

Loop-Erased Self-Avoiding Random Walk in Two and Three Dimensions

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Received June 9, 1987; revision received September 25, 1987

If $\hat{S}(n)$ is the position of the self-avoiding random walk in \mathbb{Z}^d obtained by erasing loops from simple random walk, then it is proved that the mean square displacement $E(|\hat{S}(n)|^2)$ grows at least as fast as the Flory predictions for the usual SAW, i.e., at least as fast as $n^{3/2}$ for $d=2$ and $n^{6/5}$ for $d=3$. In particular, if the mean square displacement of the usual SAW grows like $n^{1.18\dots}$ in $d=3$, as expected, then the loop-erased process is in a different universality class.

KEY WORDS: Self-avoiding random walk; loop-erased walk; Laplacian random walk; polymer models; Flory exponents.

1. INTRODUCTION

A self-avoiding walk (SAW) of length n on the integer lattice \mathbb{Z}^d is an ordered sequence of points $[x_0=0, \dots, x_n]$ with $|x_i - x_{i-1}| = 1$ and $x_i \neq x_j$ for $i \neq j$. The study of SAWs arose in the study of polymer chains, and since has been of interest in mathematical physics. The first theoretical study of such walks dates back to Flory (see Ref. 3 and references therein for early heuristic and numerical work), who produced a nonrigorous argument to suggest

$$\langle |x_n|^2 \rangle \approx \begin{cases} n^{6/(d+2)}, & d = 1, 2, 3 \\ n, & d \geq 4 \end{cases} \quad (1.1)$$

Here $\langle \cdot \rangle$ denotes expectation with respect to the uniform or counting measure on SAWs. In $d=4$, a logarithmic correction was predicted.

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After considerable heuristic and numerical work, the expected behavior of $\langle |x_n|^2 \rangle$ is: $n^{3/2}$ for $d=2$ (as Flory predicted); $n^{1.18\dots}$ for $d=3$ (a little lower than Flory's prediction); for $d=4$, $n(\log n)^\alpha$, where $\alpha=1/4$ according to a renormalization group calculation; and for $d>4$, n . For $d>4$, much progress has been made toward a rigorous proof.^(2,13)

In Ref. 5, I introduced a new measure on self-avoiding walks for $d \geq 3$ by erasing the loops from the paths of simple (unrestricted) random walks. The same process has recently appeared independently under the name of Laplacian random walk.^(10,11) For this process it was shown that for $d>4$, $\langle |x_n|^2 \rangle \sim cn$,⁽⁵⁾ and for $d=4$, $\langle |x_n|^2 \rangle \sim b_n n$, where b_n grows at least as fast as $(\log n)^{1/3}$ but no faster than $(\log n)^{1/2}$, with $(\log n)^{1/3}$ being the conjectured growth rate.⁽⁶⁾ Comparing the $d=4$ result to the renormalization group calculation shows that the loop-erased process grows faster than the conjectured rate for the usual SAW. Here we discuss the loop-erased process for $d=2, 3$ (the definition will have to be modified for $d=2$) and prove that the exponents for the loop-erased process must be at least as large as the Flory exponents. More precisely, if $\hat{S}(n)$ denotes the position of the loop-erased SAW at time n , then for every $\varepsilon > 0$,

$$\lim_{n \rightarrow \infty} n^{(-3/2) + \varepsilon} E(|\hat{S}(n)|^2) = \infty, \quad d=2$$

$$\lim_{n \rightarrow \infty} n^{(-6/5) + \varepsilon} E(|\hat{S}(n)|^2) = \infty, \quad d=3$$

In particular, for $d=3$ the mean square displacement of the process grows faster than $n^{1.18\dots}$, the current predicted value for the usual SAW. It is quite possible that the exponents for \hat{S} will be larger than the Flory exponents. In fact, numerical work on walks of a small number of steps by Lyklema and Evertsz⁽¹¹⁾ suggest a preliminary guess of about 1.6 for $d=2$. For $d=3$, we expect that 1.2 will not be very far from the true exponent.

We now give a quick definition of the loop-erased process for $d \geq 3$ and show how to modify it for $d=2$. See Ref. 5 for details. Let $S(n)$ be a simple random walk in \mathbb{Z}^d ($d \geq 3$) and let

$$\tau = \min\{j: \exists i < j \text{ with } S(i) = S(j)\}$$

$$\sigma = \text{the } i \text{ for which } S(i) = S(\tau)$$

Then we send $S(n)$ to the path

$$\tilde{S}_1(n) = \begin{cases} S(n), & 0 \leq n \leq \sigma \\ S(n + (\tau - \sigma)), & \sigma \leq n < \infty \end{cases}$$

$\tilde{S}_1(n)$ is a walk with one loop erased. We now perform the same process on $\tilde{S}_1(n)$, producing a new walk $\tilde{S}_2(n)$ and keep going, letting

$$\hat{S}(n) = \lim_{j \rightarrow \infty} \tilde{S}_j(n)$$

The transience of the simple random walk in $d \geq 3$ allows us to make this definition. It can be shown that this definition is equivalent to the walk generated by assigning transition probabilities

$$\begin{aligned} P\{\hat{S}(n+1) = x_{n+1} \mid [\hat{S}(0), \dots, \hat{S}(n)] = [x_0, \dots, x_n]\} \\ = \Phi(x_{n+1}) \Big/ \sum_{|y-x_n|=1} \Phi(y) \end{aligned} \tag{1.2}$$

where

$$\Phi(y) = P_y\{S(j) \notin \{x_0, \dots, x_n\}, j = 0, 1, 2, \dots\}$$

For $d = 2$, we define the loop-erased process by using a variant of (1.2). Let

$$\Phi_m(y) = P_y\{S(j) \notin \{x_0, \dots, x_n\}, j = 0, 1, 2, \dots, m\}$$

It can be shown⁽⁴⁾ that for any finite set $A \subset \mathbb{Z}^2$, $x, y \notin A$,

$$\lim_{m \rightarrow \infty} \frac{P_x\{S(j) \notin A, j = 0, \dots, m\}}{P_y\{S(j) \notin A, j = 0, \dots, m\}} \tag{1.3}$$

exists (assuming x and y are connected to ∞). Hence we define the loop-erased process for $d = 2$ by the transition probability

$$\begin{aligned} P\{\hat{S}(n+1) = x_{n+1} \mid [\hat{S}(0), \dots, \hat{S}(n)] = [x_0, \dots, x_n]\} \\ = \lim_{m \rightarrow \infty} \left[\Phi_m(x_{n+1}) \Big/ \sum_{|y-x_n|=1} \Phi_m(y) \right] \end{aligned} \tag{1.4}$$

The above definition for $d = 2$ is not very practical. We will use a slightly different measure, suggested by an idea of Lyklema and Evertsz.⁽¹¹⁾ Let M be a (large) number and let

$$\begin{aligned} R_M &= \{z = (z_1, z_2) \in \mathbb{Z}^2: |z_i| \leq M\} \\ \partial R_M &= \{z \in R_M: y \notin R_M \text{ for some } y, |y - z| = 1\} \end{aligned}$$

We can take simple random walks starting at the origin that end when they reach ∂R_M . On this finite path, we do loop-erasing, and produce a finite self-avoiding walk of at least M steps. If $n \leq M$, we get a measure $\hat{P}_{n,M}$ on

n -step SAWs. In Section 5 we show that if \hat{P}_n is the measure produced by (1.4), then

$$\hat{P}_{n,n^3}(\omega) = \hat{P}_n(\omega)[1 + O(1/\sqrt{n})] \quad (1.5)$$

where the $O(\cdot)$ term is uniform over all n -step SAWs ω . Hence, in order to estimate $E(|\hat{S}(n)|^2)$ we can use \hat{P}_{n,n^3} rather than \hat{P}_n (or in other words, n^3 looks like ∞ for an n -step walk).

In this paper, we will assume that the reader is familiar with basic results about $\hat{S}(n)$, as developed in Refs. 5 and 6. If we define $\hat{S}(n)$ with a finite cutoff, we get the same type of results with the natural modification (see Ref. 10); for example, if n is fixed and we let

$$\xi = \xi_n = \inf\{j \geq 1: S(j) \in \partial R_{n^3}\}$$

and consider the loop-erased process using finite walks stopped at time ξ , we get the transition probability

$$\begin{aligned} P\{\hat{S}(m+1) = x_{m+1} \mid [\hat{S}(0), \dots, \hat{S}(m)] = [x_0, \dots, x_m]\} \\ = \tilde{\Phi}_n(x_{m+1}) \Big/ \sum_{|y-x_m|=1} \tilde{\Phi}_n(y) \end{aligned} \quad (1.6)$$

where

$$\tilde{\Phi}_n(y) = P_y\{S(j) \notin \{x_0, \dots, x_m\}, j = 0, 1, \dots, \xi\}$$

The remainder of this paper contains two independent parts. Section 2 gives a nonrigorous description of the problem, motivating the way in which the Flory exponents arise. Readers not interested in mathematical details may want to read this section only. The last three sections prove the main result, Theorem 3.1. It is assumed that the reader has read the previous work on the loop-erased process, in particular Sections 3 and 6 of Ref. 5 and Section 2 of Ref. 6. The basic outline of the proof is given in Section 3, reducing the problem to an estimate (3.1), which is proved in Section 4. Some technical questions about the simple random walk in \mathbb{Z}^2 are discussed in Section 5: the justification that “ $n^3 = \infty$ ” for the self-avoiding walk, i.e., (1.5), is proven, as well as an estimate needed in Section 3.

2. NONRIGOROUS DERIVATION OF THE EXPONENT

Here we give an idea of how the Flory exponents appear for $\hat{S}(n)$. We will leave out details and make no attempt to be mathematically rigorous. We write $f(n) \approx g(n)$ if $\log f(n)$ and $\log g(n)$ are asymptotic. The key

question to ask is how many of the first n points of a simple random walk remain after loops have been erased. If we let $\tau(n)$ denote the number of points remaining, our goal is to find the α such that

$$E(\tau(n)) \approx n^\alpha \tag{2.1}$$

If (2.1) holds, then n points of a self-avoiding walk should correspond to $n^{1/\alpha}$ points of a simple random walk, i.e.,

$$E(|\hat{S}(n)|^2) \approx E(|S(n^{1/\alpha})|^2) \approx n^{1/\alpha} \tag{2.2}$$

If we let I_n denote the indicator function of the event “the n th point is not erased,” then (2.1) gives

$$E(I_n) \approx n^{\alpha-1} \tag{2.3}$$

One can show that for $d = 2$,

$$P\{S(j) \neq S(k), 0 \leq j \leq n, 2n \leq k \leq n^3\} \approx (\log n)^{-1}$$

and for $d \geq 3$,

$$P\{S(j) \neq S(k), 0 \leq j \leq n, 2n \leq k < \infty\} \geq c > 0$$

Hence we expect $E(I_{n,2n}) \approx E(I_n)$, where $I_{n,2n}$ denotes the indicator function of the event “the n th point is not erased by time $2n$.”

We consider a simple random walk of length $2n$ and define

$$L_0 = \sup\{j \leq 2n: S(0) = S(j)\}$$

and if $L_k < 2n$, we define L_{k+1} by

$$L_{k+1} = \sup\{j \leq 2n: S(L_k + 1) = S(j)\}$$

Let \bar{k} be such that $L_{\bar{k}} = 2n$. Then

$$2n = L_0 + \sum_{j=1}^{\bar{k}} (L_j - L_{j-1})$$

and the k th point of the corresponding SAW is $S(L_k)$. What we have done is to split the walk into a sequence of loops with the property that the k th loop does not intersect the set $\{S(L_0), \dots, S(L_{k-1})\}$:

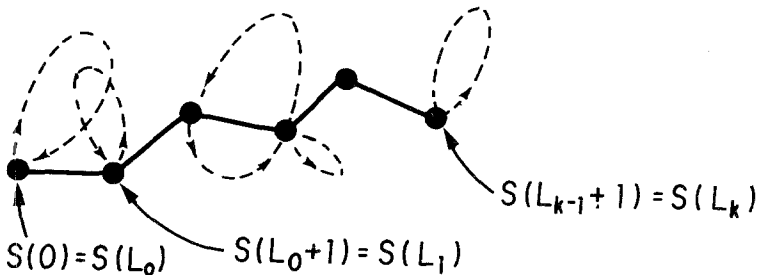


Fig. 1. The dotted lines represent erased loops. The solid line is the remaining SAW.

We define ρ_j by

$$\rho_0 = L_0$$

and for $j > 0$,

$$\rho_j = \begin{cases} L_k - L_{k-1} & \text{if } j = L_{k-1} + 1 \text{ for some } k \\ 0 & \text{otherwise} \end{cases}$$

Clearly, $E(\sum_{j=0}^{2n} \rho_j) \approx 2n \approx n$ or

$$E(\rho_n) \approx 1 \tag{2.4}$$

We now try to estimate $E(\rho_n)$. If we erase loops from the path only through time n , we get a self-avoiding path starting at 0 and ending at $S(n)$. Let A_n denote the (random) set of points in this path and $\bar{A}_n = A_n \setminus \{S(n)\}$. Then $\rho_n \neq 0$ if and only if $S(k) \notin \bar{A}_n, n + 1 \leq k \leq 2n$, and $\{\rho_n = m + 1\}$ is the set

$$\{S(k) \notin \bar{A}_n, n + 1 \leq k \leq 2n; S(n + m) = S(n); S(k) \neq S(n), m + 1 \leq k \leq 2n\}$$

What is the probability of this set? It is standard that $P\{S(n + m) = S(n)\} \approx m^{-d/2}$. The remaining conditions essentially require the path to avoid \bar{A}_n three times

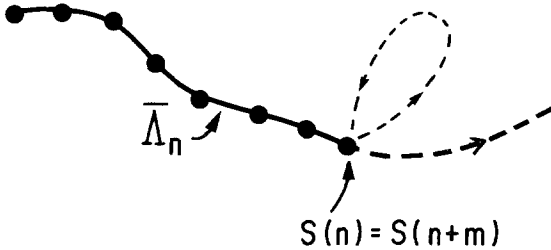


Fig. 2. The dotted lines represent the paths of $S(k)$ for $k > n$. If $\rho_n \neq 0$, then this does not intersect \bar{A}_n , the SAW up to $S(n)$.

[that is for small i , we need $S(n + i) \notin \bar{A}_n, S((n + m) - i) \notin \bar{A}_n$, and $S((n + m) + i) \notin \bar{A}_n$]. This suggests that given \bar{A}_n , a good estimate for the probability would be (for m not too small)

$$m^{-d/2} [F_n(S(n), A_n)]^3 \tag{2.5}$$

Here $F_n(x, A) = P_x\{S(j) \notin A, j = 1, \dots, n\}$. We have clearly made only an approximation to the probability, and making some of these ideas rigorous

is the role of Lemma 4.1 of this paper. However, if we accept (2.5), we get by summing that

$$E(\rho_n | A_n) \approx n^{2-d/2} [F_n(S(n), A_n)^3]$$

or

$$E(\rho_n) = n^{2-d/2} E[F_n(S(n), A_n)^3]$$

By (2.3), this is of order 1, so we get

$$E[F_n(S(n), A_n)^3] \approx n^{d/2-2} \tag{2.6}$$

In this paper we prove one direction of (2.6),

$$E[F_n(S(n), A_n)^3] \lesssim n^{d/2-2} \tag{2.7}$$

but we conjecture, in fact, that (2.6) holds.

The quantity we are interested in is $E(I_{n,2n})$, which is $E(F_n(S(n), A_n))$. It is not clear how to take the power outside of the expectation in (2.6); in fact, we do not know (even from a nonrigorous point of view) whether

$$E[F_n(S(n), A_n)^3] \approx \{E[F_n(S(n), A_n)]\}^3 \tag{2.8}$$

If (2.6) and (2.8) were true, then we would have

$$E(F_n(S(n), A_n)) \approx n^{d/6-2/3}$$

which gives, by (2.3), $\alpha = d/6 + 1/3$, or by (2.2),

$$E(|\hat{S}(n)|^2) \approx n^{d/(d+2)}$$

which is the Flory prediction. For positive random variables X , $E(X^3) \geq [E(X)]^3$, so (2.7) allows us to prove rigorously

$$\alpha \leq d/6 + 1/3$$

But determining the exact exponent is still an open question.

There is an open problem about simple random walks that is similar to this. Let Π_n be all the points of a random walk path of length n (i.e., do not erase loops) and let

$$H_n = F_n(0, \Pi_n)$$

$E(H_n)$ is the probability that the paths of two independent random walks

starting at 0 do not intersect. The asymptotic behavior of $E(H_n)$ for $d = 2, 3$ is unknown, although it can be shown that

$$E(H_n^2) \approx \begin{cases} n^{-1}, & d = 2 \\ n^{-1/2}, & d = 3 \\ (\log n)^{-1}, & d = 4 \end{cases}$$

(see Ref. 7 and references therein for a discussion of this problem). For $d = 4$ it can be shown that $E(H_n^2) \approx [E(H_n)]^2$ and hence that $E(H_n) \approx (\log n)^{-1/2}$. For $\hat{S}(n)$ in $d = 4$, it was shown that $E(I_n^3) \approx (\log n)^{-1}$ and it was from analogy with this problem that the conjecture $E(I_n) \approx (\log n)^{-1/3}$ was made, i.e., that $E(|\hat{S}(n)|^2)$ grows like $n(\log n)^{1/3}$. For $d = 2, 3$, it is not clear whether one should expect $E(H_n)^2 \approx E(H_n^2)$; in fact, for $d = 1$, $E(H_n)^2 \not\approx E(H_n^2)$. Determining the exponent for $E(I_n)$ seems at least as hard as finding the exponent for $E(H_n)$; however, if $E(H_n)^2 \approx E(H_n^2)$, we would expect that $E(I_n)^3 \approx E(I_n^3)$.

3. THE MAIN THEOREM

If $A \subset \mathbb{Z}^d$, $x \in \mathbb{Z}^d$, and $S(n)$ is simple random walk in \mathbb{Z}^d , we define $F_n(x, A) = P_x\{S(j) \notin A, j = 1, \dots, n\}$. Now, let S be simple random walk starting at 0, and for fixed j , consider $S(i)$, $0 \leq i \leq j$. On this finite walk we can erase loops, and get a self-avoiding walk of length no more than j , starting at 0 and ending at $S(j)$. We call the (random) set of points in this walk A_j . If $n \geq j$, we let $I_{j,n}$ be the indicator function of the event “the j th point is not erased by time n ,” or, more precisely, the event

$$\{S(k) \notin A_j, k = j + 1, \dots, n\}$$

Clearly, for fixed j , the sets decrease with n . Also,

$$E(I_{j,n}) = E(F_{n-j}(S(j), A_j))$$

In Section 4 we will prove our main estimate that for $d = 2, 3$, any $\varepsilon > 0$,

$$\sum_{j=0}^n E(I_{j,2n}) \leq o(n^{(d+2)/6+\varepsilon}) \tag{3.1}$$

Here we show how (3.1) gives our main result:

Theorem 3.1. If $\hat{S}(n)$ is loop-erased, self-avoiding random walk and $\varepsilon > 0$, then

$$\lim_{n \rightarrow \infty} n^{-3/2+\varepsilon} E(|\hat{S}(n)|^2) = \infty, \quad d = 2 \tag{3.2}$$

$$\lim_{n \rightarrow \infty} n^{-6/5+\varepsilon} E(|\hat{S}(n)|^2) = \infty, \quad d = 3 \tag{3.3}$$

Proof. For $d=3$ we assume that $\hat{S}(n)$ has no cutoff; for $d=2$, let

$$\xi_n = \inf\{j \geq 1: S(j) \in \partial R_{n^3}\}$$

and we will assume that \hat{S} is cut off at ξ_n , as described in Section 1 (and hence is a slightly different process for each n). By (1.5), it is sufficient to prove (3.2) for this cutoff walk. Fix n , \hat{S} , and let

$$\sigma_n(m) = \sup\{j: \hat{S}(m) = S(j)\}$$

and let τ_n be the inverse of σ_n in the sense

$$\tau_n(j) = m \quad \text{if} \quad \sigma_n(m) \leq j < \sigma_n(m+1)$$

Then

$$\hat{S}(n) = S(\sigma_n(n)) \tag{3.4}$$

$$\tau_n(\sigma_n(m)) = m, \quad \text{all } m \tag{3.5}$$

$$\tau_n(j) - \tau_n(j-1) \in \{0, 1\}$$

The indicator function of the event $\{\tau_n(j) - \tau_n(j-1) = 1\}$ is exactly I_{j, ξ_n} if $d=2$ or $I_{j, \infty}$ if $d=3$. Hence, for any $k \leq n^2$, by (3.1), for every $\varepsilon > 0$,

$$\begin{aligned} E(\tau_n(k)) &\leq \sum_{j=0}^k E(I_{j, \xi_n}) + 1 \\ &\leq \sum_{j=0}^k E(I_{j, 2k}) + 1 \\ &= O(k^{(d+2)/6 + \varepsilon}) \end{aligned}$$

If we apply this to $k = \frac{1}{2}n^{6/(d+2) - \varepsilon}$, we see that for every $\varepsilon > 0$

$$P\{\tau_n(\frac{1}{2}n^{6/(d+2) - \varepsilon}) \geq n\} = o(1), \quad n \rightarrow \infty$$

From this and (3.5) we see for $\varepsilon > 0$,

$$\lim_{n \rightarrow \infty} P\{\sigma_n(n) \leq n^{6/(d+2) - \varepsilon}\} = 0 \tag{3.6}$$

We now use an estimate for simple random walk: for every $\varepsilon > 0$, there exists a $c_\varepsilon > 0$ such that

$$\begin{aligned} P\{|S(j)|^2 \leq n^{6/(d+2) - 2\varepsilon} \text{ for some } n^{6/(d+2) - \varepsilon} \leq j \leq \xi_n\} \\ \leq 1 - c_\varepsilon, \quad d=2 \end{aligned}$$

$$\begin{aligned} P\{|S(j)|^2 \leq n^{6/(d+2) - 2\varepsilon} \text{ for some } n^{6/(d+2) - \varepsilon} \leq j < \infty\} \\ \leq 1 - c_\varepsilon, \quad d=3 \end{aligned}$$

The result for $d=3$ is easy, using transience of the simple random walk [one can estimate the probability by the expected number of j with $|S(j)|^2 \leq n^{6/(d+2)-2\epsilon}$] and in fact the probability goes to 0 as $n \rightarrow \infty$. For $d=2$, it is a little more delicate; we prove it in Lemma 5.4(b). These estimates combined with (3.4) and (3.6) give the theorem.

4. THE ESTIMATE ON AMOUNT ERASED

Here we prove (3.1) using the ideas in Refs. 5 and 6. Our goal is to estimate

$$\sum_{j=0}^n E(I_{j,2n})$$

For any j , let

$$\rho_{j,2n} = [\inf\{k > j: I_{k,2n} = 1\}] - j$$

Then it is easy to see by telescoping that

$$\sum_{j=0}^n I_{j-1,2n} \rho_{j,2n} \leq 2n + 1 \tag{4.1}$$

where $I_{-1,2n} = 1$. The term $\rho_{j,2n}$ can be thought of as the size of the loop at time j . The results of Section 6 of Ref. 5 state that the conditional distribution of $\rho_{j,2n}$ given $\{I_{j-1,2n} = 1\}$ and A_j is the size of a loop at $S(j)$ conditioned not to enter the set $A_j \setminus \{S(j)\}$.

Let us make a more precise statement of this. Let $A \subset \mathbb{Z}^d$, $0 \notin A$, and let $S(n)$ be simple random walk starting at 0. Let

$$\Delta_m^A = \sup\{j \leq m: S(j) = 0, S(k) \notin A, k = 1, 2, \dots, j\}$$

Then, conditioned on A_j and $\{I_{j-1,2n} = 1\}$, $\rho_{j,2n}$ has the same distribution as $\Delta_{2n-j}^{A_j} + 1$, where

$$\Gamma_j = \{y - S(j): y \in A_j, y \neq S(j)\}$$

We state a lemma for general A .

Lemma 4.1. For every $\epsilon > 0$, there exists a $c_\epsilon > 0$ such that for $A \subset \mathbb{Z}^d$ ($d = 2, 3$) with $F_n(0, A) \geq n^{-3}$, $0 \notin A$,

$$E(\Delta_n^A) \geq c_\epsilon n^{2-d/2-\epsilon} [F_n(0, A)]^2 \tag{4.2}$$

Before proving the lemma, let us show how this gives (3.1). If we let $J_{j,n}$ be the indicator function of $\{F_n(S(j), A_j) \geq n^{-3}\}$, Lemma 4.1 gives

$$E(\rho_{j,2n} | I_{j-1,2n} = 1, J_{j,n} = 1, A_j) \geq c_\varepsilon n^{2-d/2-\varepsilon} F_n(S(j), A_j)^2$$

and hence

$$E(I_{j-1,2n} J_{j,n} \rho_{j,2n} | A_j) \geq c_\varepsilon n^{2-d/2-\varepsilon} F_n(S(j), A_j)^3 J_{j,n}$$

and

$$E(I_{j-1,2n} J_{j,n} \rho_{j,2n}) \geq c_\varepsilon n^{2-d/2-\varepsilon} E(F_n(S(j), A_j)^3 J_{j,n})$$

We write $F_{j,n} = F_n(S(j), A_j)$. Then

$$\begin{aligned} \sum_{j=0}^n E(I_{j,2n}) &\leq \sum_{j=0}^n E(F_{j,n}) \\ &\leq \sum_{j=0}^n E(J_{j,n} F_{j,n}) + O\left(\frac{1}{n^2}\right) \\ &\leq \left[(n+1)^2 \sum_{j=0}^n [E(J_{j,n} F_{j,n})]^3 \right]^{1/3} + O\left(\frac{1}{n^2}\right) \\ &\leq \left[(n+1)^2 \sum_{j=0}^n E(J_{j,n} F_{j,n}^3) \right]^{1/3} + O\left(\frac{1}{n^2}\right) \\ &\leq (n+1)^{2/3} \left[\sum_{j=0}^n n^{(d/2)-2+\varepsilon} \frac{1}{c_\varepsilon} E(I_{j-1,2n} \rho_{j,2n}) \right]^{1/3} + O\left(\frac{1}{n^2}\right) \end{aligned}$$

But by (4.1)

$$\sum_{j=0}^n E(I_{j-1,2n} \rho_{j,2n}) \leq 2n + 1$$

Hence

$$\sum_{j=0}^n E(I_{j,2n}) \leq O(n^{(d+2)/6+\varepsilon/3})$$

which gives (3.1).

To prove Lemma 4.1, let $\varepsilon > 0$ be given. It suffices to show the result for n sufficiently large. By standard exponential estimates for the simple random walk (see, e.g., VII, §4 of Ref. 12) there exists a $\delta = \delta(\varepsilon) > 0$ such that

$$\begin{aligned} P\{|S(j)| > n^{1/2+\varepsilon/d} \text{ for some } 1 \leq j \leq n\} \\ \leq O(e^{-n^\delta}) = o(1/n^3) \end{aligned}$$

Choose n sufficiently large so that the above probability is less than $1/(2n^3)$. Let

$$p^A(j, x) = P_0\{S(j) = x, S(i) \notin A, i = 1, 2, \dots, j\}$$

Then, if $F_n(0, A) \geq n^{-3}$, we have

$$\sum_{|x| \leq n^{1/2 + \varepsilon/d}} p^A(j, x) \geq \frac{1}{2} F_n(0, A)$$

But

$$\begin{aligned} p^A(2j, 0) &= \sum_{x \in \mathbb{Z}^d} p^A(j, x)^2 \\ &\geq \sum_{|x| \leq n^{1/2 + \varepsilon/d}} [p^A(j, x)]^2 \\ &\geq K_d n^{-d/2 - \varepsilon} [F_n(0, A)]^2 \end{aligned}$$

Also

$$\begin{aligned} P\{\Delta_n^A = 2j\} &\geq p^A(2j, 0) P_0\{S(j) \neq 0, j = 0, 1, \dots, n\} \\ &\geq \begin{cases} K_3 p^A(2j, 0), & d = 3 \\ K_2 (\log n)^{-1} p^A(2j, 0), & d = 2 \end{cases} \end{aligned}$$

Therefore,

$$\begin{aligned} E(\Delta_n^A) &\geq \sum_{j=0}^{n/2} P\{\Delta_n^A = 2j\} (2j) \\ &\geq \begin{cases} O(n^{2-d/2-\varepsilon}), & d = 3 \\ O(n^{2-d/2-\varepsilon} (\log n)^{-1}), & d = 2 \end{cases} \end{aligned}$$

Since $\varepsilon > 0$ was arbitrary, we get (4.2).

5. RANDOM WALK IN TWO DIMENSIONS

Throughout this section $S(n)$ denotes a simple random walk in \mathbb{Z}^2 . Let $x = (x_1, x_2) \in \mathbb{Z}^2$ and

$$p(n, x) = \begin{cases} P_0\{S(2n) = x\}, & x_1 + x_2 \text{ even} \\ P_0\{S(2n+1) = x\}, & x_1 + x_2 \text{ odd} \end{cases}$$

The asymptotic behavior of $p(n, x)$ is well understood. We summarize in Lemma 5.1 the facts we will need; all of these facts can be derived from the

local central limit theorem (see Chapter 7 of Ref. 14) and hence we omit the proof. Throughout this section we will use $O(\cdot)$ and $o(\cdot)$ notation. We set the following conventions: the error terms describe behavior as $n \rightarrow \infty$; they are uniform over all $w, x, y, z \in \mathbb{Z}^2$ and $A \subset \mathbb{Z}^2$; they may depend on exponents (denoted by $\alpha, \beta, \gamma, \delta, \varepsilon$) and the constant K .

Lemma 5.1. For every $\alpha, \beta, \varepsilon > 0, K > 0$:

- (a) $p(n, 0) = (1/\pi n)[1 + O(1/n)]$.
- (b) For all n and $x, p(n, x) \leq p(n, 0)$.
- (c) For $|x| \leq Kn^2$ and $m \geq n^{2\alpha + \varepsilon}$,

$$p(m, x) = p(m, 0)[1 + o(1)]$$

- (d) There exists $\delta = \delta(\beta, \varepsilon) > 0$ such that if $|x| \geq n^{(\beta + \varepsilon)/2}$, $p(n, x) = O(e^{-n^\delta})$.

For any $\alpha > 0$, let

$$R_\alpha = R_{\alpha, n} = \{(z_1, z_2) \in \mathbb{Z}^2: |z_i| \leq n^\alpha\}$$

and

$$\partial R_\alpha = \{z \in R_\alpha: y \notin R_\alpha \text{ for some } |y - z| = 1\}$$

For $x, y \in \mathbb{Z}^2, m_1 \leq m_2$, let

$$V_y(m_1, m_2) = \sum_{j=m_1}^{m_2} I\{S(j) = y\}$$

(here I denotes indicator function) and

$$g(x, y, m_1, m_2) = E_x(V_y(m_1, m_2)) = \sum_{j=m_1}^{m_2} P_x\{S(j) = y\}$$

Lemma 5.2. For any $\alpha < \beta < \gamma, K > 0$:

- (a) If $|x| \geq n^\beta$ and $y \in R_\alpha$,

$$g(x, y, 0, Kn^{2\gamma}) \leq \frac{1}{\pi} (\gamma - \beta)(\log n)[1 + o(1)]$$

- (b) If $x, y \in R_\alpha$, then

$$g(x, y, 0, Kn^{2\gamma}) \geq \frac{1}{\pi} (\gamma - \alpha)(\log n)[1 + o(1)]$$

Proof. Let $\varepsilon > 0$. Then, using Lemma 5.1,

$$\begin{aligned} \text{(a)} \quad 2g(x, y, 0, n^{2\gamma}) &\leq \sum_{0 \leq j \leq Kn^{2\gamma}} p(j, x - y) \\ &\leq n^{2\beta - 2\varepsilon} o(e^{-n^\delta}) + \sum_{(1/2)n^{2\beta - 2\varepsilon} \leq j \leq Kn^{2\gamma}} p(j, 0) \\ &= o(1) + \frac{2}{\pi} (\log n)(\gamma - \beta + \varepsilon)[1 + o(1)] \end{aligned}$$

$$\begin{aligned} \text{(b)} \quad 2g(x, y, 0, Kn^{2\gamma}) &\geq \sum_{n^{2(\alpha + \varepsilon)} \leq j \leq (1/2)n^{2\gamma}} p(j, 0)[1 + o(1)] \\ &= \frac{2}{\pi} (\log n)(\gamma - \alpha - \varepsilon)[1 + o(1)] \end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, we get the result.

Lemma 5.3. For any $0 < \alpha < \beta < \gamma$, $K > 0$, if $x \notin R_\beta$,

$$P_x\{S(j) \notin R_\alpha, j = 1, \dots, Kn^{2\gamma}\} \geq \frac{\beta - \alpha}{\gamma - \alpha} [1 + o(1)]$$

Proof. Consider

$$W = \sum_{y \in R_\alpha} V_y(0, 2Kn^{2\gamma})$$

By Lemma 5.2(a)

$$E(W) \leq |R_\alpha| \frac{1}{\pi} (\gamma - \beta)(\log n)[1 + o(1)]$$

where $|\cdot|$ denotes cardinality. Let $\eta = \inf\{j \geq 1: S(j) \in R_\alpha\}$. Then Lemma 5.2(b) combined with a standard Markov argument gives

$$E(W | \eta \leq Kn^{2\gamma}) \geq |R_\alpha| \frac{1}{\pi} (\gamma - \alpha)(\log n)[1 + o(1)]$$

Since

$$E(W) \geq E(W | \eta \leq Kn^{2\gamma}) P\{\eta \leq Kn^{2\gamma}\}$$

we get

$$P\{\eta \leq Kn^{2\gamma}\} \leq \frac{\gamma - \beta}{\gamma - \alpha} [1 + o(1)]$$

Lemma 5.4. Let $0 < \alpha < \beta < \gamma < \infty$ and $\xi = \inf\{j \geq 1: S(j) \in \partial R_\gamma\}$.

(a) If $x \notin R_\beta$,

$$P_x\{|S(j)| \notin R_\alpha, j = 1, \dots, \xi\} \geq \frac{\beta - \alpha}{\gamma - \alpha} [1 + o(1)]$$

(b)

$$P_0\{|S(j)| \notin R_\alpha, j = n^{2\beta}, \dots, \xi\} \geq \frac{\beta - \alpha}{\gamma - \alpha} [1 + o(1)]$$

Proof. (a) Let $\varepsilon > 0$. By the central limit theorem we can find K_ε such that

$$P_x\{|S(K_\varepsilon n^{2\gamma})| \notin R_\gamma\} \geq (1 - \varepsilon)[1 + o(1)]$$

But

$$\begin{aligned} &P_x\{S(j) \notin R_\alpha, j = 1, \dots, \xi\} \\ &\geq P_x\{S(j) \notin R_\alpha, j = 1, \dots, K_\varepsilon n^{2\gamma}, S(K_\varepsilon n^{2\gamma}) \notin R_\gamma\} \\ &\geq \left(\frac{\beta - \alpha}{\gamma - \alpha} - \varepsilon\right) [1 + o(1)] \end{aligned}$$

(b) Let $\varepsilon > 0$. By the central limit theorem, $P\{|S(n^{2\beta})| \leq n^{\beta - \varepsilon}\}$ goes to zero. Hence we can apply part (a).

If $A \subset \mathbb{Z}^2$, $|A| < \infty$, let

$$\tau_A = \inf\{j \geq 1: S(j) \in A\}$$

Let $\bar{A} = \{y \notin A: \text{there exists a path from } y \text{ to } \infty \text{ avoiding } A\}$. By Ref. 4, if $x, y \in \bar{A}$,

$$\lim_{M \rightarrow \infty} \frac{P_x\{\tau_A > M\}}{P_y\{\tau_A > M\}}$$

exists. We will need a slightly stronger version of this result, which gives a rate of convergence.

Lemma 5.5. Let $A \subset R_1$, $x, y \in R_1 \cap \bar{A}$. Then, if $\xi = \inf\{j \geq 1: S(j) \in \partial R_3\}$,

$$\lim_{M \rightarrow \infty} \frac{P_x\{\tau_A > M\}}{P_y\{\tau_A > M\}} = \frac{P_x\{\tau_A > \xi\}}{P_y\{\tau_A > \xi\}} \left[1 + O\left(\frac{1}{n^{3/2}}\right)\right]$$

Proof. For fixed n , it is routine to prove

$$\lim_{M \rightarrow \infty} P_x\{\tau_A > 2M \mid \tau_A > M\} = 1$$

and hence $P_x\{\tau_A > 2M\} \sim P_x\{\tau_A > M\}$. Similarly, one can show

$$\begin{aligned} \lim_{M \rightarrow \infty} \frac{P_x\{\tau_A > M\}}{P_y\{\tau_A > M\}} &= \lim_{M \rightarrow \infty} \frac{P_x\{\tau_A > M + \xi\}}{P_y\{\tau_A > M + \xi\}} \\ &= \frac{P_x\{\tau_A > \xi\}}{P_y\{\tau_A > \xi\}} \lim_{M \rightarrow \infty} \frac{P_x\{\tau_A > M + \xi \mid \tau_A > \xi\}}{P_y\{\tau_A > M + \xi \mid \tau_A > \xi\}} \end{aligned}$$

In Lemma 5.8 we show that for $z \in \partial R_3$,

$$P_x\{S(\xi) = z \mid \tau_A > \xi\} = P_y\{S(\xi) = z \mid \tau_A > \xi\} \left[1 + O\left(\frac{1}{n^{3/2}}\right) \right] \quad (5.1)$$

which implies, for every $M > 0$,

$$P_x\{\tau_A > M + \xi \mid \tau_A > \xi\} = P_y\{\tau_A > M + \xi \mid \tau_A > \xi\} \left[1 + O\left(\frac{1}{n^{3/2}}\right) \right]$$

This gives the result. (We have assumed the result of Ref. 4, i.e., that the limit exists. A little more work could be done to prove this independently.)

The key remaining step is (5.1), which intuitively states that a random walk, by the time it hits ∂R_3 , has forgotten its starting point. The unconditioned hitting distribution was discussed in Lemma 4.4(a) of Ref. 8 using a result in Ref. 1. We state this as a lemma:

Lemma 5.6. If $x \in R_\alpha$, then for $z \in \partial R_3$,

$$P_x\{S(\xi) = z\} = P_0\{S(\xi) = z\} [1 + O(n^{\alpha-3})]$$

We emphasize here that the $O(\cdot)$ is independent of $x \in R_\alpha$ and $z \in \partial R_3$.

Lemma 5.7. If $A \subset R_1$ and $x \in R_{3/2} \setminus R_{4/3}$, then for $z \in \partial R_3$

$$P_x\{S(\xi) = z \mid \xi < \tau_A\} = P_x\{S(\xi) = z\} [1 + O(n^{-3/2})]$$

Proof. By Lemma 5.4(a)

$$P\{\xi < \tau_A\} \geq \frac{1}{6}[1 + o(1)] \quad (5.2)$$

But,

$$\begin{aligned} P_x\{S(\xi) = z\} &= P_x\{S(\xi) = z \mid \xi > \tau_A\} P\{\xi > \tau_A\} \\ &\quad + P_x\{S(\xi) = z \mid \xi < \tau_A\} P\{\xi < \tau_A\} \end{aligned} \quad (5.3)$$

By Lemma 5.6, for $y \in R_{3/2}$,

$$P_y\{S(\xi) = z\} = P_0\{S(\xi) = z\} [1 + O(n^{-3/2})]$$

Since $A \subset R_{3/2}$, an easy Markov argument gives

$$\begin{aligned} P_x\{S(\xi) = z \mid \xi > \tau_A\} &= P_0\{S(\xi) = z\} [1 + O(n^{-3/2})] \\ &= P_x\{S(\xi) = z\} [1 + O(n^{-3/2})] \end{aligned}$$

Using this with (5.2) and (5.3) gives the result.

Lemma 5.8. With the assumptions of Lemma 5.5

$$P_x\{S(\xi) = z \mid \tau_A > \xi\} = P_y\{S(\xi) = z \mid \tau_A > \xi\} \left[1 + O\left(\frac{1}{n^{3/2}}\right) \right] \quad (5.4)$$

Proof. Let $\eta = \inf\{j \geq 1: S(j) \in \partial R_{3/2}\}$, $\varphi = \tau_A \wedge \xi$, $\psi = \tau_A \wedge \eta$. Then for $z \in \partial R_3$,

$$P_x\{S(\varphi) = z\} = \sum_{w \in \partial R_{3/2}} P_x\{S(\psi) = w\} P_w\{S(\varphi) = z\}$$

By Lemma 5.7, for $w \in \partial R_{3/2}$,

$$P_w\{S(\varphi) = z\} = P_0\{S(\xi) = z\} P_w\{\tau_A > \xi\} \left[1 + O\left(\frac{1}{n^{3/2}}\right) \right]$$

Also,

$$P_x\{\tau_A > \xi\} = \sum_{w \in \partial R_{3/2}} P_x\{S(\psi) = w\} P_w\{\tau_A > \xi\}$$

Hence

$$P_x\{S(\varphi) = z\} = P_x\{\tau_A > \xi\} P_0\{S(\xi) = z\} [1 + O(n^{-3/2})]$$

A similar expression holds for y , and hence we have (5.1).

Finally, we note that from Lemma 5.5 we get (1.5). Using (1.4) and (1.6), we see at each step the two transition probabilities agree up to order $O(1/n^{3/2})$. Hence, for any n -step ω ,

$$\begin{aligned} \hat{P}_{n,n^3}(\omega) &= \hat{P}_n(\omega) \prod_{j=1}^n \left[1 + O\left(\frac{1}{n^{3/2}}\right) \right] \\ &= \hat{P}_n(\omega) \left[1 + O\left(\frac{1}{\sqrt{n}}\right) \right] \end{aligned}$$

ACKNOWLEDGMENTS

This research was supported by NSF grant DMS-85-02293 and an Alfred P. Sloan Research Fellowship.

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