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FAST TRACK COMMUNICATION

The unusual asymptotics of three-sided prudent polygons

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Online at stacks.iop.org/JPhysA/43/342001**Abstract**

We have studied the area-generating function of prudent polygons on the square lattice. Exact solutions are obtained for the generating function of two-sided and three-sided prudent polygons, and a functional equation is found for four-sided prudent polygons. This is used to generate series coefficients in polynomial time, and these are analysed to determine the asymptotics numerically. A careful asymptotic analysis of the three-sided polygons produces a most surprising result. A transcendental critical exponent is found, and the leading amplitude is not quite a constant, but is a constant plus a small oscillatory component with an amplitude approximately 10^{-8} times that of the leading amplitude. This effect cannot be seen by any standard numerical analysis, but it may be present in other models. If so, it changes our whole view of the asymptotic behaviour of lattice models.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

A well-known long-standing problem in combinatorics and statistical mechanics is to find the generating function for self-avoiding polygons or polyominoes on a two-dimensional lattice, enumerated by area. These are models of biological vesicles that can expand or contract [1], and also occur in models of magnetism, such as the Ising model.

Prudent walks were introduced to the mathematics community by Pr ea in an unpublished manuscript [2] and more recently reintroduced by Duchi [4]. A prudent walk is a connected path on \mathbb{Z}^2 such that, at each step, the extension of that step along its current trajectory will

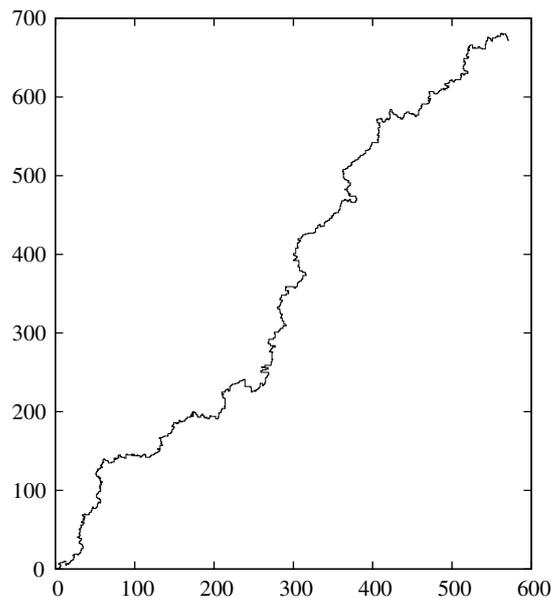


Figure 1. Typical prudent walk of $n = 2000$ steps, generated via Monte Carlo simulation using a pivot algorithm [3].

never intersect any previously occupied vertex. Such walks are clearly self-avoiding. We take the empty walk, given by the vertex $(0, 0)$ to be a prudent walk. Figure 1 shows a typical prudent walk of $n = 2000$ steps, generated via Monte Carlo simulation using a pivot algorithm. Note the roughly linear behaviour—it is believed, although unproven, that the mean-square end-to-end distance grows like n^2 for prudent walks, i.e. that the exponent ν defined through $\langle R^2 \rangle_N \sim AN^{2\nu}$ is exactly 1.

The *bounding box* of a prudent walk is the minimal rectangle containing the walk. The bounding box may reduce to a line or even to a point in the case of the empty walk. One significant feature of two-dimensional prudent walks is that the end-point of a prudent walk is always on the boundary of the bounding box. At every step of the walk, the step just taken either lies on the perimeter of the existing bounding box of the walk or it extends the bounding box (while still lying on the perimeter of the newly extended box). Note that this is not a bijection. There are walks with each step lying on the perimeter of the bounding box that are not prudent. Such walks we call *perimeter walks*. Prudent walks are, generally speaking, not reversible. If a path from the origin to the end-point defines a prudent walk, it is not necessary that the path from the end-point to the origin will also be a prudent walk. Ordinary SAW are of course reversible.

Even though prudent walks are a subset of self-avoiding walks, the problem of their enumeration is still not solved. Accordingly, certain subsets of prudent walks have been studied. These are called *one-sided*, *two-sided* and *three-sided* prudent walks. The original problem corresponds to *four-sided* prudent walks, but we will refer to them just as prudent walks (see figure 2 for examples). Every step of a one-sided prudent walk must end on the northern side of its bounding box. Every step of a two-sided prudent walk must end on the northern or eastern sides of its bounding box.

Every step of a three-sided prudent walk must end on the northern, eastern or western sides of its bounding box. Here we will be concerned with the polygon analogue. A prudent

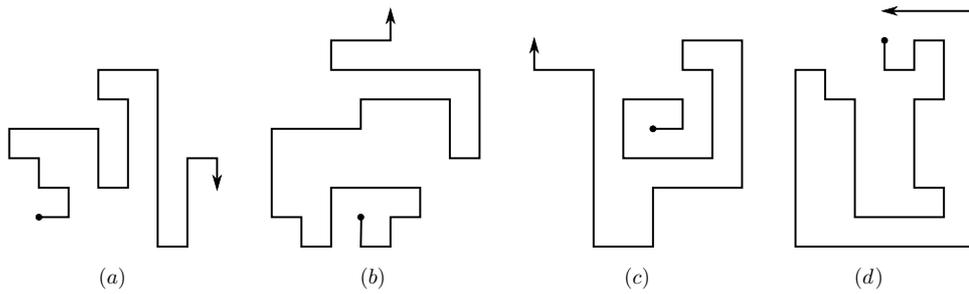


Figure 2. Examples of (a) a two-sided prudent SAW; (b) a three-sided prudent SAW; (c) an (unrestricted) prudent SAW; and (d) a prudent SAW leading to a prudent SAP.

polygon is a prudent walk of $2n - 1$ steps that ends on a lattice site adjacent to the origin. Then the addition of a single bond suffices to close the walk, forming a $2n$ -step polygon, as shown in figure 2(d). The case of two-sided prudent walks was solved by Duchi [4] who also gave a functional equation for four-sided prudent walks. The case of three-sided prudent walks was subsequently solved by Bousquet-Mélou [5], who also solved a version of the model on the triangular lattice. Bousquet-Mélou used the kernel method [6] to solve the three-sided case, which had a rather complicated solution, given in terms of the q -series.

The polygon version of the problem was introduced by one of us (AJG) and studied by Schwerdtfeger [7] who solved the problem in the case of the *perimeter*-generating function of two-sided and three-sided prudent polygons, using a method of solution similar to that used by Bousquet-Mélou for the walk case. For the unrestricted, or four-sided case, Garoni *et al* [8] used a transfer-matrix formulation to generate the first 500 terms in the generating function (equivalent to 1000 step polygons). Schwerdtfeger [7] subsequently gave an equivalent, but more elegant, functional equation for the four-sided case. Garoni *et al* [8] gave an analysis of the 500-term series. Despite the substantial length of the series, the results were not as precise as one might have expected. The number of polygons of perimeter $2n$ was found to grow like $A\mu^{2n}n^g$, where the estimates $\mu^2 \approx 4.415$ and $g \approx 2.5$ were given. The estimate of g in particular was rather uncertain, being very sensitive to the value of μ used in its estimation.

The rest of this communication is about the behaviour of prudent polygons enumerated by *area* rather than perimeter. That case is in one sense easier, in that as we move from two-sided, to three-sided to four-sided, the exponential growth factor μ appears to remain unchanged³. For perimeter enumeration, μ changes as we move through the same cycle of models. While for the four-sided case, enumerated by area, we have not solved the problem, we do at least know the exact value of μ^2 , which is 4. This makes the series analysis more precise than in the perimeter enumeration case.

Let a_n denote the number of polygons, of a given class, enclosing an area n . Typically, indeed, until this work we would have said invariably, the asymptotic behaviour of a_n is

$$a_n \sim B\mu^n n^g. \quad (1)$$

Here μ is the growth constant, g is the critical exponent (sometimes $1 + g$ is referred to as the critical exponent, as that is the exponent that occurs in the singular behaviour of the generating function $A(z) = \sum a_n z^n \sim D(1 - \mu z)^{-(1+g)}$), and B is a critical amplitude (sometimes D is referred to as the critical amplitude). For most solvable models, μ is algebraic, g is a simple rational fraction and B (or the simply related D) is a real number.

³ This is proved for two-sided and three-sided polygons, but only verified to high precision for four-sided polygons.



Figure 3. A prudent SAW corresponding to a one-sided prudent SAP.

We will show that for one-sided and two-sided prudent polygons, enumerated by area, that is precisely the case. However, for three-sided prudent polygons, we prove that this is not the case. First, we find a non-rational critical exponent, $g = \log_2 3 \approx 1.584$. However, the most astonishing result is that the limit as n tends to infinity of $a_n/(\mu^n n^g)$ does not exist! That is to say, there is no unique critical amplitude. Indeed, we find that

$$a_n \sim \beta(\log_2 n) \mu^n n^g, \quad \mu = 2, g = \log_2 3,$$

where $\beta(n)$ is a periodic function with mean value 0.108 38 and amplitude of the periodic oscillation around 10^{-9} . Thus, the ratio $a_n/(\mu^n n^g)$ oscillates with a known periodicity!

Given that such a small variation in amplitude is extraordinarily difficult to detect numerically, this result raises the question as to just how common this behaviour is? Are there other models for which the standard asymptotics as given by equation (1) does not prevail? If so, it opens a whole new chapter in the study of exactly solved models.

A comprehensive and detailed discussion of the asymptotic analysis will be published elsewhere [9]. Here we will give only a sketch of the derivation, as our aim in this communication is to focus on the implications of the result for other lattice models of interest in mathematical physics.

2. The behaviour of prudent polygons

2.1. One-sided prudent polygons

One-sided prudent polygons are simply a single row or column of cells. An example of a prudent SAW leading to a one-sided prudent polygons is shown in figure 3. The area-generating function is, self-evidently,

$$A_1(q) = \frac{2q}{1 - q},$$

while the semi-perimeter-generating function is

$$P_1(x) = \frac{2x^2}{1 - x}.$$

The singularity in either case is a simple pole at $q = 1$ or $x = 1$ for the area- or perimeter-generating function, respectively.

2.2. Two-sided prudent polygons

Two-sided prudent polygons ending at $(0, 1)$ in a counterclockwise direction appear as upside-down bar graphs. A bar graph is either a single column or can be constructed by adding a column to the right of another bar graph, and thus the bar-graph-generating function $B(q)$ satisfies

$$B(q) = \frac{q}{1 - q} + \frac{q}{1 - q} B(q).$$

We wish to determine the asymptotic expansion around $q = 1/2$. We define a small parameter $t = 1 - 2q$. The sum then becomes approximately

$$-\sum_{m,l} a_{m,l} \frac{2^{-m}}{1+t \cdot 2^{l+2}}, \tag{5}$$

and we are interested in the asymptotic behaviour around $t = 0$.

The Mellin transform of a function $f(x)$ is

$$\phi(s) = \int_0^\infty x^{s-1} f(x) dx,$$

and our analysis of (5) follows the methods of [12]. The Mellin transform of $\frac{1}{1+\alpha x}$ is $\pi \alpha^{-s} / \sin \pi s$. The Mellin transform of equation (5) is therefore

$$-\sum_{m,l} a_{m,l} 2^{-m} 2^{-s(l+2)} \pi / \sin \pi s = -2^{-2s} \pi / \sin \pi s \cdot a\left(\frac{1}{2}; 2^{-s}\right). \tag{6}$$

Now

$$a\left(\frac{1}{2}; z\right) = \frac{-4(3/2; 1/2)_\infty (z/2; 1/2)_\infty}{(3z/2; 1/2)_\infty (1/2; 1/2)_\infty}.$$

The singularities closest to the right of the fundamental strip of (6) occur when

$$1 - \frac{3}{2} 2^{-s} = 0$$

or

$$s_k = \log_2 3 - 1 + \frac{2k\pi i}{\log 2}, \quad k \in \mathbb{Z}. \tag{7}$$

Near $s \approx s_0$, the rhs of equation (6) becomes

$$\frac{16\pi}{9 \log 2 \sin(\pi s_0)} \cdot \frac{(3/2; 1/2)_\infty (1/3; 1/2)_\infty}{(1/2; 1/2)_\infty^2} \times \frac{1}{s - s_0}.$$

The inverse Mellin transform can now be taken, which just involves replacing $\frac{1}{s-s_0}$ by $(1 - 2q)^{-s_0}$. Reintroducing the prefactor multiplying the sum in equation (3), we find the leading asymptotic behaviour to be

$$\frac{\pi}{9 \log 2 \sin(\pi s_0)} \cdot \frac{(3/2; 1/2)_\infty (1/3; 1/2)_\infty}{(1/2; 1/2)_\infty^2} \times \frac{1}{(1 - 2q)^{s_0}}. \tag{8}$$

The transfer of the asymptotic form (8) of $A_3(q)$ at its singularity $q = 1/2$ to the coefficients $a_n^{(3)}$ is permitted, subject to various side conditions, and here we resort to singularity analysis as described in [11]. This leads us to expect the asymptotics to behave, in the usual way, as

$$a_n^{(3)} \sim \kappa \cdot n^g \cdot 2^n, \tag{9}$$

where

$$\kappa = \frac{\pi}{9 \log 2 \sin(\pi s_0) \Gamma(s_0 + 2)} \cdot \frac{(3/2; 1/2)_\infty (1/3; 1/2)_\infty}{(1/2; 1/2)_\infty^2} = 0.108\,384\,2947\dots \tag{10}$$

and

$$g = s_0 + 1 = \log_2 3 = 1.584\,962\,501\dots$$

in seemingly good agreement with our series analysis. However, there are two surprises. The first is the transcendental value of the exponent. This is very rare for two-dimensional lattice models. What is even rarer is the fact that there are other terms ('harmonics') of the same

asymptotic order as (9), but of a numerically minute amplitude and an oscillating character. In particular, recall that only the term $k = 0$ in equation (7) was taken. If we now include the next two terms, corresponding to $k = \pm 1$, we get an additional term, to be added to the dominant term, of the form

$$\kappa' \cdot n^g \cdot 2^n,$$

where

$$\kappa' = c_1 \cos(2\pi \log_2 n) + c_2 \sin(2\pi \log_2 n), \tag{11}$$

where $c_1, c_2 \approx 10^{-9}$. Taking $k = \pm 2$ adds a further oscillatory term with an even smaller amplitude. Thus, we see that the leading amplitude does not, in fact, exist in a technical sense. That is to say, the limit

$$\lim_{n \rightarrow \infty} \frac{a_n^{(3)}}{n^g \cdot 2^n}$$

does not exist! Numerically, we are unlikely to ever observe this, as the ‘effective amplitude’ is indeed given by equation (10) and varies from this value as n increases by no more than about one part in 10^8 . Knowing that this term is present, and having available very long series of hundreds of terms, we can see clear numerical evidence of this [9].

The sub-dominant term in the asymptotic expansion is expected to be proportional to $n \cdot 2^n$. Partly heuristic algebra of q -identities, supported by extensive numerical evidence, suggests that the coefficient of this term is identically zero. Details of this derivation are given in [9]. It is not subject to an additional oscillatory component. The next terms we expect are proportional to $n^{g-1} \log n$ and n^{g-1} . If we write

$$a_n^{(3)} \sim 2^n (\kappa \cdot n^g + \kappa_1 \cdot n + \kappa_2 \cdot n^{g-1} \log n + \kappa_3 \cdot n^{g-1})$$

and fix κ to the value given in equation (10), κ_1 to zero and $g = \log_2 3$, we can solve a pair of linear equations, corresponding to successive n values, and find estimators of κ_2 and κ_3 . The estimates are $\kappa_2 = -0.4 \pm 0.15$ and $\kappa_3 = 0.5 \pm 0.5$. As well as the leading term, already discussed, these last two terms should also possess the property of a small additive oscillatory component to the amplitude. These oscillations are entirely masked by the very large uncertainties we quote in our amplitude estimates, but the effect can be seen by a careful Maple analysis, which we have done [9].

3. The full problem or four-sided polygons

A prudent SAW leading to an unrestricted or four-sided prudent polygons is shown in figure 3. For unrestricted perimeter polygons enumerated by area, we can construct a functional equation. Polygons ending at $(1, 0)$ in a clockwise direction can be rotated and/or reflected to give all other four-sided polygons, so the generating function for these polygons is precisely $1/8$ of the overall generating function. We partition this sub-class of polygons into three classes \mathcal{X}, \mathcal{Y} and \mathcal{Z} , with respective generating functions $X^{(1,0)}(q, u, v), Y^{(1,0)}(q, u, v)$ and $Z^{(1,0)}(q, u, v)$. In all three cases q measures the area; for \mathcal{X} , u measures the width and v measures the height; for \mathcal{Y} , u measures the height and v measures the width; and for \mathcal{Z} , u measures the width -1 and v measures the height. We find that

$$\begin{aligned} X^{(1,0)}(q, u, v) &= \frac{qv}{1-q} [X^{(1,0)}(q, u, v) - X^{(1,0)}(q, qu, v)] \\ &+ \frac{qv}{1-q} [Y^{(1,0)}(q, v, u) - Y^{(1,0)}(q, v, qu)] \\ &+ \frac{quv}{1-q} [Z^{(1,0)}(q, u, v) - qZ^{(1,0)}(q, qu, v)] \end{aligned} \tag{12}$$

$$\begin{aligned}
 Y^{(1,0)}(q, u, v) &= quv + \frac{qv}{1-q} [Y^{(1,0)}(q, u, v) - Y^{(1,0)}(q, qu, v)] \\
 &+ \frac{qv^2}{1-q} [Z^{(1,0)}(q, v, u) - Z^{(1,0)}(q, v, qu)] \\
 &+ quv [X^{(1,0)}(q, qv, u) + Y^{(1,0)}(q, u, qv) + qvZ^{(1,0)}(q, qv, u)] \quad (13)
 \end{aligned}$$

$$\begin{aligned}
 Z^{(1,0)}(q, u, v) &= \frac{qv}{1-q} [Z^{(1,0)}(q, u, v) - Z^{(1,0)}(q, qu, v)] \\
 &+ qvY^{(1,0)}(q, qv, u) + quvZ^{(1,0)}(q, u, qv). \quad (14)
 \end{aligned}$$

An explanation of the sub-classes \mathcal{X} , \mathcal{Y} and \mathcal{Z} and the derivation of this equation is given in [9], and is based on a construction by Schwerdtfeger [7]. The generating function for four-sided polygons is

$$A^{(4)}(q) = 8(X^{(1,0)}(q, 1, 1) + Y^{(1,0)}(q, 1, 1) + Z^{(1,0)}(q, 1, 1)) = \sum a_n^{(4)} q^n. \quad (15)$$

We are unable to solve this functional equation, nor extract its asymptotics. Accordingly, we turn to series analysis. The functional equation can be iterated to generate long series in polynomial time. The first few terms $a_1^{(4)}, \dots, a_{15}^{(4)}$ are

8, 16, 40, 96, 232, 560, 1336, 3176, 7480, 17 528, 40 776, 94 336, 21 6976,
496 432, 1130 120.

The full series can be found at www.ms.unimelb.edu.au/~tonyg. We cannot prove that the dominant term in the asymptotics is the exponential growth term 2^n , but our numerical estimates, plus comparison with other solved models, suggest that this is likely to be true. We cannot say if the same phenomenon of a non-existent critical amplitude will occur in this case, but even if so, it will not affect our numerical study, which is too crude to detect possible effects of the magnitude observed for the three-sided case.

We have used a variety of techniques of series analysis [10], including the method of differential approximants, and standard sequence extrapolation algorithms to estimate the critical exponent. Assuming $a_n^{(4)} \sim \lambda \cdot 2^n \cdot n^{g_4}$, in order to estimate the exponent g_4 we extrapolated the sequence

$$n(a_n^{(4)} / (2 \cdot a_{n-1}^{(4)} - 1) \sim g_4.$$

This sequence is very slowly converging, despite the fact that we have some 800 terms in the sequence. The best we can do is estimate $2.58 < g_4 < 2.61$, where, as is usual in series analysis, the bounds are confidence limits and are not rigorous. It is tempting to conjecture that the exponent g_4 in this case is just 1 greater than that for the three-sided case, g_3 , so that $g_4 = 1 + \log_2(3) = 2.584 96 \dots$

We have investigated this conjecture with some success. First, we considered the Hadamard quotient of the series for four-sided polygons and that of the derivative of the series for three-sided polygons. Differentiation increases the exponent by 1. If the conjecture is true, the coefficients of the Hadamard quotient should tend to a constant. With 800 terms in the quotient series, the ratio does seem to be approaching a constant. If $a_n^{(3)}$ denotes the number of three-sided polygons of area n and $a_n^{(4)}$ denotes the number of four-sided polygons of area n , extrapolating the quotient $h_n = n \cdot a_n^{(3)} / a_n^{(4)}$, we find a limit of 3.25 ± 0.05 . Next, we tested the assumption that the asymptotics for the four-sided case is just given by the derivative of the three-sided case. We fitted successive quartets of coefficients $a_j, a_{j+1}, a_{j+2}, a_{j+3}$ to

$$2^n (\kappa \cdot n^{g_4} + \kappa_1 \cdot n^2 + \kappa_2 \cdot n^{g_4-1} \log n + \kappa_3 \cdot n^{g_4-1}).$$

Estimates of κ are well converged to $\kappa \approx 0.033\,41 \pm 0.000\,03$. This implies that the ‘amplitude’ of the three-sided polygons should be $0.033\,41 \pm 0.000\,03 \times 3.25 \pm 0.05 = 0.108 \pm 0.002$ which agrees well with the direct estimate, calculated above, of $0.108\,384\dots$. On balance, we believe the conjecture is more likely to be true than not.

4. Conclusion

We have studied the area-generating function of prudent polygons in two dimensions, and their restrictions to one-sided, two-sided and three-sided versions. The results are consistent with our expectations for the rather simple one- and two-sided cases.

For the three-sided case, a careful asymptotic analysis reveals surprising asymptotic behaviour. First, we find an irrational critical exponent, which is rare for two-dimensional solvable models. Second, we find that the leading ‘amplitude’ strictly speaking does not exist. Instead, we find that we have what could perhaps be described as a *pseudo amplitude* which is a numerical approximation accurate to some eight decimal digits. But in fact there is an additional, additive term, periodic with periodicity $\log_2 n$ and amplitude approximately 10^{-9} .

Given that such a small variation in amplitude is extraordinarily difficult to detect numerically, this result raises the question as to just how common this behaviour is? Are there other models for which the standard asymptotics as given by equation (1) does not prevail? If so, it raises an intriguing new chapter in the study of exactly solved models. A numerical analysis for the four-sided or ‘full’ prudent polygon case is given. The growth constant remains unchanged from that of the solvable two- and three-sided cases, and the exponent appears to be 1 greater than the corresponding exponent for the three-sided case.

Acknowledgments

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