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Polygonal polyominoes on the square lattice

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Abstract

We study a proper subset of polyominoes, called *polygonal polyominoes*, which are defined to be self-avoiding polygons containing any number of holes, each of which is a self-avoiding polygon. The staircase polygon subset, with staircase holes, is also discussed. The internal holes have no common vertices with each other, nor any common vertices with the surrounding polygon. There are no 'holes-within-holes'. We use the finite-lattice method to count the number of polygonal polyominoes on the square lattice. Series have been derived for both the perimeter and area generating functions. It is known that while the critical point is unchanged by a finite number of holes, when the number of holes is unrestricted the critical point changes. The area generating function coefficients grow exponentially, with a growth constant greater than that for polygons with a finite number of holes, but less than that of polyominoes. We provide an estimate for this growth constant and prove that it is strictly less than that for polyominoes. Also, we prove that, enumerating by perimeter, the generating function of polygonal polyominoes has zero radius of convergence and furthermore we calculate the dominant asymptotics of its coefficients using rigorous bounds.

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1. Introduction

In an earlier paper [1] the problem of *punctured polygons* was studied. Punctured polygons are self-avoiding polygons (SAPs) with a fixed finite number of holes or punctures, each hole being a SAP. Similarly, staircase polygons with a finite number of staircase holes were also investigated. Topologically, the objects look like the cross section of a slab of Emmenthaler cheese or foam rubber. There is a boundary polygon, containing disjoint polygons which do not touch the boundary. It was shown that the connective constant is unchanged for any finite number of holes. This result was first proved for area enumeration in [2,3], and for enumeration by perimeter in [1]. Further, when enumerating by area, the critical exponent was found to increase by 1 per puncture [2, 3], while when enumerating by perimeter the critical exponent was found to increase by $3/2$ per puncture [1].

A SAP can be defined as a walk on a lattice which returns to the origin and has no other self-intersections. Alternatively we can define a SAP as a connected sub-graph (of a lattice) whose vertices are of degree 2. The history and significance of this problem is nicely discussed in [4]. Generally SAPs are considered distinct up to a translation, so if there are p_n SAPs of length n there are $2np_n$ returns (the factor of two arising since the walk can go in two directions). A polygonal polyomino, hereinafter abbreviated to PP, is defined as a SAP with an arbitrary number of holes, with the perimeter of each hole itself being a SAP. In other words a polygonal polyomino is a SAP enclosing an arbitrary number of SAPs each of which contains no further SAP. Another name for a polygonal polyomino is an *arbitrarily punctured polygon*. A staircase PP (hereinafter called an SPP) is a staircase polygon containing an arbitrary number of disjoint staircase holes.

The model is of interest for several reasons. Firstly, it interpolates between two important, unsolved problems: the enumeration by area of polygons and of polyominoes. All available numerical evidence supports the conclusion that the growth constants, or, equivalently, critical points of these two models differ. A simple proof of this result is given in section 3.1. We know that [2], with a finite number of punctures, the growth constant of polygons does not change. The proposed model aids in our understanding of the key features in regulating asymptotic behaviour of lattice objects. In fact we also know that allowing an arbitrary number of punctures gives an increase in the connective constant [2] compared to finitely punctured polygons, though, we find and prove here, not to the same value as that for polyominoes. Thus the model truly interpolates, being exponentially more numerous than polygons, and exponentially less numerous than polyominoes. This then permits us to conclude that the dominant class of polyominoes is those with vertices of degree four. Another reason the model is interesting is that it corresponds to a previously undiscussed model of site animals, by virtue of the well known bond–site transformation that exists between polyominoes and site animals. It is also well known that polygons model biological vesicles. These may contain occlusions, or bubbles, which would then be modelled more realistically by polygonal polyominoes, rather than polyominoes.

The two principal questions one can ask are 'how many polygonal polyominoes, distinct up to a translation, are there of perimeter $2n$?' and 'how many polygonal polyominoes, distinct up to a translation, are there of area m?' To avoid any possible confusion in our definition of polygonal polyominoes, we restate that the punctures are disjoint—there are no degree four vertices in the objects we are considering.

For unpunctured polygons, enumerated by perimeter, the most recent results are reported in [5], where polygons of perimeter up to 90 steps are given. In that paper analysis of the polygon perimeter generating function led to the conclusion that

$$P^{(0)}(x) = \sum_n p_{2n}^{(0)} x^n \sim B_1^{(0)}(x) + B_2^{(0)}(x)(1-\mu^2 x)^{2-\alpha} \tag{1.1}$$

where $p_{2n}^{(0)}$ is the number of unpunctured polygons of perimeter $2n$, and more generally, $p_{2n}^{(k)}$ is the number of k-punctured polygons of total perimeter $2n$, $\mu = 2.638\,158\,530\,34(10)$, $\alpha = 1/2$, $B_1^{(0)}(1/\mu^2) \approx 0.036$ and $B_2^{(0)}(1/\mu^2) \approx 0.234\,913$. It was also concluded that there was no evidence for a non-analytic correction-to-scaling exponent, so that the asymptotic form of the coefficients behaves as

$$p_{2n}^{(0)} \mu^{-2n} \sim n^{-\frac{5}{2}}[b_1 + b_2/n + b_3/n^2 + b_4/n^3 + \cdots]. \tag{1.2}$$

The connective constant μ is of course the same as that for self-avoiding walks on the same lattice [4].

For polygon areas the most recent published work appears to be [1], in which the first 42 terms of the area generating function were given and analysed. In that work it was found that

$$A^{(0)}(y) = \sum_m a_m^{(0)} y^m \sim C_1^{(0)}(y) + C_2^{(0)}(y)\log(1-\kappa y) \tag{1.3}$$

where $a_m^{(0)}$ is the number of unpunctured polygons of area m, and, more generally, $a_m^{(k)}$ is the number of k-punctured polygons of area m, $\kappa = 3.970\,943\,97(9)$ and various amplitudes are estimated. It was also found that the asymptotic form of the coefficients satisfied

$$a_m^{(0)}\kappa^{-m} \sim m^{-1}[c_1 + c_2/m + c_3/m^2 + c_4/m^3 + \cdots]. \tag{1.4}$$

Estimates of the first few amplitudes c_i were also given.

Note that κ is slightly smaller than the growth constant for the related problem of *polyominoes* [6]. For the polyomino problem, Jensen and Guttmann [7] estimated the connective constant, on the basis of an enumeration to 46 terms, to be $\tau \approx 4.062\,570(8)$.

Note that polygons are just the hole-free subset of square-lattice polyominoes. Further, PPs differ from polyominoes only by the exclusion of configurations in which corners of polygons are allowed to touch. That is to say, configurations with vertices of degree four are permitted for polyominoes, but not for PPs.

For PPs, the basic problem is, analogously, the calculation of the generating functions

$$\hat{P}(x) = \sum_n \hat{p}_{2n} x^n \tag{1.5}$$

and

$$\hat{A}(y) = \sum_m \hat{a}_m y^m \tag{1.6}$$

where

$$\hat{p}_{2n} = \sum_k p_{2n}^{(k)} \tag{1.7}$$

and

$$\hat{a}_m = \sum_k a_m^{(k)}. \tag{1.8}$$

From the generating functions, one then wishes to deduce the asymptotic behaviour. We use the method of series analysis to investigate the PP area generating function. That the coefficients $\hat{a}_m = \hat{\kappa}^{m+o(m)}$ was proved in [2], along with the result that $\hat{\kappa} > \kappa$, but no estimate of $\hat{\kappa}$ (or κ) was given, nor its relationship to τ.

For the perimeter generating function we prove here that the radius of convergence is zero and furthermore that the coefficients grow like $\hat{p}_{2n} = (2n)^{n/2+o(n)}$. The radius of convergence of the analogous full polyomino generating function can be deduced to be zero from earlier work on strongly embedded lattice animals (which are none other than polyominoes) counted by monomer–solvent contacts [8] since the number of monomer–solvent contacts equals the total perimeter of the animals on the lattice dual to that which the animals sit. Note that the set of PPs is a subset of full polyominoes. On the other hand the bounds we give for PPs also hold for full polyominoes so that their number also grows as $\hat{p}_{2n} = (2n)^{n/2+o(n)}$, strengthening the result in [8].

In [1] the finite-lattice method for enumerating punctured polygons is described. It is directly applicable to PP, without modification. We have calculated four series, given in table 1. These are the number of SPPs enumerated by area, the number of SPPs enumerated by perimeter, the number of PPs enumerated by area and the number of PPs enumerated by perimeter.

Table 1. The number of polygonal polyominoes of perimeter $2n$, $\hat{p}_{2n}$, or area m, $\hat{a}_m$, and the number of staircase polygonal polyominoes of perimeter $2n$, $\hat{p}^{\rm st}_{2n}$, or area m, $\hat{s}_m$.

n/m	$\hat{p}_{2n}$	$\hat{a}_m$	$\hat{p}^{\rm st}_{2n}$	$\hat{s}_m$
1		1		1
2	1	2	1	2
3	2	6	2	4
4	7	19	5	9
5	28	63	14	20
6	124	216	42	46
7	588	756	132	105
8	2939	2685	430	243
9	15292	9650	1442	561
10	82168	35018	4956	1303
11	453376	128084	17400	3026
12	2558074	471623	62251	7047
13	14712038	1746492	226506	16419
14	86029132	6499356	836911	38314
15	510455002	24290272	3136182	89454
16	3068304865	91123171	11906908	209056
17	18658787150	342984175	45761338	488810
18	114663168405	1294829776	177903128	1143686
19	711391109162	4901319978	699167112	2677074
20	4452321247688	18597856445	2776219871	6269438
21	28090360338572	70723784744	11132523840	14687799
22	178550339417087	269486503694	45062497156	34423317
23	1142799275636690	1028736811230	184057276510	80702234
24	7361841911349777	3933715966653	758328417263	189258382
25	47712828183763674	15065252411607	3150593560374	443958607
26	311000299384633777	57779548335314	13195743501195	1041704375
27	2038098982983283068	221896915543750	55701570631532	2444830929
28	13424712837039445351	853232815247444	236912169511538	5739200960
29	88856471571466071022	3284632794812871	1015068593253684	13475465449
30	590850295002210397823	12658330973848610	4380259237747256	31646214004
31	3946205909981551632692	48832263708330818	19033328755899266	74332573028
32	26467556786917603655310	188560709059134046	83264420967604579	174627329054
33	178239966838155965583688	728760817757448226	366655205085330754	410313815426
34	1204995095957680793591247	2818940663555496816	1624942378351678887	964245433466
35	8176962665640957003999066	10912731697954602186	7246555406950817070	2266328149674
36	55688824203643528928729635	42277454370938037803	32514274178033294859	5327442926759
37	380592941318712979509072986	163905930541724093228	146758647164785266546	12524850563664
38	2609885948594665135129922550	635879771229410643736	666287722771906045149	29449740628657
39	17955835774830449233266689242	2468511047239077707194	3042232146776071911832	69253703703773
40	123928596735035984074403512167	9588731818158416489325	13968241947440882579006	162875182415300
41	857987154196013528132355504048		64485004508208085784530	383102538326512
42	5957960953815698380702078725480		299291364610157172753062	901200454419191
43	41494342039847412784054011043806		1396371555510788767947710	2120177203865944
44			6548380870934717496464667	4988449724380572
45			30863810827538886791713408	11738161778732289
46			146186095139239811033955305	27623209128180245
47			695766125351305249088108606	65010917109342081
48			3327227388843853057755195874	153015435868159426
49			15985505420293285150710955822	360180105732172583
50			77154096305090215295655323668	847888100764886424
51			374063765552778126305462873154	1996138067317609179
52			1821599276183366136170795057986	4699750155916801866
53			8909395975714092838161196818354	11065985987591398039
54			43762350849164935682443996974055	26057674785502843842
55			215863782802515724690579508172220	61363552769734094377
56			1069193876276445150407221637411850	144515279072674364214
57			5317437665869390636753224605363860	340364808419076278807
58			26551572351632434658366505912095893	801682439416494282830
59			133104721251439553661654788479523704	1888366048221085250103
60			669863574297537386790186209007157407	4448313430293910458776
61			3384106669969830191675921010590498804	10479227865658340635331
62			17160990384334924879892650065013543652	24688076117070001221977
63			87348979596532466909056055181091335100	58165926803554877074945
64			446239239235538076430340141572814690508	137048064231130032590612
65			2287968370937735984302682976966485803978	322923342753661211750433
66				760935261366896243806045
67				1793152365922104505662634
68				4225784928956712385335430
69				9959047794642276203449266
70				23471887252057509601564025
71				55321955801180461643930996
72				130396499371079231113708937
73				307363871855369467378963987
74				724532355612579177700943905
75				1707970821956519674564551300
76				4026432615357178761395593420

The methods of series analysis are discussed in section 2. The area series and the results of the analysis are presented in section 3 along with our rigorous results. The perimeter series and the discussion of their behaviour are presented in section 4 along with our rigorous results. In section 5 we show how the change in the connective constant for PPs relates to the *amplitudes* of the generating functions for k-punctured polygons.

2. Analysis of the series enumerations

Both area series are characterized by coefficients which grow exponentially, with sub-dominant terms given by a critical exponent. (The first clause is rigorously true as discussed above, the second unproved, except for solved models, but is universally accepted.) The generic generating function behaviour is $G(z) = \sum_n g_n z^n \sim D(z)(1 - \sigma z)^{-\xi}$, and hence the coefficients of the generating function $g_n = [z^n]G(z) \sim D(1/\sigma)/\Gamma(\xi)\ \sigma^n\ n^{\xi-1}$. The radius of convergence of the generating function is usually given by the critical point, which is at $z = 1/\sigma$, where σ is often referred to as the *connective constant*.

We used a number of methods to analyse the series studied in this paper. Firstly, to obtain the singularity structure of the generating function we used the numerical method of differential approximants [9]. In particular, we used this method to estimate the growth constant σ and the critical exponent ξ. For PPs we were able to conjecture an exact value for ξ. Imposing this conjectured exponent permitted a refinement of the estimate of the growth constant—providing so-called biased estimates.

While the foregoing analysis method worked well for PPs, it worked less well for SPPs. In that case we reverted to simpler methods based on the ratio method and its refinements [9].

For the first stage of the analysis, the method of differential approximants, we proceeded as follows. 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. For each order L of the inhomogeneous polynomial we averaged over those approximants to the series which used at least the first 80–90% of the terms of the series, and used approximants such that the difference between N, M and K did not exceed 2. These are therefore 'diagonal' approximants. Some approximants were excluded from the averages because the estimates were obviously spurious. The error quoted for these estimates reflects the spread (basically one standard deviation) among the approximants. Note that these error bounds should *not* be viewed as a measure of the true error as they cannot include possible systematic sources of error. However systematic error can also be taken into account in favourable situations, as, for example, in the case of SAP enumerated by perimeter [5]. Again, in the interests of space, we present only our results, and not the intermediate detail from which our estimates were made. An example in full detail for a similar series to those investigated in this study can be found in [5]. We turn now to the analysis of the series.

3. Polygonal polyominoes by area

Before giving the results of our series analysis we present some bounds on the growth constants of PPs and SPPs enumerated by area.

3.1. Bounds for the growth constant of polygonal polyominoes enumerated by area

We have already defined κ as the growth constant, or connective constant, for the number of polygons enumerated by the number of cells, or, equivalently, area. We have also denoted by τ the connective constant for polyominoes (enumerated by the number of cells, or equivalently, by area), and denoted by $\hat{\kappa}$ the analogous constant for polygonal polyominoes. The existence of all three constants follows directly from concatenation arguments and the existence of an upper bound to the nth root of the coefficient of the term conjugate to area n. A review of such arguments can be found in [10]. We note again that in [2] the existence of $\hat{\kappa}$ was proved and $\kappa < \hat{\kappa}$ was also proved. We provide an alternative proof of this result below and expand the inequality to include τ.

We can similarly define three such constants for staircase polygons, staircase polygonal polygons and staircase polyominoes enumerated by area. Let these be η, $\hat{\eta}$ and ζ respectively.

Prior to our numerical analysis, we first outline a proof that $\kappa < \hat{\kappa} < \tau$, and $\eta < \hat{\eta} < \zeta$, based on a recent theorem due to Madras [11] (theorem 2.1, p 366).

Applied to the types of 'cluster' (embedded graph) enumerated by area that we are considering, the theorem may be loosely stated as follows. Let $\mathcal{G}_n$ be such a cluster of area n, and $\lambda = \lim_{n\to\infty}(\mathcal{G}_n)^{1/n}$. Let it contain an arbitrary number of *patterns* P satisfying axioms given below. (Importantly, this arbitrary number is at least linear in n.) For example, polyominoes can contain an arbitrary number of figure-eight graphs[1].

Let $\mathcal{G}_n[\leqslant m, P]$ be the set of such clusters containing at most m translates of a pattern P. Then there exists an $\epsilon > 0$ such that

$$\lambda > \limsup_{n\to\infty} (\mathcal{G}_n[\leqslant \epsilon n, P])^{1/n}. \tag{3.1}$$

Note that the inequality is strict.

Consider as a pattern a unit square. SAPs and k-punctured SAPs contain only a finite number (k) of these patterns. PPs on the other hand contain an arbitrary number. It therefore follows that $\kappa < \hat{\kappa}$. Repeating the argument with a different pattern, that of two unit squares joined corner to corner, a so-called *figure eight* topology, we again see that PPs have none of these, while polyominoes have an arbitrary number. Thus $\hat{\kappa} < \tau$.

The three axioms that must be satisfied are as follows. (i) *Translational invariance*. This is immediately satisfied by the problem specification. (ii) If the clusters are *weighted*, the weight function must satisfy a certain property. In our case, all weights are unity, and the property is thus automatically satisfied. The final axiom is relevant. It states that one can define a new cluster by altering sites and bonds inside a specified set of sites (the pattern in question) and a translation from a specified site to create a (possibly translated) occurrence of a specified pattern, while leaving everything outside the new cluster unchanged. To ensure that this axiom is satisfied, we have to ensure that the surgery carried out, in which a frame or window is placed around a pattern, in going from one model to another does not change the topology of a pattern. In our case the concern is that a polygon pattern might change to a figure eight. This situation can be accommodated by making the frame of finite thickness (one lattice spacing) rather than of zero thickness.

The analogous result for staircase polygons, PPs and polyominoes also follows immediately. That is to say, $\eta < \hat{\eta} < \zeta$.

3.2. Analysis of staircase polygonal polyominoes by area

For SPPs we have generated a 75-term series. We denote the generating function $\hat{S}(y) = \sum \hat{s}_m y^m$, where $\hat{s}_m$ is the number of SPPs of area m. Differential approximant analysis gave predominantly defective approximants, and a strong indication of several confluent singularities. Accordingly we abandoned that method of analysis, and instead looked at the results of the ratio method. Ratio plots, enhanced by Neville table extrapolation, gave sequences of estimates of the connective constant that were monotonically increasing. This behaviour allowed us to conclude that the growth constant $\hat{\eta} > 2.36$, and in fact $\hat{\eta} \approx 2.365$,

[1] These are two polygons sharing a vertex, which is thus of degree four.

where we expect the error to be confined to the last quoted digit. For staircase polygons with a finite number of staircase holes, [1], the growth constant is known to be $\eta = 2.309\,138\ldots < \hat{\eta}$. With such an imprecise estimate of the connective constant for SPPs, it is not surprising that we can only imprecisely estimate the exponent. While the staircase polygon area generating function has a simple pole singularity, the SPP generating function appears to have a slightly sharper singularity, but we really cannot say much more than that

$$\hat{S}(y) = \sum_m \hat{s}_m y^m \sim E\,(1 - \hat{\eta} y)^{-\theta} \tag{3.2}$$

and hence

$$\hat{s}_m = [y^m]\hat{S}(y) \sim \hat{\eta}^m m^{\theta-1} \tag{3.3}$$

where $\hat{\eta} = 2.365 \pm 0.005$, and $\theta = 1.25 \pm 0.25$.

Thus it is possible that the generating function has a simple pole, just like its unpunctured counterpart—but with a different connective constant. While we consider this the most likely scenario, the series analysis does indicate a slightly higher value for the exponent.

3.3. Analysis of polygonal polyominoes by area

For polygonal polygons, we have obtained 40 terms in the generating function $\hat{A}(y)$. Our analysis based on the method of differential approximants strongly suggests that the generating function $\hat{A}(y)$ behaves similarly to its unpunctured counterpart, but with a slightly larger connective constant. More precisely, we find

$$\hat{A}(y) = \sum_m \hat{a}_m y^m \sim \hat{C}_1(y) + \hat{C}_2(y)\log(1 - \hat{\kappa} y) \tag{3.4}$$

with $\hat{\kappa} \approx 3.980\,503$, where we expect the error to be restricted to the last quoted digit. Hence, our numerical results are consistent with the proven inequality $\kappa < \hat{\kappa} < \tau$.

However, unlike the situation for unpunctured polygons, we were unable to obtain convincing numerical evidence for the nature of the sub-dominant singularities, except to find that the situation appears more complex than that for unpunctured polygons, in which case we found that the asymptotic form of the coefficients satisfied (1.4).

4. Polygonal polyominoes by perimeter

Before giving the results of our series analysis we present some bounds on the number of PPs and SPPs enumerated by perimeter and associated rigorous results for the dominant asymptotic behaviour of these numbers.

4.1. Bounds for the number of arbitrarily punctured polygons enumerated by perimeter

Recall that $p_{2n}^{(k)}$ is the number of punctured polygons with k polygonal holes of total perimeter $2n$. The polygons and all the holes are taken to be SAPs on the square lattice. Furthermore all polygons mutually avoid each other. Let $\hat{p}_{2n}$ be the number of punctured polygons with an arbitrary number of such holes of total perimeter $2n$ (i.e. polygonal polyominoes). Hence,

$$\hat{p}_{2n} = \sum_{k=0}^{\infty} p_{2n}^{(k)}. \tag{4.1}$$

Note, however, the sum (4.1) has only a finite number of terms for any fixed n and there exists a number k_x depending on n such that $k_x(n)$ is the maximum number of holes possible for a

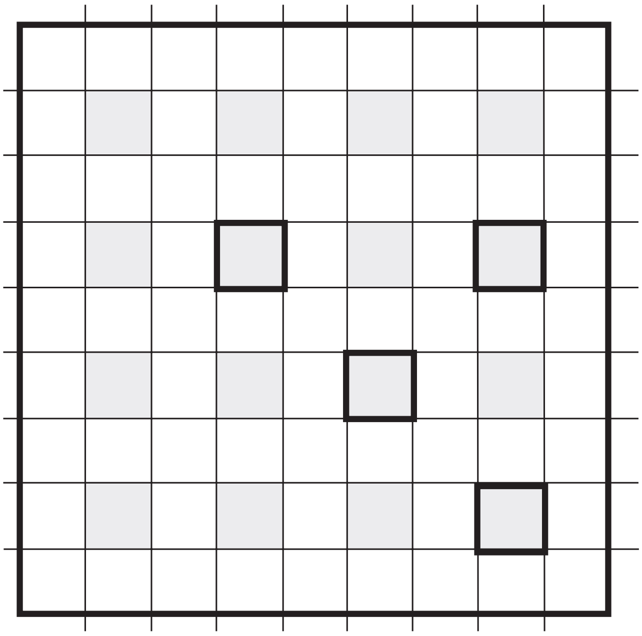

Figure 1. The figure portrays a configuration of the lower bound $L_{52}^{(4)}$. Here, $m = 4$ so a large square of side 9 makes up the outside polygon while $k = 4$ so four unit squares have been arranged on the sparse checker-board that is indicated by the grey shaded faces.

punctured polygon of total perimeter $2n$ and so $p_{2n}^{(k)} = 0$ for $k > k_x$. We note that $p_{2n}^{(0)}$ is simply the number of SAPs of perimeter $2n$. Also, let $\hat{p}_{2n}^{\mathrm{st}}$ be the number of punctured polygons of total perimeter $2n$ with an arbitrary number of such holes where all the polygons involved are staircase polygons on the square lattice (i.e. staircase polygonal polyominoes—SPPs).

In this section we shall accomplish two tasks. Firstly, we construct upper and lower bounds for $\hat{p}_{2n}$. Secondly, we shall use these bounds to show that the limit

$$\lim_{n\to\infty} \frac{\log \hat{p}_{2n}}{2n \log 2n} \tag{4.2}$$

exists and is equal to 1/4. Hence, the normal free energy defined as the limit

$$\lim_{n\to\infty} \frac{1}{2n} \log \hat{p}_{2n} \tag{4.3}$$

is infinite.

To begin, since every SPP is a PP it should be clear that

$$\hat{p}_{2n}^{\mathrm{st}} \leqslant \hat{p}_{2n}. \tag{4.4}$$

We shall first construct various lower bounds for $\hat{p}_{2n}$, which we label $L_{2n}^{(k)}$. Consider a square of side $2m + 1$ on the square lattice and k unit square polygons (each having perimeter four). The total perimeter for such a collection is

$$2n = 4(2m + 1 + k). \tag{4.5}$$

Now consider placing the k unit square polygons inside the larger square to form punctured polygons. Let us restrict the places where we put the unit squares so they are mutually avoiding by construction: we shall restrict these placement positions to the sparse-checkerboard positions as in figure 1. There are m^2 such placement positions inside the larger square. Let $L_{2n}^{(k)}$ be the number of ways of placing k unit square polygons inside a square of side $2m+1$ to give a total perimeter as in (4.5). Each configuration so generated is a valid punctured polygon since each of the constituents are SAPs (they are all squares) and they have been constructed to be mutually avoiding. The numbers $L_{2n}^{(k)}$ are given by

$$L_{4(2m+1+k)}^{(k)} = \binom{m^2}{k}. \tag{4.6}$$

Since squares are also staircase polygons we immediately have that

$$L_{4(2m+1+k)}^{(k)} \leqslant \hat{p}_{4(2m+1+k)}^{\mathrm{st}} \leqslant \hat{p}_{4(2m+1+k)} \tag{4.7}$$

for all $m \geqslant 1$ and for $0 \leqslant k \leqslant m^2$. This gives us lower bounds for all even values of $n \geqslant 6$. To obtain lower bounds for n odd simply consider enlarging the outer square of our constructed configurations for n even by two steps: one can do this by adding a face adjacent to and outside the square to the inside of the punctured polygon (that is, shifting a step in the square outwards one face of the lattice and adding steps to the other two sides of that face). There are $4(2m+1)$ places to add these steps. This procedure gives a set of configurations that are punctured polygons of total perimeter

$$2n = 4(2m+1+k) + 2. \tag{4.8}$$

Hence we can choose $L_{4(2m+1+k)+2}^{(k)} = (8m+4)L_{4(2m+1+k)}^{(k)}$. So for any value of total perimeter, $2n \geqslant 12$, one can always find k and m so that

$$L_{2n}^{(k)} \leqslant \hat{p}_{2n}^{\mathrm{st}} \leqslant \hat{p}_{2n}. \tag{4.9}$$

For sufficiently large n there are many allowed values of k and m.

Next we construct an upper bound U_{2n}, and then bound this number by an easily calculated value $\bar{U}_{2n}$. Consider an area on the square lattice inside a square of side $n-1$ including the boundary of this square, but do not place a square polygon on the boundary as we did for the lower bound above. Any SAP of perimeter less than or equal to $2n$ can be placed inside such a square by simple translation since the maximum horizontal or vertical extent of such a polygon is $n-1$ lattice units. Since any punctured polygon of total perimeter $2n$ has an outside polygon of perimeter less than or equal to $2n$ they can always be fitted inside this 'imaginary' bounding square. The bounding square's area has $b = 2n^2 - 2n$ lattice bonds. Now observe that any SAP can be constructed from the concatenation of a number of four-step oriented self-avoiding walks with perhaps the inclusion of a single six-step oriented self-avoiding walk. Hence all punctured polygons of total perimeter $2n$ can be constructed by placing a number of four-step oriented self-avoiding walks and six-step oriented self-avoiding walks on the square lattice inside the bounding square. Let us now consider the sets of all four-step oriented self-avoiding walks and six-step oriented self-avoiding walks which are unique up to translation and rotation by $\pi/2$. Denote their cardinality by c_4 and c_6 respectively. Choose ℓ_0 such four-step walks and ℓ_1 such six-step walks such that

$$4\ell_0 + 6\ell_1 = 2n. \tag{4.10}$$

In this way we have chosen walks whose total length is $2n$. Let $\ell = \ell_0 + \ell_1$ be the total number of objects chosen at any one time. Place these walks on the square lattice such that the first step of each walk is inside the bounding square described above and such that these first steps are on different bonds of the lattice. By considering all possible placements of all possible sets of 4 and six-step walks chosen with all values of ℓ_0 and ℓ_1 obeying (4.10) we have constructed a set of configurations that is a superset of the set of punctured polygons of total perimeter $2n$.

Note that we have ignored the mutual avoidance of the walks. Let U_{2n} be the number of four- and six-step walks so placed. Hence

$$\hat{p}_{2n}^{\mathrm{st}} \leqslant \hat{p}_{2n} \leqslant U_{2n} \tag{4.11}$$

for all $n \geqslant 2$. The numbers U_{2n} are given as

$$U_{2n} = \sum_{\ell_0} c_4^{\ell_0} \, c_6^{\ell_1} \binom{b}{\ell} \tag{4.12}$$

with (4.10) always satisfied. We now note that $\ell_0 \leqslant n/2$, $\ell_1 \leqslant n/3$ and $n/3 \leqslant \ell \leqslant n/2$. Using these inequalities one can bound U_{2n} as

$$\begin{aligned} U_{2n} &\leqslant c_4^{n/2} c_6^{n/3} \sum_{\ell=n/3}^{n/2} \binom{b}{\ell} \\ &\leqslant c_4^{n/2} c_6^{n/3} \frac{n}{6} \binom{b}{n/2}. \end{aligned} \tag{4.13}$$

Hence if we define

$$\bar{U}_{2n} = c_4^{n/2} c_6^{n/3} \frac{n}{6} \binom{2n^2 - 2n}{n/2} \tag{4.14}$$

we have

$$\hat{p}_{2n}^{\mathrm{st}} \leqslant \hat{p}_{2n} \leqslant U_{2n} \leqslant \bar{U}_{2n} \qquad \text{for all} \quad n \geqslant 2. \tag{4.15}$$

Now we come to the second part of our work in this section and analyse the dominant asymptotics of $\hat{p}_{2n}$ using our bounds. We make extensive use of the following result: let $a(n) \gg n \gg 1$ such that $\lim_{n\to\infty} n/a(n) = 0$, then

$$\log \binom{a(n)}{n} \sim n \log \left(\frac{a(n)}{n} \right) \qquad \text{as} \quad n \to \infty \tag{4.16}$$

and the asymptotic error is of order $\mathrm{O}(n)$. Using this we can show that

$$\lim_{n\to\infty} \frac{\log \bar{U}_{2n}}{2n \log 2n} = \frac{1}{4}. \tag{4.17}$$

Demanding that $k = \mathrm{o}(m^2)$ and $k > \alpha m$ for some $\alpha > 0$ we also have

$$\frac{\log L_{2n}^{(k)}}{2n \log 2n} \sim \frac{k}{4k + 8m} \qquad \text{as} \quad m \to \infty. \tag{4.18}$$

Hence, by choosing $k = \lfloor m \log_2 m \rfloor$ (which is always possible), for any even (odd) value of n one solves (4.5) (respectively (4.8)) for m, and noting that $m \to \infty$ as $n \to \infty$, we have

$$\lim_{n\to\infty} \frac{\log L_{2n}^{(k^*)}}{2n \log 2n} = \frac{1}{4} \tag{4.19}$$

where k^* is the sequence of k values chosen according to the algorithm above. Using the Sandwich theorem for limits we have the existence of the limit (4.2) and the value

$$\lim_{n\to\infty} \frac{\log \hat{p}_{2n}}{2n \log 2n} = \frac{1}{4}. \tag{4.20}$$

This result is also true for SPPs. Our results immediately imply that the free energy, defined by (4.3), is infinite for both staircase and regular self-avoiding punctured polygons. We note in passing that the above bounds also hold for full polyominoes counted by perimeter since in the upper bound mutual avoidance is ignored.

4.2. Analysis of SPPs and PPs by perimeter

We have enumerated all SPPs up to and including those of perimeter 130, and all PPs up to and including those of perimeter 86. The bounds obtained in the previous section imply that we should analyse not the ordinary generating function, but rather a modified exponential generating function. The results above imply that the leading asymptotic term is $p_n \sim (n/4)!$ for either a PP or an SPP of perimeter n.

Accordingly, we first divided by this factor, and studied the resulting generating functions with coefficients $q_n = p_n/(n/4)!$. For SPPs, the coefficients q_n obtained in this way increase up to terms corresponding to polygon perimeter 86, and then decreased. For PPs, the corresponding coefficients are monotonically increasing for all coefficients to hand. However the ratio of coefficients is decreasing, and the sequence of ratios extrapolates to a value less than 1, which implies that, for n sufficiently large, the coefficients q_n will also reach a maximum and then decrease.

A difficulty in any further analysis is that we have no reasonable expectation as to the sub-dominant asymptotic form. The fact that the terms at first increase and then decrease implies that the sub-dominant form is going to be complicated, involving the interplay of at least two different terms. A plausible first guess is that the next term is of the form $q_n \sim \mu^n$. If so, ratios of coefficients $r_n = q_n/q_{n-1}$ should converge to μ. The observed behaviour of the coefficients r_n implies that we are quite far from the asymptotic regime. Applying a variety of standard extrapolation procedures [9] is inconclusive. For PPs we have some evidence that $\mu(\text{PP}) \approx 0.6$, while for SPPs it appears that $\mu(\text{SPP}) \approx 0.4$. These estimates come from combining the results of five different extrapolation schemes, where the spread of estimates implies that we can only quote one significant digit, and even this is uncertain. In both cases errors of about ± 01 would encompass most estimates. We remark in passing that a functional form of the type $q_n \sim \mu^n \lambda^{\sqrt{n}} n^g$ is one of a number of possible forms that can give rise to sequences that behave as observed, but our attempts to fit to this form have not been successful.

In an attempt to confirm these tentative extrapolations we studied the ratio of the coefficients of the SPP and PP generating functions. That is, we studied the sequence $\{r_n\}$ where $r_n = p_n(\text{PP})/p_n(\text{SPP}) = q_n(\text{PP})/q_n(\text{SPP})$. In this way the leading asymptotic part of course cancels, and hopefully any sub-sub-dominant terms, such as $\log n$ or n^g, are weakened. Extrapolating the sequence $\{r_n\}$ should then provide an estimate of the ratio $\mu(\text{PP})/\mu(\text{SPP})$. This study gave results that were reasonably consistent across several extrapolation techniques, all giving rise to the estimated limit 1.25 ± 0.02. This is consistent with, but more precise than, the individual estimates given above, whose ratios are 1.5 ± 0.5.

Thus we conclude this section with the rather tentative conclusions that the first sub-dominant term appears to be μ^n, where $\mu(\text{PP}) \approx 0.6$ and $\mu(\text{SPP}) \approx 0.4$. Further, we find evidence from the behaviour of the coefficients that the sub-sub-dominant term is stronger than n^g.

5. Critical point renormalization

We have noted [1] that for a k-punctured polygon, the coefficients of the area generating function grow like κ^n, with $\kappa = 3.9709\ldots$, while PPs (which can have any number of punctures), have coefficients which grow like $\hat{\kappa}^n$ where $\hat{\kappa} = 3.9805\ldots$.

One mechanism for the renormalization of the growth constant is given by the k-dependence of the *amplitudes* of the generating function of k-punctured polygons. The proposed mechanism is illustrative rather than definitive. That is to say, we propose a plausible mechanism, but there are others.

Let $A^{(k)}(y)$ be the generating function of k-punctured polygons by area. It was found [1] that

$$A^{(k)}(y) \sim C^{(k)}(y) y^{3+\ell k}(1-\kappa y)^{-k} \tag{5.1}$$

for $k > 0$[2]. The generating function for PPs is clearly obtained by summing $A^{(k)}(y)$ over k, so that

$$\begin{aligned}\hat{A}(y) &= \sum_k A^{(k)}(y) \sim A^{(0)}(y) + y^3 \sum_{k\geqslant 1} C^{(k)}\,(1/\kappa)\, y^{\ell k}(1-\kappa y)^{-k} \\ &= A^{(0)}(y) + y^3 \sum_{k\geqslant 1} C^{(k)}(1/\kappa)\,\theta^k \end{aligned}\tag{5.2}$$

where $\theta = \frac{y^\ell}{1-\kappa y}$.

Now if $C^{(k)}(1/\kappa) \sim c^{-k}/k^n$, then

$$\hat{A}(y) \sim A^{(0)}(y) + y^3 \sum_{k\geqslant 1} \left(\frac{\theta}{c}\right)^k \Big/ k^n = A^{(0)}(y) + y^3 Li_n\left(\frac{\theta}{c}\right). \tag{5.3}$$

That is, the singular behaviour is given by an nth-order polylogarithm. The polylogarithm function is singular when its argument is unity, hence it is singular at $c = \frac{y^\ell}{1-\kappa y}$, that is, when $1 - \kappa y - y^\ell/c = 0$, so that the growth constant is increased. In the special case $n = 1$, the polylogarithm is a simple logarithm, and we find

$$\hat{A}(y) = A^{(0)}(y) - y^3 \log\big((1-\kappa y - y^\ell/c)/(1-\kappa y)\big) \tag{5.4}$$

which is just the behaviour we observe for PPs: that is to say, a renormalized critical point, and an (unchanged) logarithmic singularity, as is observed numerically.

6. Conclusion

We have investigated polygonal polyominoes and staircase polygonal polyominoes enumerated both by area and perimeter.

We have shown that the perimeter generating functions have zero radius of convergence and asymptotic growth $\hat{p}_{2n} = (2n)^{n/2+o(n)}$. Analysis suggests that the sub-dominant term is μ^n. Estimates of μ of limited precision are given.

For the area generating function we have proved that $\eta < \hat{\eta} < \zeta$ for staircase polygons, SPPs and staircase polyominoes, and $\kappa < \hat{\kappa} < \tau$ for polygons, PPs and polyominoes. Numerically we have found

$$\hat{S}(y) = \sum_m \hat{s}_m y^m \sim E\,(1-\hat{\eta} y)^{-\theta} \tag{6.1}$$

where $\hat{\eta} = 2.365 \pm 0.005$, and $\theta = 1.25 \pm 0.25$, for SPPs, and

$$\hat{A}(y) = \sum_m \hat{a}_m y^m \sim \hat{C}_1(y) + \hat{C}_2(y)\log(1-\hat{\kappa} y) \tag{6.2}$$

with $\hat{\kappa} \approx 3.980\,503$, for PPs.

[2] Here $\ell \approx 5$, and just reflects the fact that the lowest-order non-zero coefficient of the generating function is clearly an increasing function of k. The exponent ℓ is in fact k-dependent, but takes the quoted value on average. For $k = 0$ the singularity is logarithmic and the pre-factor power of y is absent.

E-mail or WWW retrieval of series

The series for the various generating functions studied in this paper can be obtained via e-mail by sending a request to I.Jensen@ms.unimelb.edu.au or via the world-wide web on the URL http://www.ms.unimelb.edu.au/˜iwan/ by following the instructions.

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