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Scaling of the atmosphere of self-avoiding walks

A L Owczarek[1] **and T Prellberg**[2]

[1] Department of Mathematics and Statistics, The University of Melbourne, Victoria 3010, Australia
[2] School of Mathematical Sciences, Queen Mary, University of London, Mile End Road, London E1 4NS, UK

E-mail: a.owczarek@ms.unimelb.edu.au and t.prellberg@qmul.ac.uk

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Abstract
The number of free sites next to the end of a self-avoiding walk is known as the *atmosphere* of the walk. The average atmosphere can be related to the number of configurations. Here we study the distribution of atmospheres as a function of length and how the number of walks of fixed atmosphere scale. Certain bounds on these numbers can be proved. We use Monte Carlo estimates to verify our conjectures in two dimensions. Of particular interest are walks that have zero atmosphere, which are known as *trapped*. We demonstrate that these walks scale in the *same* way as the full set of self-avoiding walks, barring an overall constant factor.

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

Consider an n-step self-avoiding walk $\omega = (\omega_0, \omega_1, \ldots, \omega_n)$ with $n + 1$ sites $\omega_i \in \mathbb{Z}^d$ for $d \geqslant 2$, and steps having unit length, i.e. $|\omega_{i+1} - \omega_i| = 1$.

The number of edges that can be appended to the last visited vertex ω_n to create an $(n + 1)$-step is called the *atmosphere* of the walk ω (see figure 1). Clearly the smallest value of the atmosphere is zero, in which case the walk is called *trapped*. A zero-step self-avoiding walk has atmosphere $2d$, and for $n \geqslant 1$ any n-step self-avoiding walk has atmosphere of at most $2d - 1$.

We partition the set of n-step self-avoiding walks by the value of their atmospheres. Denote by c_n the number of n-step self-avoiding walks starting at $\omega_0 = 0$, and by $c_n^{(a)}$ the number of n-step self-avoiding walks starting at $\omega_0 = 0$ with atmosphere a.

The subject of this paper is the fraction of n-step self-avoiding walks with fixed atmosphere,

$$p_n^{(a)} = \frac{c_n^{(a)}}{c_n}, \qquad (1)$$

and its limiting behaviour as $n \to \infty$.

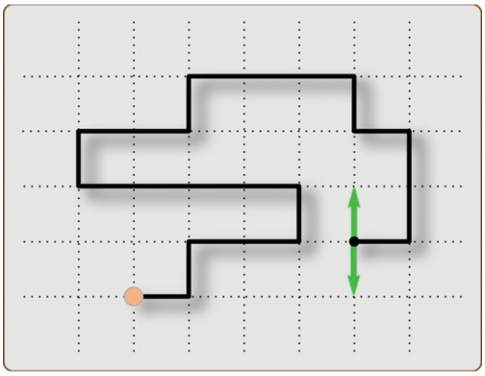

Figure 1. A self-avoiding walk on the square lattice $\mathbb{Z}^2$ with $n = 20$ steps and an atmosphere $a = 2$.

(This figure is in colour only in the electronic version)

The atmosphere was introduced by Rechnitzer and van Rensburg [1] for self-avoiding walks. Since it is well established theoretically, though not proven, that

$$c_n \sim A_1 \mu^n n^{\gamma-1} \tag{2}$$

they immediately pointed out that the *mean* atmosphere could be used to estimate the connective constant μ and exponent γ since

$$\langle a \rangle = \sum_a a p_n^{(a)} = \frac{\sum_a a c_n^{(a)}}{c_n} = \frac{c_{n+1}}{c_n}. \tag{3}$$

Subsequently they have generalized this elegant idea to self-avoiding walks near walls [2] and recently to self-avoiding polygons [3]. It is worth pointing out that the notion of atmosphere is also central to kinetic-growth algorithms such as the Rosenbluth algorithm [4] and PERM [5] (although it is not referred to by that name in the description of these algorithms).

Motivating this paper is recent interest in various subsets of walks that do not *trap* [6, 7] including prudent walks [8–10]. The question that naturally arises for each class of walks is *'Does the number of walks in the class scale in the same way as the full set of self-avoiding walks'*; that is, as in equation (2) with the same values of μ and γ.

It is then natural to consider the limits

$$p^{(a)} = \lim_{n\to\infty} \frac{c_n^{(a)}}{c_n}. \tag{4}$$

In this paper we demonstrate results in the literature [11, 12] can be used to prove

$$\liminf_{n\to\infty} \frac{c_n^{(a)}}{c_n} > 0, \tag{5}$$

and so that if one assumes the limit exists then one has immediately that

$$p^{(a)} > 0. \tag{6}$$

Going further and assuming the scaling in equation (2) we can therefore predict

$$c_n^{(a)} \sim A_1^{(a)} \mu^n n^{\gamma-1}, \tag{7}$$

where

$$A_1^{(a)} = p^{(a)} A_1. \tag{8}$$

Hence walks that trap, that is, those with atmosphere zero will have the same connective constant and same value of exponent γ as all self-avoiding walks. Conversely the same is true for walks that do not trap.

Furthermore we use the Monte Carlo Algorithm flatPERM [13] to provide estimates for $p_n^{(a)}$ up to length $n = 512$ on the square lattice $\mathbb{Z}^2$, and use the corrections-to-scaling to extrapolate high-precision estimates of $p^{(a)}$.

Theory. Intuitively one would expect that the probability that the end of a long self-avoiding walk ω ends at the corner of a cube Q of fixed size, but otherwise does not intersect with the cube, i.e. being confined to the exterior of the cube except for its endpoint, is non-zero. Therefore one can append to this walk, a short walk, contained within the cube with fixed atmosphere. Using a related argument, we shall prove below that the *limit inferior* of $p_n^{(a)}$ is bounded away from zero.

Our main result is the following theorem, which is a corollary of a theorem in [11].

Theorem 1. *Let* $0 \leqslant a < 2d$. *Then*

$$\liminf_{n\to\infty} p_n^{(a)} > 0,$$

and

$$\limsup_{n\to\infty} p_n^{(a)} < 1.$$

This theorem is very similar to a result concerning tail patterns of self-avoiding walks.

Definition 2. *A self-avoiding walk* $P = (p_0, p_1, \ldots, p_k)$ *is called a tail pattern if there is a self-avoiding walk* $\omega = (\omega_0, \omega_1, \ldots, \omega_n)$ *such that* $P = (\omega_{n-k}, \omega_{n-k+1}, \ldots, \omega_n)$. *P is called a proper tail pattern if for all sufficiently large n there is a self-avoiding walk having P as a tail pattern.*

Let $c_n[P]$ be the number of n-step self-avoiding walks with tail pattern P. We have the following result, which is taken from [11, 12].

Proposition 3. *If P is a proper tail pattern then*

$$\liminf_{n\to\infty} \frac{c_n[P]}{c_n} > 0.$$

When applying this proposition for the proof of theorem 1, we find that the main difficulty is that the atmosphere of a proper tail pattern P and the atmosphere of a self-avoiding walk having P as a tail pattern can be different.

Proof of theorem 1. It is sufficient to show that for any atmosphere a with $0 \leqslant a < 2d$ there exists a proper tail pattern P_a with atmosphere a and the additional property that any sufficiently long self-avoiding walk having P_a as a tail pattern also has atmosphere a. The first inequality then follows as an immediate consequence of proposition 3, as $c_n^{(a)} \geqslant c_n[P_a]$, and therefore

$$\liminf_{n\to\infty} p_n^{(a)} = \liminf_{n\to\infty} \frac{c_n^{(a)}}{c_n} \geqslant \liminf_{n\to\infty} \frac{c_n[P_a]}{c_n} > 0.$$

The upper bound follows now from the observation that $\sum_{a=0}^{2d-1} p_n^{(a)} = 1$, as

$$\begin{aligned}\limsup_{n\to\infty} p_n^{(a)} &= \limsup_{n\to\infty}\left(1 - \sum_{a'\neq a} p_n^{(a')}\right)\\ &\leqslant 1 + \sum_{a'\neq a} \limsup_{n\to\infty}\left(-p_n^{(a')}\right)\\ &= 1 - \sum_{a'\neq a} \liminf_{n\to\infty} p_n^{(a')} < 1.\end{aligned}$$

The pattern P_a is constructed as follows. Consider a self-avoiding walk ω which starts at the origin, visits precisely $2d - a$ neighbouring vertices and ends on the corner of a cube Q containing it. Continue ω by a self-avoiding walk ω' on the set of vertices ∂Q which have distance 1 from Q and which is Hamiltonian on ∂Q. The pattern P_a which is obtained by reversal of steps is a proper tail pattern. It has atmosphere a, and by construction the atmosphere of any sufficiently long self-avoiding walk having P as a tail pattern must also be a. □

Note that the idea of this proof generalizes easily to different notions of atmosphere, such as a k-step atmosphere given by the number of $(n+k)$-step self-avoiding walks which can be grown from an n-step self-avoiding walk.

Simulation results. Backed up by the rigorous results, we now consider results of simulations for self-avoiding walks on the square lattice $\mathbb{Z}^2$. Using flatPERM, a flat-histogram kinetic growth algorithm, we have grown 10^9 walks at length 512. The flatPERM algorithm is a stochastic growth algorithm [13], which performs an estimation of the whole density of states (here, atmospheres) and can be interpreted as an approximate counting algorithm. The algorithm combines the pruned-enriched Rosenbluth method (PERM) [5] with umbrella sampling techniques [15]. The configurations of interest are grown from scratch adding a step at each step. We parameterize the configuration space in such a manner that the algorithm explores it evenly; here, the algorithm aims to generate the same number of samples for each value of the atmosphere. As a consequence of using a flat-histogram method with respect to the atmosphere, we could boost the occurrence of zero-atmosphere walks roughly by a factor of 3, with minimal computational overhead.

From figure 2 it is clear that the quantities $p_n^{(a)}$ approach an asymptotic value quickly as $n \to \infty$ with only small corrections to scaling.

Figure 3 shows that these corrections are asymptotically linear in $1/n$. We therefore conjecture on the basis of our simulations that the limit

$$p^{(a)} = \lim_{n\to\infty} \frac{c_n^{(a)}}{c_n}$$

indeed exists. A linear fit can be used to obtain estimates for $p^{(a)}$, and we find that

$$p^{(0)} = 0.009\,096(4) \tag{9}$$

$$p^{(1)} = 0.054\,76(1) \tag{10}$$

$$p^{(2)} = 0.225\,00(2) \tag{11}$$

$$p^{(3)} = 0.711\,14(3) \tag{12}$$

for self-avoiding walks on the square lattice $\mathbb{Z}^2$. Using the relation $\mu = \sum_k k p^{(k)}$ for the connective constant μ, we obtain the estimate

$$\mu = 2.638\,18(3), \tag{13}$$

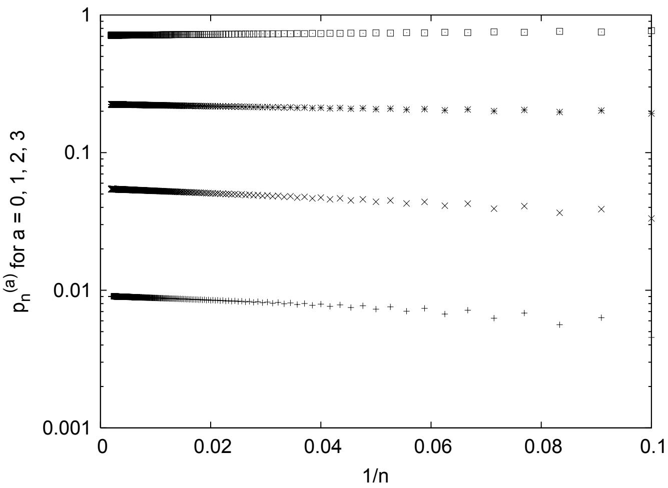

Figure 2. A plot of the probability $p_n^{(a)}$ of an n-step self-avoiding walk on the square lattice $\mathbb{Z}^2$ having atmosphere a. $p_n^{(a)}$ for $a = 0, 1, 2, 3$ (from bottom to top) on a logarithmic scale versus $1/n$ are shown. We note that there are only small corrections to scaling.

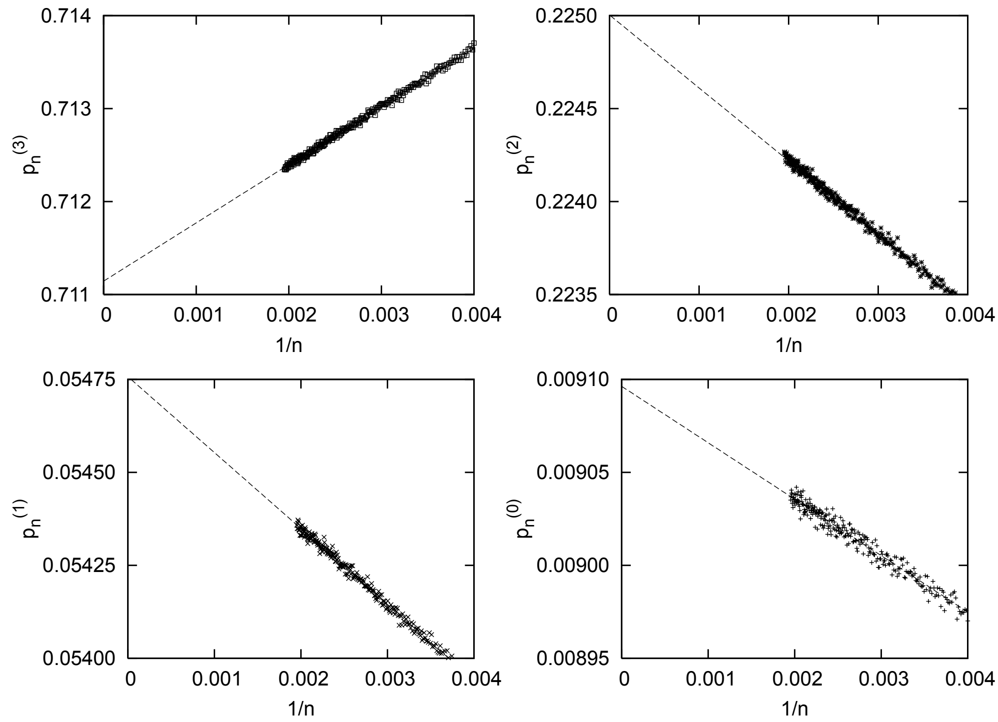

Figure 3. A plot of the probability $p_n^{(a)}$ of an n-step self-avoiding walk on the square lattice $\mathbb{Z}^2$ having atmosphere a. $p_n^{(a)}$ for $a = 0$ (bottom right), 1 (bottom left), 2 (top right), 3 (top left) on a linear scale versus $1/n$, together with linear fits of $p_n^{(a)}$ to $1/n$ computed from all walks with at least 100 steps are shown.

which is consistent with $\mu = 2.638\,158\,5303\ldots$ [14]. Just as is the case with connective constants, atmospheres are of course non-universal quantities, in contrast to, say, critical exponents, and should be accorded the appropriate importance.

Due to the close connection between atmospheres and the connective constant, we expect the value of the atmospheres to be unchanged when considering self-avoiding walks near a wall.

The notion of atmospheres for polygons as introduced in [3] is somewhat different from the notion of atmosphere for walks. For polygons, the atmosphere depends on the actual algorithm used for adding and deleting edges, and one needs to consider outer and inner atmospheres. Moreover, while the atmosphere for walks is bounded, the atmosphere for polygons is not. It would be desirable to derive similar results to those presented here for polygon atmospheres.

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