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End Patterns of Self-Avoiding Walks

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Consider a fixed "end pattern" (a short self-avoiding walk) that can occur as the first few steps of an arbitrarily long self-avoiding walk on $\mathbb{Z}^d$. It is a difficult open problem to show that as $N \to \infty$, the fraction of N-step self-avoiding walks beginning with this pattern converges. It is shown that as $N \to \infty$, this fraction is bounded away from zero, and that the ratio of the fractions for N and $N+2$ converges to one. Similar results are obtained when patterns are specified at both ends, and also when the endpoints are fixed.

KEY WORDS: Self-avoiding walk; self-avoiding polygon; pattern; reptation algorithm.

1. INTRODUCTION

An *N-step self-avoiding walk* (SAW) is an ordered sequence of *distinct* points $(\omega_0, ..., \omega_N)$ of the d-dimensional integer lattice $\mathbb{Z}^d$ $(d \geqslant 2)$ such that consecutive points are unit distance apart. Let S_N be the set of N-step SAWs having $\omega_0 = 0$, and let c_N denote $|S_N|$, the cardinality of S_N. For a fixed nonzero point $z \in \mathbb{Z}^d$, let $c_N(z)$ be the cardinality of

$$S_N(z) := \{\omega \in S_N : \omega_N = z\}$$

Hammersley[1,2] proved that there exists a constant $\mu > 1$ such that

$$\lim_{N \to \infty} (c_N)^{1/N} = \mu \tag{1.1}$$

and that for each fixed nonzero $z = (z^{(1)}, ..., z^{(d)}) \in \mathbb{Z}^d$,

$$\lim_{N \to \infty} [c_N(z)]^{1/N} = \mu \tag{1.2}$$

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[In (1.2), N is restricted to be of the same parity as $|z| := |z^{(1)}| + |z^{(2)}| + \cdots + |z^{(d)}|$. This will be implicitly adopted as a convention for the remainder of this paper.] It is also known[3] that $\mu^N \leqslant c_N \leqslant \mu^N e^{0(N^{1/2})}$, and that[2] for $|z| = 1$, $c_N(z) \leqslant N\mu^N$. It is believed, however, that asymptotically

$$c_N \approx \mu^N N^{\gamma - 1} \qquad \text{and} \qquad c_N(z) \approx \mu^N N^{\alpha_{\text{sing}} - 2}$$

(for z fixed and nonzero) as $N \to \infty$. Here γ and α_{sing} are critical exponents which (unlike μ) are believed to be universal among all lattices of a given dimension d. (Slade[8] has proven that $\gamma = 1$ in high dimensions.)

A *pattern* is a (short) SAW that can occur as part of a longer SAW. Formally, a pattern P can be any SAW $P = (p_0,..., p_n)$. A pattern P is said to occur at the jth step of the SAW $\omega = (\omega_0,..., \omega_N)$ if there exists a vector $v \in \mathbb{Z}^d$ such that $\omega_{j+k} = p_k + v$ for $k = 0,..., n$. Kesten[4] proved that if a pattern can occur several times on a long SAW, then it must occur quite often on most SAWs. More precisely, let $\chi_N(m, P)$ be the number of ω in S_N for which P occurs at most at m different steps. Then there exists an $\varepsilon > 0$ such that

$$\limsup_{N \to \infty} \left(\frac{\chi_N(\varepsilon N, P)}{c_N} \right)^{1/N} < 1 \tag{1.3}$$

A pattern $P = (p_0,..., p_n)$ is said to occur at the front (respectively, tail) of the SAW $\omega = (\omega_0,..., \omega_N)$ if P occurs at the 0th [respectively, $(N-n)$th] step of ω. For patterns P and R, and for $z \in \mathbb{Z}^d$, define

$$\begin{aligned} F_N(P) &= \{\omega \in S_N : P \text{ occurs at the front of } \omega\} \\ T_N(R) &= \{\omega \in S_N : R \text{ occurs at the tail of } \omega\} \\ S_N(P, R) &= F_N(P) \cap T_N(R) \\ c_N(P) &= |F_N(P)| \\ c_N(P, R) &= |S_N(P, R)| \\ c_N(z; P) &= |S_N(z) \cap F_N(P)| \\ c_N(z; P, R) &= |S_N(z) \cap S_N(P, R)| \end{aligned}$$

Thus, $c_N(P)/c_N$ is the probability that an N-step SAW (chosen uniformly at random) begins with the pattern P. It is conjectured that $\lim_{N \to \infty} c_N(P)/c_N$ exists for every pattern P; if true, this would define a probability distribution for the "SAW of infinite length." (Lawler[5] has proven this conjecture in high dimensions, using the methods of Slade.[8]) The present results are somewhat weaker. In Section 2, it is proven that if P is a pattern which can occur at the front of arbitrarily long SAWs [i.e., if $c_N(P)>0$ for all sufficiently large N], then

$$\liminf_{N\to\infty}\frac{c_N(P)}{c_N}>0 \tag{1.4}$$

Analogous results are proven for $c_N(P, R)$, $c_N(z; P)$, and $c_N(z; P, R)$ (the result is weaker for the latter two cases when $|z|>1$; see Theorems 2.2 and 2.3). Section 3 extends the following results of Kesten[4]:

$$\lim_{N\to\infty}\frac{c_{N+2}}{c_N}=\mu^2 \tag{1.5}$$

$$\lim_{N\to\infty}\frac{c_{N+2}(z)}{c_N(z)}=\mu^2 \tag{1.6}$$

Specifically, if $c_N(P)>0$ for all large N, then

$$\lim_{N\to\infty}\frac{c_{N+2}(P)}{c_N(P)}=\mu^2 \tag{1.7}$$

with analogous results for $c_N(P, R)$, $c_N(z; P)$, and $c_N(z; P, R)$. Section 4 gives a simple application of the results to the analysis of a particular Monte Carlo algorithm for SAWs.

These results are obviously weaker than one would like, yet proving the existence of the limit in (1.4) is a notoriously difficult problem, analogous to the existence of the thermodynamic limit for states in the absence of either monotonicity properties or convergent expansions (the latter is the key tool in refs. 5 and 8). This contrasts with the easier thermodynamic limit of the free energy [analogous to (1.1) for the SAW]. Despite their apparent simplicity, many basic questions about SAWs remain unanswered. For example, let $P=(p_0,..., p_n)$ be a pattern with $p_n^{(1)}\geqslant p_i^{(1)}$ for $0\leqslant i<n$. Is it true that at least half of the SAWs in $F_N(P)$ (for $N>n$) have $\omega_N^{(1)}\geqslant p_n^{(1)}$? Such a "reflection principle" would be a most useful result, but nobody can prove it. One also encounters problems of parity on the $\mathbb{Z}^d$ lattice; for example, it is an open question whether one can improve (1.5) to $\lim_{N\to\infty} c_{N+1}/c_N=\mu$. Similarly, although $c_{N+2}\geqslant c_N$ is elementary, it is not at all easy to prove $c_{N+1}\geqslant c_N$ for all N. This last result has been obtained only very recently.[7]

To close this section, I set some additional terminology and notation. Let u_N be the number of N step SAWs with $\omega_0=0$ and $|\omega_N|=1$, and let η_{N+1} be the number of such SAWs such that ω_0 is lexicographically smaller than every other point of the SAW. Alternatively,[2] η_N is the number of *oriented N-step self-avoiding polygons* (oriented simple closed curves of length N passing through N points of $\mathbb{Z}^d$, without specified starting point), modulo translation. Thus, one has[2,4] $\eta_{N+1} = u_N/(N+1)$, and $\mathbb{Z}^d$, without specified starting point), modulo translation. Thus, one has[2,4] $u_N = 2dc_N(z)$ if $|z| = 1$. A *cube* is any set of the form

$$\{x \in \mathbb{Z}^d: a^{(i)} \leqslant x^{(i)} \leqslant a^{(i)} + b \qquad \text{for all} \quad i = 1,..., d\}$$

where $a^{(1)},..., a^{(d)}$, and b are integers, with $b > 0$. A front (respectively, tail) pattern P is called *proper* if there exist arbitrarily long SAWs with P occurring at the front (respectively, tail).

2. OCCURRENCE OF END PATTERNS

In this section I prove (1.4) and its extensions, which say in effect that if certain end patterns can occur on long walks, then the probability that they occur is bounded away from zero as $N \to \infty$. [Here I refer to the uniform probability measures on S_N or on $S_N(z)$.]

Theorem 2.1. Let $P = (p_0,..., p_n)$ be a proper front pattern, and let $R = (r_0,..., r_{n'})$ be a proper tail pattern. Then

$$\liminf_{N \to \infty} \frac{c_N(P)}{c_N} > 0 \tag{2.1}$$

and

$$\liminf_{N \to \infty} \frac{c_N(P, R)}{c_N} > 0 \tag{2.2}$$

Proof. Since $c_N(P) \geqslant c_N(P, R)$, it would suffice to prove the latter assertion. However, for expository purposes, I will prove both, since they require the same basic ideas, and the former has fewer complications.

Since P is a proper front pattern, there exist $m > m_0 > n$ and a SAW $\omega^P = (\omega_0^P,..., \omega_m^P)$ such that P occurs at the front of ω^P,

$$\omega_j^P \in \{x \in \mathbb{Z}^d: 1 \leqslant x^{(i)}, i = 1,..., d\} \qquad \text{for} \quad j = 0,..., m_0$$
$$\omega_j^P \in \{x \in \mathbb{Z}^d: x^{(1)} = 0\} \qquad \text{for} \quad j = m_0 + 1,..., m$$

and $\omega_m^P = 0$. Let D be the cube $\{x \in \mathbb{Z}^d: 0 \leqslant x^{(i)} \leqslant m, i = 1,..., d\}$. Observe that $\omega_i^P \in D$ for each $i = 0,..., m$. Let $q = (m+1)^d - 1$. Let $\omega^D = (\omega_0^D,..., \omega_q^D)$ be a SAW such that $\omega_q^D = 0$, ω_0^D is another extreme point of D, and the remaining $q-1$ points of ω^D are precisely the remaining $q-1$ points of D. Such a walk "exactly fills D" and its existence is proven in ref. 4, Lemma 3.

Observe that for each $\omega \in F_N(\omega^D)$, if we define

$$\omega_i^* = \begin{cases} \omega_i^P & \text{for} \quad i = 0,..., m \\ \omega_{i-q+m} & \text{for} \quad i = m+1,..., N-m+q \end{cases}$$

then $\omega^* = (\omega_0^*,..., \omega_{N-m+q}^*)$ is a SAW, and it has ω^P as a front pattern. This transformation induces a map from $F_N(\omega^D)$ to $F_{N-m+q}(\omega^P)$ which is clearly one-to-one. Also, $F_N(\omega^P) \subset F_N(P)$, so it follows that

$$c_N(P) \geqslant c_N(\omega^P) \geqslant c_{N+q-m}(\omega^D)$$

Thus, (2.1) will be proven once we prove

$$\liminf_{N \to \infty} \frac{c_{N+q-m}(\omega^D)}{c_N} > 0 \tag{2.3}$$

By (1.3) and (1.1),

$$\limsup_{i \to \infty} [\chi_i(0, \omega^D)]^{1/i} < \mu$$

so there exist I and $\varepsilon > 0$ such that

$$\chi_i(0, \omega^D) \leqslant [(1-\varepsilon)\,\mu]^i \qquad \text{for all} \quad i \geqslant I \tag{2.4}$$

Fix an even integer $k \geqslant I$.

Let σ_{mj} be the set of SAWs $\omega \in S_m$ such that ω^D occurs at the jth step of ω, and let $U_{m,k} = \bigcup_{j=0}^k \sigma_{mj}$. Then

$$|S_{N-m+q+k} \backslash U_{N-m+q+k,k}| \leqslant \chi_k(0, \omega^D)\, c_{N-m+q} \leqslant \mu^k (1-\varepsilon)^k\, c_{N-m+q}$$

Therefore

$$\begin{aligned} c_{N-m+q+k} - c_{N-m+q}\mu^k(1-\varepsilon)^k &\leqslant |U_{N-m+q+k,k}| \\ &\leqslant \sum_{j=0}^{k} |\sigma_{N-m+q+k,j}| \\ &\leqslant \sum_{j=0}^{k} c_j\, |F_{N-m+q}(\omega^D)|\, c_{k-j} \end{aligned}$$

Division by $c_N \mu^k$ gives

$$\frac{c_{N-m+q+k}}{\mu^k c_N} - (1-\varepsilon)^k \frac{c_{N-m+q}}{c_N} \leqslant \left(\sum_{j=0}^{k} \frac{c_j c_{k-j}}{\mu^k} \right) \frac{c_{N-m+q}(\omega^D)}{c_N} \tag{2.5}$$

Since k and $q-m$ are both even (and fixed), we have, from (1.5),

$$\lim_{N\to\infty}\frac{c_{N-m+q+k}}{\mu^k c_N}=\mu^{q-m}=\lim_{N\to\infty}\frac{c_{N-m+q}}{c_N}$$

So, as $N\to\infty$, the left side of (2.5) converges to a strictly positive number. Thus, (2.3) follows, and (2.1) is proven.

The proof of (2.2) requires some extra details, but the ideas are similar. In addition to the above definitions, there exist $m'>m_0'$, with $m_0'+n'<m'$, and a SAW ω^R in $S_{m'}$ such that R occurs at the tail of ω^R,

$$\omega_j^R\in\{x\in\mathbb{Z}^d\colon 1\leqslant x^{(i)},\ i=1,\dots,d\}\qquad\text{for}\quad j=m_0',\dots,m'$$
$$\omega_j^R\in\{x\in\mathbb{Z}^d\colon x^{(1)}=0\}\qquad\text{for}\quad j=0,\dots,m_0'-1$$

and $\omega_0^R=0$. Let D' be the cube $\{x\in\mathbb{Z}^d\colon 0\leqslant x^{(i)}\leqslant m',\ i=1,\dots,d\}$, and let $\omega^{D'}=(\omega_0^{D'},\dots,\omega_{q'}^{D'})$ be a SAW that exactly fills D' with $\omega_0^{D'}=0$, $\omega_{q'}^{D'}$ another extreme point of D' and $\omega^{D'}$ exactly fills D' [and so $q'=(m'+1)^d-1$]. The roles of ω^R, D', and $\omega^{D'}$ will be exactly analogous to the roles of ω^P, D, and ω^D.

We also need the SAW $\hat{\omega}^R=(\hat{\omega}_0^R,\dots,\hat{\omega}_{m'+1}^R)$ obtained by "adding" a single edge to ω^R, as follows. Let

$$\hat{\omega}_i^R=\begin{cases}\omega_i^R & \text{for}\quad i=0,\dots,m_0'-1\\ \omega_{i-1}^R+(1,0,0,\dots,0) & \text{for}\quad i=m_0',\dots,m'+1\end{cases}$$

It is not hard to see that $\hat{\omega}^R$ is a SAW, and that it is contained in D', begins at 0, and has R as a tail pattern.

As in (2.4), there exist I' and $\varepsilon'>0$ such that

$$\chi_i(0,\omega^{D'})\leqslant[(1-\varepsilon')\,\mu]^i\qquad\text{for all}\quad i\geqslant I'\tag{2.6}$$

Fix $k\geqslant\max\{I,I'\}$ such that k is even and

$$(1-\varepsilon)^k<1/4\qquad\text{and}\qquad(1-\varepsilon')^k<1/4\tag{2.7}$$

Let $v_{N,k}$ be the number of SAWs in S_N in which ω^D occurs at none of the first k steps and $\omega^{D'}$ occurs at none of the last k steps. Then

$$\begin{aligned}\sum_{j=0}^{k}\sum_{j'=0}^{k}c_j c_{N-j-j'}(\omega^D,\omega^{D'})\,c_{j'}&\geqslant c_N-v_{N,k}\\ &\geqslant c_N-\chi_k(0,\omega^D)\,c_{N-k}-c_{N-k}\chi_k(0,\omega^{D'})\\ &\geqslant c_N-2c_{N-k}\mu^k/4\end{aligned}$$

[using (2.4), (2.6), and (2.7)], and therefore

$$\max_{0 \leqslant t \leqslant 2k} c_{N-t}(\omega^D, \omega^{D'}) \geqslant c_N \left(1 - \frac{\mu^k c_{N-k}}{2c_N}\right)\left(\sum_{j=0}^{k} c_j\right)^{-2}$$

Thus, (2.2) will be proven if it can be shown that, for all $t \geqslant 0$,

$$c_{N-t}(\omega^D, \omega^{D'}) \leqslant c_{N-q-q'+m+m'}(P, R) \tag{2.8}$$

To prove (2.8), I will construct a one-to-one mapping from $S_{N-t}(\omega^D, \omega^{D'})$ to $S_{N-q-q'+m+m'}(P, R)$. For $t=0$ or 1, this is easy: given a SAW in $S_{N-t}(\omega^D, \omega^{D'})$, replace the front pattern ω^D by ω^P and replace the tail pattern $\omega^{D'}$ by ω^R or $\hat{\omega}^R$, according to whether t is 0 or 1. For $t \geqslant 2$, let l be the integer satisfying $t=2l$ if t is even and $t=2l+1$ if t is odd. For a SAW ω in $S_{N-t}(\omega^D, \omega^{D'})$, let $u = \min\{i: \omega_i^{(1)} \geqslant \omega_j^{(1)}$ for all $j=0,..., N-t\}$. To define the mapping, consider three cases:

Case I: $q \leqslant u < N-t-q'$: Replace the edge from ω_u to ω_{u+1} by the $(2l+1)$-step SAW from ω_u to $\omega_u + (l, 0, 0,..., 0)$ to $\omega_{u+1} + (l, 0, 0,..., 0)$ to ω_{u+1}. Then replace the front pattern ω^D by ω^P and replace the tail pattern $\omega^{D'}$ by ω^R or $\hat{\omega}^R$, according to whether t is even or odd.

Case II: $u \geqslant N-t-q$: Replace ω^D by ω^P and replace $\omega^{D'}$ by the pattern consisting of the t-step SAW from $(0, 0,..., 0)$ to $(t, 0,..., 0)$ followed by ω^R.

Case III: $u < q$: Similar to case II, but with the t-step segment immediately following ω^P.

The above three cases define the desired one-to-one mapping, so (2.8) is proven and (2.2) follows.

Theorem 2.2. Fix a point $z \in \mathbb{Z}^d$ with $|z| = 1$. Let $P = (p_0,..., p_n)$ be a front pattern and let $R = (r_0,..., r_{n'})$ be a tail pattern such that $c_N(z; P, R) > 0$ for all sufficiently large (odd) N. Then

$$\liminf_{\substack{N \to \infty \\ N \text{ odd}}} \frac{c_N(z; P, R)}{c_N(z)} > 0 \tag{2.9}$$

Proof. Without loss of generality, $p_0 = 0$ and $r_{n'} = z$. Let P' be the pattern $(r_0,..., r_{n'}, p_0,..., p_n)$. Then P' can occur many times on long SAWs, so, for some $\varepsilon > 0$,

$$\limsup_{N \to \infty} [\chi_N(\varepsilon N, P')]^{1/N} < \mu \tag{2.10}$$

by (1.3) and (1.1). Let Π_N be the set of $\omega \in S_N(z)$ such that P' occurs at least εN times on ω; then (2.10), (1.1), and (1.2) imply $|\Pi_N| \geqslant |c_N(z)|/2$ for sufficiently large N.

If $\omega \in \Pi_N$ and P' occurs at the jth step of ω, then $(\omega_{j+n'+1}, \omega_{j+n'+2},..., \omega_N, \omega_0,..., \omega_{j+n'})$ is a SAW; if we translate this so that its initial point is the origin, we obtain a SAW ω^* in $S_N(z) \cap S_N(P, R)$. In words, ω^* is obtained by adding the bond (ω_N, ω_0) to ω, forming an oriented self-avoiding polygon, and then removing the $(r_{n'}, p_0)$ edge from an occurrence of P' (followed by a translation). Given ω^*, there are at most N possible ω that it could have come from (the polygon is uniquely determined, but each such oriented polygon could come from $N+1$ different SAWs with $|\omega_N - \omega_0| = 1$). Thus, each obtained $\omega^* \in S_N(z) \cap S_N(P, R)$ comes from at most N different ω's in Π_N. Conversely, each $\omega \in \Pi_N$ gives rise to at least εN different ω^*'s in $S_N(z) \cap S_N(P, R)$. Therefore, $Nc_N(z; P, R) \geqslant \varepsilon N\, |\Pi_N|$. Combining this with $|\Pi_N| \geqslant |c_N(z)|/2$ (for large N) proves (2.9).

Theorem 2.3. Fix a nonzero point $z \in \mathbb{Z}^d$. Let $P = (p_0,..., p_n)$ be a proper front pattern and let $R = (r_0,..., r_{n'})$ be a proper tail pattern such that $c_N(z; P, R) > 0$ for all sufficiently large N (of the same parity as $|z|$). Then, if $|z|$ is odd,

$$\liminf_{\substack{N \to \infty \\ N \text{ odd}}} \frac{c_N(z; P, R)}{u_N} > 0 \tag{2.11}$$

and if $|z|$ is even, (2.11) holds when N is replaced by $N+1$ in the numerator.

Proof. To get a handle on the geometry, consider an arbitrary SAW $\tilde{\omega}$ in $S_k(z) \cap S_k(P, R)$ for some k. Let b be large enough so that $|\tilde{\omega}_i| < b$ for all $0 \leqslant i \leqslant n$ and $N - n' \leqslant i \leqslant N$. Let D be the cube $\{x: |x^{(i)}| \leqslant b$ for all $i = 1,..., d\}$. Then there exist two SAWs $\omega^P = (\omega_0^P,..., \omega_m^P)$ and $\omega^R = (\omega_0^R,..., \omega_{m'}^R)$ having no vertices in common, contained entirely in D, having ω_m^P and ω_0^R as extreme points of D, and satisfying $\omega_i^P = \tilde{\omega}_i$ for $0 \leqslant i \leqslant m$ and $\omega_i^R = \tilde{\omega}_{N+i-m'}$ for $m' - n' \leqslant i \leqslant m'$. We can also require that $\omega^D = (\omega_0^D,..., \omega_q^D)$ is a SAW with $\omega_0^D = \omega_0^R$, $\omega_q^D = \omega_m^P$, and such that ω^D exactly fills D (ref. 4, Lemma 3).

Put $y = (1, 0,..., 0)$; let $\omega \in S_N(y) \cap T_N(\omega^D)$. [If $S_N(y) \cap T_N(\omega^D)$ is empty, put $y = (-1, 0,..., 0)$ instead.] Define a SAW ω^* obtained from ω by removing the tail pattern ω^D and replacing it with ω^R at the tail and ω^P and $(y, 0)$ at the front; explicitly, $\omega^* = (\omega_0^P,..., \omega_m^P, \ \omega_0 + (\omega_m^P - y),..., \omega_{N-q} + (\omega_M^P - y), \omega_1^R,..., \omega_{m'}^R)$. Then it is easy to see that ω^* is an M step SAW, where $M \equiv M(N) = N - q + m + m' + 1$, and that $\omega^* \in S_M(z) \cap S_M(P, R)$. (Therefore, M has the same parity as $|z|$.) Since the transformation from ω to ω^* is one-to-one, it follows that $|S_N(y) \cap T_N(\omega^D)| \leqslant$

$c_M(z; P, R)$. So, when $|z|$ is odd, this inequality combines with Theorem 2.2 and (1.6) to give

$$\liminf_{m \to \infty} \frac{c_M(z; P, R)}{u_M} \geqslant \liminf_{N \to \infty} \left(\frac{|S_N(y) \cap T_N(\omega^D)|}{2dc_N(y)} \frac{u_N}{u_M} \right) > 0$$

The case where $|z|$ is even is exactly analogous.

Corollary 2.4. Fix y, $z \in \mathbb{Z}^d$ with $|y| = 1$. Then there exists a constant $A = A(z)$ such that for all sufficiently large odd N,

$$c_N(y) \leqslant A c_N(z) \qquad \text{if } |z| \text{ is odd}$$

$$c_N(y) \leqslant A c_{N+1}(z) \qquad \text{if } |z| \text{ is even}$$

We remark that if the reverse inequalities also hold (for different A), then Theorem 2.2 holds for every fixed z.

3. RATIO LIMIT THEOREMS

In this section I prove a theorem which extends the known results[4] (1.5) and (1.6). (The rates in the theorem are exactly the same as those in ref. 4.)

Theorem 3.1. (i) Let $P = (p_0,..., p_n)$ be a proper front pattern, and let $R = (r_0,.., r_{n'})$ be a proper tail pattern. Then there exist constants A_1 and A_2 (depending on P and R) such that

$$\left| \frac{c_{N+2}(P)}{c_N(P)} - \mu^2 \right| \leqslant A_1 N^{-1/3} \tag{3.1}$$

and

$$\left| \frac{c_{N+2}(P, R)}{c_N(P, R)} - \mu^2 \right| \leqslant A_2 N^{-1/3} \tag{3.2}$$

for all sufficiently large N.

(ii) In addition to the above hypotheses, fix a nonzero $z \in \mathbb{Z}^d$. If $c_N(z; P, R) > 0$ for all sufficiently large N (of the same parity as $|z|$), then there exist constants A_3, A_4, A_5, and A_6 (depending on z, P, and R) such that

$$-A_3 N^{-1/3} \leqslant \frac{c_{N+2}(z; P)}{c_N(z; P)} - \mu^2 \leqslant A_4 N^{-1/4} \tag{3.3}$$

$$-A_5 N^{-1/3} \leqslant \frac{c_{N+2}(z; P, R)}{c_N(z; P, R)} - \mu^2 \leqslant A_6 N^{-1/4} \tag{3.4}$$

for all sufficiently large N (of the same parity as $|z|$).

Remark. (3.1) is a consequence of (3.2), since

$$\left|\frac{c_{N+2}(P)}{c_N(P)} - \mu^2\right| = \left|\sum_R \left(\frac{c_{N+2}(P, R)}{c_N(P, R)} - \mu^2\right) \frac{c_N(P, R)}{c_N(P)}\right|$$
$$\leqslant \max_R \left|\frac{c_{N+2}(P, R)}{c_N(P, R)} - \mu^2\right|$$

where R ranges over all n'-step proper tail patterns and N is large. Similarly, (3.3) follows from (3.4).

Before I prove (3.2) and (3.4), I prove two lemmas which generalize the inequality

$$c_{M+N} \geqslant (1/2d)\, c_N \eta_M \tag{3.5}$$

which is Lemma 1 of ref. 4.

Lemma 3.2. For P and R as in Theorem 3.1(i), there exists a constant $\delta \equiv \delta(P, R) > 0$ such that

$$c_{N+M}(P, R) \geqslant \delta c_N \eta_M \geqslant \delta c_N(P, R)\, \eta_M \tag{3.6}$$

$$c_{N+M}(P, R) \leqslant \delta^{-1} c_N(P, R)\, c_M \tag{3.7}$$

for sufficiently large N and all M.

Proof. (3.6) follows from (3.5) and Theorem 2.1 if we put $\delta = 1/2 \liminf_{N \to \infty} c_N(P, R)/c_N$. (3.7) follows from the inequalities

$$c_{N+M}(P, R) \leqslant c_{N+M} \leqslant c_N c_M \leqslant \delta^{-1} c_N(P, R)\, c_M$$

Lemma 3.3. For P, R, and z as in Theorem 3.1(ii),

$$c_{N+M}(z; P, R) \geqslant (1/2d)\, c_N(z; P, R)\, \eta_M \tag{3.8}$$

for all M and sufficiently large N (of correct parity).

Proof. Choose A large enough so that for any $\omega \in S_N(z) \cap S_N(P, R)$, one has

$$\omega_j \in \{x \in \mathbb{Z}^d \colon |x^{(i)}| < A,\ i = 1,\dots, d\}$$

for all $0 \leqslant j \leqslant n$ and $N - n' \leqslant j \leqslant N$ (that is, the end patterns must be contained in the above cube). Now, given $\omega \in S_N(z) \cap S_N(P, R)$ for some $N > (2A+1)^d$, choose the integer ξ so that $\omega_j^{(i)} = \xi$ for some $i \in \{1,\dots, d\}$ and some $j \in \{0,\dots, N\}$, and so that $|\xi|$ is as large as possible. (Observe that since $N > (2A+1)^d$, we must have $|\xi| > A$ and $n < j < N - n'$.) Let k_0 be the subscript of the lexicographically largest point of ω in the hyperplane $x^{(i)} = \xi$. Now proceed as in the proof of Lemma 1 of ref. 4, attaching an M-step self-avoiding polygon to ω at ω_{k_0} (the points of the polygon are all on the side of the hyperplane $x^{(i)} = \xi$ that contains no points of ω). The resulting SAW, ω^*, is in $S_{N+M}(z) \cap S_{N+M}(P, R)$. Every $(N+M)$-step ω^* obtained in this way is different, because there can be only one cube centered at the origin which contains exactly $N+1$ points of ω^* (those $N+1$ points give $\omega \in S_N$, and the remaining M points give the polygon). Since the polygon can be chosen in at least $\eta_M/2d$ ways, and ω in $c_N(z; P, R)$ ways, (3.8) is proven.

I now return to the proof of (3.2) and (3.4). Much of the proof is the same as the proofs of (1.5) and (1.1) in ref. 4. Instead of reproducing the details, I refer the reader to ref. 4 and restrict myself here to describing the changes that must be made.

Proof of Theorem 3.1. Define $\phi_N^1 \equiv \phi_N^1(P, R) = c_{N+2}(P, R)/c_N(P, R)$ and $\phi_N^2 \equiv \phi_N^2(z; P, R) = c_{N+2}(z; P, R)/c_N(z; P, R)$. First we require the following result: There exist constants B_1 and B_2 such that

$$\phi_{N+2}^j \geqslant \phi_N^j - B_j/N \tag{3.9}$$

This is the exact analog of Theorem 2 of ref. 4. The proof is essentially identical; we must, however, prohibit any changes affecting the end patterns P and R (see Kesten's remark at the end of ref. 4, Section 3). Everything else in the proof is the same, until the final line, where we require $\liminf_{N \to \infty} \phi_N^j > 0$. For $j = 1$, $\phi_N^1 \geqslant [c_{N+2}(P, R)/c_{N+2}]\, c_{N+2}/c_N$, so the result follows from Theorem 2.1 and (1.5); for $j = 2$, the result follows from (3.8) because $\eta_2 = d$.

Now I proceed to Theorem 4 of ref. 4. Define ρ_N^j by $\phi_N^j = \mu^2 + \rho_N^j N^{-1/3}$. The upper bound on ρ_N^1 uses (3.7) (for large N) instead of Eq. (3.10) of ref. 4: the δ^{-1} constant is unimportant (it can be absorbed, for example, by increasing α_1).

For the upper bound on ρ_N^2, I use $c_N(z) \geqslant K u_N$ for some constant K (from Corollary 2.4), as well as (3.5) and (1.1) of ref. 4:

$$\begin{aligned}\frac{c_{N+2M}(z; P, R)}{c_N(z; P, R)} &\leqslant \frac{c_{N+2M}}{K u_N} \\ &\leqslant \frac{1}{K} \mu^{2M} \exp[\alpha_1 (N+2M)^{1/2}] \exp[\alpha_4 (N+1)^{1/2}] \\ &\leqslant \mu^{2M} \exp[\alpha (N+2M)^{1/2}]\end{aligned}$$

for an appropriate $\alpha > 0$. Then Kesten's argument, with $m = [(\rho_N^2/2B_2)\,N^{2/3}]$, gives

$$N^{-1/3}\rho_N^2 \log[1 + (\rho_N^2/2\mu^2)\,N^{-1/3}] \leq 2B_2\alpha N^{-1/2}[1 + (\rho_N^2/2B_2)\,N^{-1/3}]^{1/2}$$

from which we deduce $\rho_N^2 N^{-1/3} = O(N^{-1/4})$.

The proof of the lower bound for ρ_N^j is the same as Kesten's, except that $c_N/c_{N-2m'} \geq \eta_{2m'}/2d$ is replaced by $c_N(P, R)/c_{N-2m'}(P, R) \geq \delta\eta_{m'}$ [from (3.6)] for $j = 1$, and the analogous result from (3.8) for $j = 2$.

4. AN EXAMPLE

As an application, I discuss the nonergodicity of the "reptation" Monte Carlo algorithm for SAWs (see references in ref. 6, Section 3). Also known as the "slithering snake," this algorithm starts with a (given) SAW $\omega^{[0]}$ in S_N and generates a random sequence of SAWs $\omega^{[1]}$, $\omega^{[2]}$,... in S_N (here, each element of S_N should be viewed as an equivalence class of SAWs modulo translation). Given $\omega^{[i]}$, the algorithm randomly adds one step to one end of the SAW and simultaneously deletes a step from the other end; if the result is a SAW, then it is $\omega^{[i+1]}$ (if it is not a SAW, we

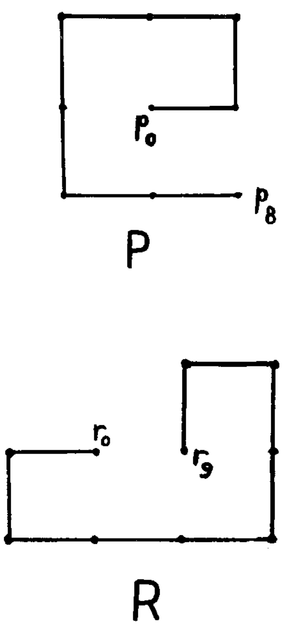

Fig. 1. An example of a proper front pattern P and a proper tail pattern R.

put $\omega^{[i+1]} = \omega^{[i]}$). Two SAWs ω^A and ω^B are said to be in the same ergodic class if the algorithm can transform ω^A into ω^B: i.e., if there exists a finite sequence $\omega^A \equiv \omega^{[0]}, \omega^{[1]}, \ldots, \omega^{[k]} \equiv \omega^B$ of SAWs which is a possible realization of the algorithm. The SAW ω^A is said to be *frozen* if it is the only SAW in its ergodic class.

The purpose of such a Monte Carlo algorithm is to generate a representative sample of all SAWs of fixed length, so the degree to which this can be done can be partly measured by d_N, the size of the largest ergodic class, relative to c_N. In $\mathbb{Z}^2$, consider the patterns P and R shown in Fig. 1. These are proper end patterns, but each is a "cul de sac": no step can be added to either end of a SAW in $S_N(P, R)$, so every SAW in $S_N(P, R)$ is frozen. Therefore, Theorem 2.1 implies that for some $\varepsilon > 0$ and for sufficiently large N, one has $d_N \leqslant (1-\varepsilon)\, c_N$. It is known[6] that a lower bound on d_N is $c_{2N}^{1/2}$, so if one assumes the scaling relation $c_N \approx \mu^N N^{\gamma - 1}$, then

$$O(N^{-(\gamma-1)/2}) \leqslant d_N/c_N \leqslant 1-\varepsilon \tag{4.1}$$

for large N. This would hold for all dimensions $d \geqslant 2$, since a cul de sac can be constructed in any dimension. It would be most interesting to know which inequality in (4.1) is sharp (if either).

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REFERENCES

1. J. M. Hammersley, *Proc. Camb. Phil. Soc.* **53**:642–645 (1957).
2. J. M. Hammersley, *Proc. Camb. Phil. Soc.* **57**:516–523 (1961).
3. J. M. Hammersley and D. J. A. Welsh, *J. Math. Oxford Ser. 2* **13**:108–110 (1962).
4. H. Kesten, *J. Math. Phys.* **4**:960–969 (1963).
5. G. Lawler, The infinite self-avoiding walk in high dimensions, Preprint.
6. N. Madras and A. D. Sokal, *J. Stat. Phys.* **47**:573–595 (1987).
7. G. L. O'Brien, private communication.
8. G. Slade, *Commun. Math. Phys.* **110**:661–683 (1987).