1 = 0$. This corresponds to a logarithmic singularity, so that in fact

$$P(z) = \sum_n p_n z^n \approx A(z)\log(1-\tau z). \tag{7}$$

We have used two methods to analyse this series. Firstly, to obtain the singularity structure of the generating function we used the numerical method of differential approximants [9]. Very briefly, in this method we approximate the generating function by the solution of a linear, inhomogeneous, ordinary differential equation (o.d.e.) with polynomial coefficients. That is to say, we insist that the power series expansion of the solution of the o.d.e. agrees, order by order, with the known coefficients of the generating function. One can increase the degree of the polynomials, and the order of the underlying differential equation until there are no more known coefficients. In practice, it has been found that a first- or second-order o.d.e. is usually sufficient to approximate the singularity structure found in problems such as this. One then solves the o.d.e. in the standard manner, the critical point being given by the closest zero on the positive real axis of the polynomial multiplying the highest derivative, while the corresponding exponent is obtained from the solution of the appropriate *indicial equation* [27]. A substantial number of such *differential approximants* are constructed, and a statistical procedure used to estimate the critical point and critical exponent [9].

Estimates of the critical point and critical exponent were obtained by averaging values obtained from first order $[L/N;M]$ and second order $[L/N;M;K]$ inhomogeneous differential approximants. These are the solutions of the differential equations $zR_M^{(1)}(z)P'(z) + R_N^{(0)}(z)P(z) = Q_L(z)$ and $z^2R_K^{(2)}P''(z) + zR_M^{(1)}(z)P'(z) + R_N^{(0)}(z)P(z) = Q_L(z)$ respectively, where R and Q are polynomials of degree given by their subscripts.

In particular, we used this method to estimate the growth constant τ and the critical exponent θ. As mentioned above, there is a prediction [21] that $\theta = -1$, which we also confirm numerically. Imposing this conjectured exponent permitted a refinement of the estimate of the growth constant—providing so-called biased estimates.

Our analysis is based on approximants such that the difference between N, M, and K didn't exceed 2. These are therefore "diagonal" approximants. Some approximants were excluded from the averages because the estimates were obviously spurious. We found many first order approximants were defective, so our analysis is based on second and third order approximants. The fact that first order approximants were defective (unlike the analogous analysis for hexagonal polygons enumerated by area, as reported in [25]) suggests the presence of non-analytic corrections to scaling in the case of the polyomino generating function. Such non-analytic terms were found to be absent for polygons enumerated by area [25]. As we find below, there appears to be a non-analytic correction-to-scaling term in the polyomino generating function, with value 3/2. Second and higher order differential approximants can accommodate non-analytic corrections-to-scaling, and so our analysis is based on these approximants. From second and third order approximants we estimate that $1/\tau = 0.1929331(3)$ and $1 + \theta = -0.0003(5)$.

As discussed earlier there is very convincing evidence that the critical exponent $\theta = -1$ exactly. This is certainly borne out by our numerical estimate above. If we assume this to be true, then we can obtain a slightly refined estimate of the critical point $1/\tau$. We observe that there is an almost linear relationship between the estimates for $1+\theta$ and $1/\tau$ and hence find that for $\theta = -1$ we can estimate $1/\tau = 0.19293295(5)$ and thus $\tau = 5.1831478(17)$. The biased and unbiased estimates are less precise than in the case of hexagonal polyominoes enumerated by area [25]. This is due to the simpler singularity structure, that is to say the absence of non-analytic corrections-to-scaling, in that case.

Once the exact value of the exponent was conjectured, and the growth constant accurately estimated, we turned our attention to the "fine structure" of the asymptotic form of the coefficients, by fitting the coefficients to the assumed form

$$p_n = [z^n]P(z) = \tau^n n^{-1} \sum_{i \geq 0} a_{i+1}/n^{f(i)}. \qquad (8)$$

In the most favourable circumstances, if there is no non-analytic correction term, then $f(i) = i$. That was found to be the case for hexagonal polygons enumerated by area [25]. In some problems there is a square-root correction term which means $f(i) = i/2$, while a logarithmic correction implies more subtle behaviour. In all cases, our procedure is to *assume* a particular form for $f(i)$, and observe how well it fits the data. With the long series we have at our disposal, it is usually easy to see if the wrong assumption has been made, as if so the sequence of amplitude estimates a_i either diverges to infinity or converges to zero. Once the correct assumption is made, convergence is usually rapid and obvious. A detailed demonstration of the method can be found in refs. [1,11].

For polyominoes it appears that there is a non-analytic correction with exponent equal to 3/2. This behaviour was first identified for square-lattice polyominoes in [12], and, as we might expect from universality arguments, the same exponent structure is evident for hexagonal polyominoes. As remarked above, for polygons enumerated by area, there appears to be no evidence for any non-analytic corrections [12,25].

We conjecture that the asymptotic form for the polyomino coefficients is as given by equation (8), with $f(0) = 0$, $f(1) = 1$, $f(2) = 3/2$, $f(3) = 2$, $f(4) = 5/2$, etc. From (8) with these values of $f(i)$ follows the asymptotic form

$$p_n = \tau^n n^{-1}[a_1 + a_2/n + a_3/n^{3/2} + a_4/n^2 + a_5/n^{5/2} + \mathrm{O}(n^{-3})]. \qquad (9)$$

Using the central estimate $\tau = 5.1831478$ quoted above, we show in Table 3 the estimates of the amplitudes $a_1, \cdots, a_5$. From the table we estimate that $a_1 \approx 0.2734618$, $a_2 \approx -0.2060$, $a_3 \approx 0.242$, $a_4 \approx -0.15$ and $a_5 \approx 0.04$, where in all cases we expect the error to be confined to the last quoted digit. The excellent convergence of all columns is strong evidence that the assumed asymptotic form is correct. If we were missing a term corresponding to, say, a quarter-integer correction, the fit would be far worse. This is explained at greater length in ref. [1]. Of course, if the correction-to-scaling exponent were 1.49 instead of 1.5 as assumed, our analysis would not be sensitive enough to detect this. There seems no reason however, to expect anything other than simple rational fractions for exponents in such problems. So good is the fit to the data that if we take the last entry in the table, corresponding to $n = 35$, and use the entries as the amplitudes $\{a_i\}$, then all the coefficients beyond the first are given either exactly (if rounded to the nearest integer), or to the same accuracy as the leading amplitude.

This analysis refers to the generating function for *fixed* polyominoes. For *free* polyominoes, the estimates of θ and τ are, as shown above, identical to the corresponding values for fixed polyominoes, while the amplitudes just need to be divided by 12.

5 Bounds on τ

5.1 Lower bound

A weak lower bound is immediately attainable from equation (2). Using p_{35} we obtain a lower bound of 4.50991.

This bound can be improved using the techniques developed by Rands and Welsh in ref. [22]. Using concatenation arguments they showed that if we define a sequence $\{c_n\}$, $c_n \geq 0$, such that

$$p_{n+1} = c_{n+1} + c_n p_1 + \ldots c_2 p_{n-1} + c_1 p_n, \qquad (10)$$

and construct the generating functions

$$\mathcal{P}(u) = 1 + \sum_{n=1}^{\infty} p_n u^n, \tag{11}$$

and

$$\mathcal{C}(u) = \sum_{n=1}^{\infty} c_n u^n, \tag{12}$$

then

$$\mathcal{P}(u) = 1 + \mathcal{P}(u)\mathcal{C}(u) \tag{13}$$

and $\mathcal{P}(u)$ is singular when $\mathcal{C}(u) = 1$. The coefficients in $\mathcal{C}(u)$ are obviously constructible to the same order as known for $\mathcal{P}(u)$. If we look at the polynomial C_N obtained by truncating $\mathcal{C}(u)$ at order N then the unique positive zero, $1/\tau_N$, of $C_N - 1 = 0$ leads to a lower bound for τ, that is $\tau_N \leq \tau$.

In ref. [22] the method was first applied to the generating function of polyominoes on the hexagonal lattice. Using the longest available series at the time of 16 terms [24], the bound $\tau \geq 4.43$ was obtained. The application of the method to our series up to area 35 leads to an improved lower bound of 4.80491. More elaborate concatenation schemes, such as that described in [22] and in ref. [28] for square lattice polyominoes, are discussed further in ref. [26].

5.2 Upper bound

A crude upper bound is $p_N \leq 2^{4n}$. This can be seen from the following argument: A polyomino of area n is bounded by a non-reversing, non-crossing walk of length at most $2 + 4n$. If a bond is visited once it is part of the boundary of the polyomino, that is it is either part of the outside boundary or it is part of the boundary of a hole. If it is visited twice it is an internal bond of the polyomino. This is illustrated in Figure 7. Note that there is usually more than one walk that defines the same polyomino. Further the area enclosed by the walk, excluding the walk itself, is connected. The last property ensures that we know that a walk of length $2 + 4n$ can define the boundary. The first and last steps can be chosen to be fixed. As the co-ordination number of the hexagonal lattice is 3, the non-returning walk has at most two choices at every step. This immediately gives the above bound.

Obtaining a good upper bound to τ is an involved computation and will be the subject of a separate paper [26]. In this article we merely outline the method, and give the result.

W. L. Lunnon [16] found an upper bound for the polyomino growth constant of 6.75. To improve this bound we apply the ideas of Klarner and Rivest [15] which were inspired by Eden [3]. Klarner and Rivest developed a method which involves successive improvement. The idea is that each polyomino is converted to a tree on the dual lattice, in this case the triangular lattice. We describe a mapping that associates a unique spanning tree with each polyomino. Then, by relaxing the rules for the construction of such a tree, we end up with an algorithm that overcounts the number of polyominoes. Unlike the generating function for the original problem, we can determine the radius of convergence of the "overcounted" polyominoes, which therefore provides an upper bound. The algorithm has the advantage of being amenable to systematic improvement.

The mapping from polyomino to tree is done by placing a site at the centre of each hexagon, and joining certain sites if their associated hexagons share an edge. This is done in such a way that cycles are excluded, and all cells included. Thus each polyomino is associated with a spanning tree, made up of so-called "twigs", (defined below) chosen from a fixed, finite set. The number of spanning trees (and hence polyominoes) is bounded above by the number of ways of concatenating the twigs. The cells in a twig are divided into two types, namely *dead* and *living*. Additionally, *forbidden* cells may be associated with a twig, though are not part of the twig, as shown in Figure 7. Every twig contains at least one dead cell, but not necessarily any living cells. Further one of the dead cells is marked by an incoming edge as a root cell. This incoming edge defines the orientation of the twig. The living cells of a twig have an orientation too, which is defined by the incoming edge of the internal tree structure. Further, the living cells of a twig are linearly ordered. This is necessary to ensure the uniqueness of the construction. Figure 7 shows the set of basic twigs we use to construct both polyominoes and larger twigs. Any polyomino can be constructed in the following way from the basic twigs: We start with a single living cell that has an incoming bond from below, and we keep a list of living cells which we use as a queue. The addition of twigs to the configuration constructed so far proceeds as follows:

- Add a new twig by placing the root cell of the twig over the oldest living cell such that the orientation of the twig and the oldest living cell coincide.
- The addition is legal if no other cells of the twig overlap with any part of the configuration and no cell of the twig occupies a cell marked as forbidden.
- Make the forbidden cells of the twig forbidden cells of the polyomino.
- Append the living cells of the twig to the list of living cells observing the order of the living cells in the twig.
- Remove the oldest cell from the list of living cells.
- Make the living cell where the twig has been added a dead cell.

This is repeated until no living cells are left. The construction of a polyomino of size four is illustrated in Figure 8. We can construct a set of larger twigs (i.e. twigs with more dead cells) from the basic twigs by using almost the same algorithm. A complete set of twigs of size n contains all configurations that can be constructed according to the above rules and that contain exactly n dead cells (and possibly living cells) or contain less than n dead cells and no living cells. One can construct any polyomino with such a set of twigs. Note that the set of basic twigs shown in Figure 7 is also the set of twigs of size 1 which have been constructed from the set of basic twigs.

The results are systematically improved by increasing the number of dead cells in the set of basic twigs. The calculations become increasingly complex with increasing twig size, requiring exponentially increasing amounts of computer time. The bound we obtain here derives from twigs with 16 dead cells. The C program ran for four weeks on a MacIntosh G3 computer.

From the determination of the twigs we proceeded similarly to Klarner and Rivest. We assign to every twig i a weight $w_i = x^{m-1}y^n$, where $m - n$ is the number of living cells of the twig and n is the number of dead cells of the twig.

If we relax the construction rules so that the legality of an addition of a twig is not checked (this being the second bullet point above) we can write down the two-variable generating function, $f(x, y) = x/(1 - \sum_i w_i)$. Note that this relaxation allows multiple occupancy of cells, and also allows forbidden cells to be occupied. It is this that is responsible for the overcounting of spanning trees (and hence polyominoes). We are interested in the diagonal terms $a_{n,n}$ of the series expansion of $f(x, y) = \sum_{m,n} a_{m,n}x^m y^n$. These terms represent the configurations that contain no living cells and in which all polyominoes are included. Therefore we obtain an upper bound for the polyomino growth constant if we can find the growth constant for the $a_{n,n}$. Klarner and Rivest [15] show how one can obtain the growth constant of the diagonal terms of a rational two variable generating function. This requires a change of variable so that the residue theorem can be applied. The diagonal function $f_D(x) = \sum_n a_{n,n}x^n$ can be written as a sum over residues.

In this way, and after substantial computation using a twig size of 16, we obtain the upper bound 5.9047. Thus we find

$$4.8049 < \tau < 5.9047. \tag{14}$$

6 Discussion and conclusion

We have proved a number of results for polyominoes, including the existence of a growth constant τ. We have established rigorous upper and lower bounds on τ, and a precise numerical estimate of $\tau = 5.1831478(17)$. We provide compelling arguments that the generating function

$$\sum p_n z^n \approx A(z)\log(1 - \tau z)[1 + B(z)(1 - \tau z)^{3/2}],$$

and provide a (numerical) expansion of $A(z)$ and $B(z)$ around $z = 1/\tau$. This analysis provides very strong evidence for the presence of a non-analytic correction term to the proposed asymptotic form for the generating function, with value $\Delta = 3/2$. Finally we give an asymptotic representation for the coefficients which we believe accurate to several significant figures for polyominoes of any size at least up to 100.

We have presented an improved algorithm for the enumeration of polyominoes, on the hexagonal lattice. The computational complexity of the algorithm is estimated to be 1.65^n for polyominoes of size n. Implementing this algorithm has enabled us to obtain polygons up to area 35.

It might be thought that such a simply formulated problem should have a "simple" solution. One piece of evidence against this belief is that decomposing the coefficients into prime factors reveals frequent occurrence of very large prime factors.

We also discuss the *size* of polyominoes. Many possible measures of size exist, and most of these are equivalent. Accordingly, we focus on the *mean-square radius of gyration*, $\langle R_g^2 \rangle_n$ of polyominoes of size n, and refer to compelling numerical arguments [12] (though not a proof) that this grows as $n^{2\nu}$, with $\nu = 0.64115(5)$, for square lattice polyominoes. Invoking universality, we expect this holds for hexagonal polyominoes too, though we have not explicitly investigated this aspect.

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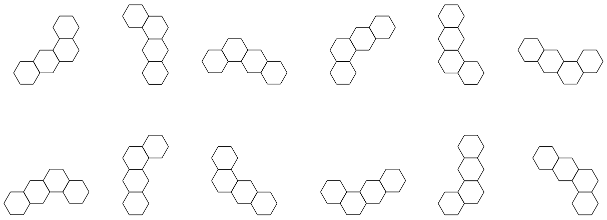

Fig. 1. A polyomino that counts as one free polyomino but as twelve fixed polyominoes

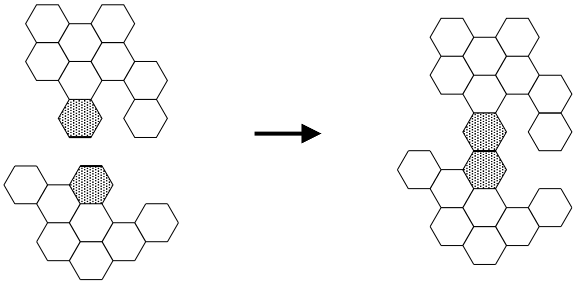

Fig. 2. The concatenation of two polyominoes.

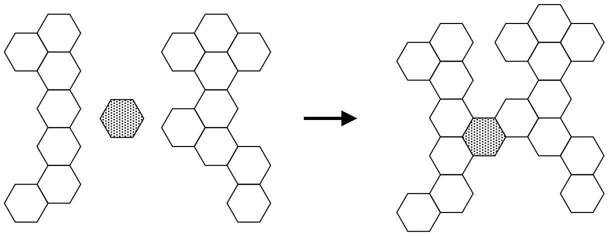

Fig. 3. One of the concatenations needed in the proof of $\theta \leq -1/2$.

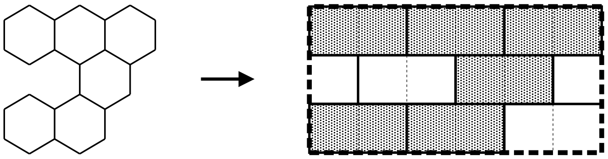

Fig. 4. A polyomino is shown with the corresponding embedding in the brick-work lattice and the bounding rectangle $Z^1_{6,3}$.

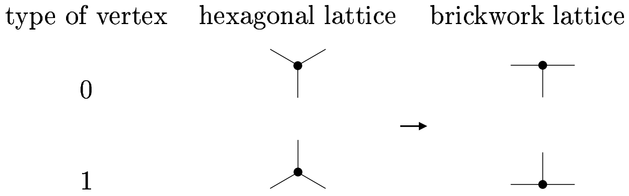

Fig. 5. The two types of vertices that appear on the brick-work lattice.

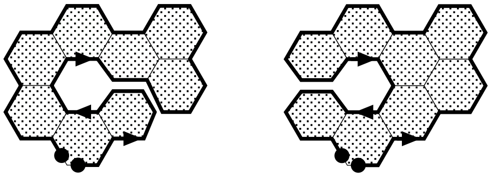

Fig. 6. This figure shows two different manifestations of a polyomino with a hole and a non-returning walk that defines the boundary.

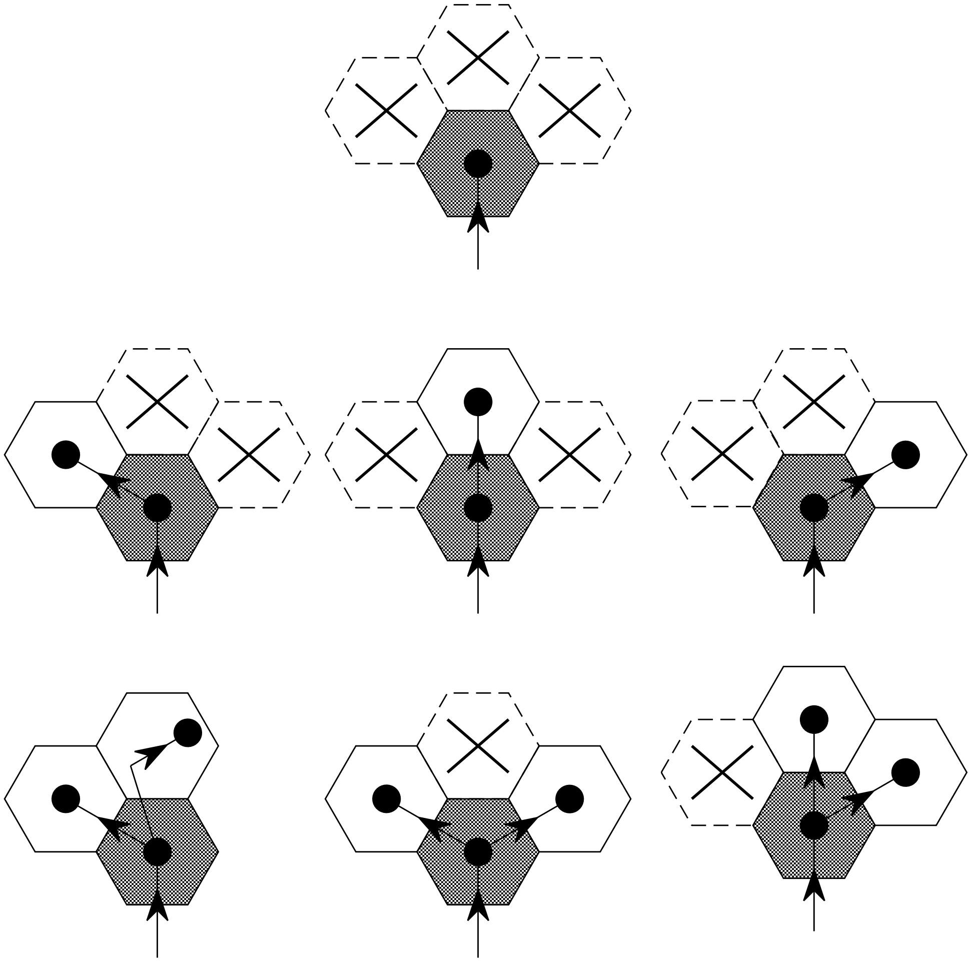

Fig. 7. This figure shows the set of basic twigs used. The dark cells are dead cells, the white cells are living cells and the cells marked with a cross are forbidden cells.

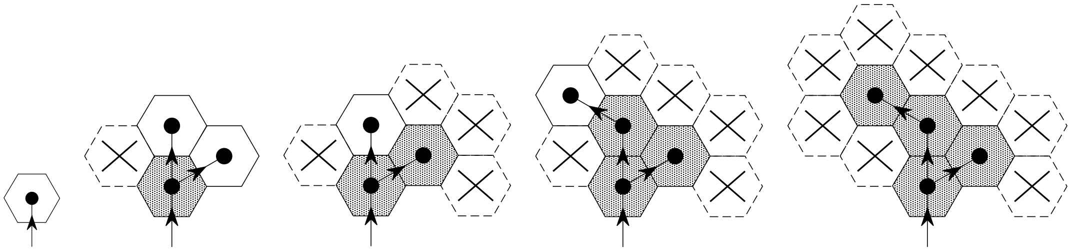

Fig. 8. This figure shows an example of a polyomino of size four being constructed by the successive addition of twigs.

Table 1

The update rules for polyominoes. A cell between the two input bonds can be part of the polyomino, denoted $\text{Output}_{\text{inside}}$, or not, denoted $\text{Output}_{\text{outside}}$. When the state '00'* is produced, the ends of the loops that have been closed have to be relabelled appropriately. "$" indicates that the polyomino can be closed and added to the total count if all other bonds on the intersection line are empty.

Input	$\text{Output}_{\text{inside}}$		$\text{Output}_{\text{outside}}$	
'00'	x '00',	'12'	'00',	x '12'
'01'	x '01',	'10'	'01',	x '10'
'02'	x '02',	'20'	'02',	x '20'
'10'	x '10',	'01'	'10',	x '01'
'11'	x '11',	'00'*	'11',	x '00'*
'12'	x '12',	$	'12',	x '00'
'20'	x '20',	'02'	'20',	x '02'
'21'	x '21',	'00'	'21',	x '00'
'22'	x '22',	'00'*	'22',	x '00'*

Table 2
The number p_h of fixed hexagonal polyominoes of area h cells.

h	p_h
1	1
2	3
3	11
4	44
5	186
6	814
7	3652
8	16689
9	77359
10	362671
11	1716033
12	8182213
13	39267086
14	189492795
15	918837374
16	4474080844
17	21866153748
18	107217298977
19	527266673134
20	2599804551168
21	12849503756579
22	63646233127758
23	315876691291677
24	1570540515980274
25	7821755377244303
26	39014584984477092
27	194880246951838595
28	974725768600891269
29	4881251640514912341
30	24472502362094874818
31	122826412768568196148
32	617080993446201431307
33	3103152024451536273288
34	15618892303340118758816
35	78679501136505611375745

Table 3
A fit to the asymptotic form of the coefficients for fixed polyominoes $p_n/\tau^n \sim n^{-1}[a_1 + a_2/n + a_3/n^{3/2} + a_4/n^2 + a_5/n^{5/2} + \cdots]$. The n^{th} estimate uses the five coefficients $p_n, p_{n-1}, \cdots, p_{n-4}$ to uniquely define the amplitude values. Estimates of the amplitudes a_1, a_2, a_3, a_4, a_5 are given.

n	a_1	a_2	a_3	a_4	a_5
15	0.2734537	−0.203715	0.218992	−0.06350	−0.06548
16	0.2734311	−0.200663	0.196603	−0.00193	−0.12564
17	0.2734515	−0.203625	0.219130	−0.06615	−0.06059
18	0.2734451	−0.202632	0.211316	−0.04312	−0.08472
19	0.2734495	−0.203350	0.217149	−0.06086	−0.06554
20	0.2734513	−0.203662	0.219757	−0.06903	−0.05643
21	0.2734530	−0.203978	0.222468	−0.07777	−0.04643
22	0.2734548	−0.204329	0.225568	−0.08802	−0.03437
23	0.2734562	−0.204614	0.228147	−0.09677	−0.02381
24	0.2734574	−0.204889	0.230698	−0.10564	−0.01287
25	0.2734585	−0.205125	0.232932	−0.11358	−0.00283
26	0.2734594	−0.205332	0.234940	−0.12088	0.00660
27	0.2734601	−0.205508	0.236683	−0.12734	0.01512
28	0.2734607	−0.205655	0.238162	−0.13294	0.02266
29	0.2734611	−0.205773	0.239381	−0.13764	0.02911
30	0.2734614	−0.205865	0.240342	−0.14142	0.03438
31	0.2734617	−0.205931	0.241048	−0.14425	0.03841
32	0.2734618	−0.205973	0.241505	−0.14611	0.04110
33	0.2734619	−0.205992	0.241718	−0.14699	0.04240
34	0.2734619	−0.205990	0.241692	−0.14688	0.04223
35	0.2734618	−0.205967	0.241431	−0.14576	0.04054