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A Lower Bound for the End-to-End Distance of the Self-Avoiding Walk

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Abstract. For an N-step self-avoiding walk on the hypercubic lattice $\mathbf{Z}^d$, we prove that the mean-square end-to-end distance is at least $N^{4/(3d)}$ times a constant. This implies that the associated critical exponent ν is at least $2/(3d)$, assuming that ν exists.

1 Introduction

A self-avoiding walk (SAW) is a path in a lattice that does not visit any site more than once. In theoretical physics and chemistry, the SAW is a standard simple model of a linear polymer molecule in solution, and it is also important as a model exhibiting critical phenomena in statistical mechanics. Seminal contributions to the nonrigorous theory of the SAW have been made by, among others, Nobel laureates Paul J. Flory (Chemistry, 1974) and Pierre-Gilles de Gennes (Physics, 1991). For a general review, see Madras and Slade [5] or Vanderzande [8]. The SAW is also of considerable mathematical interest, since it is simple to define but has been very challenging to analyze rigorously. The purpose of this paper is to prove a lower bound on a key quantity, the mean-square end-to-end distance. Our result, Proposition 1.1, is the only nontrivial lower bound that has been proven in 2 or 3 dimensions, which are the most relevant dimensions in polymer physics.

We follow the notation of Madras and Slade [5]. Let $\mathbf{Z}^d$ be the d-dimensional hypercubic lattice ($d \geq 2$ fixed). Points of $\mathbf{Z}^d$ will often be called *sites*. We write a typical element of $\mathbf{Z}^d$ (or more generally $\mathbf{R}^d$) as $z = (z_1, \dots, z_d)$. We shall refer to the following norms on $\mathbf{R}^d$:

$$\|z\|_p = \left(|z_1|^p + \cdots + |z_d|^p\right)^{1/p} \quad (\text{for } 1 \leq p < \infty) \quad \text{and}$$
$$\|z\|_\infty = \max\{|z_1|, \dots, |z_d|\}.$$

In this paper, N always denotes a positive integer. An N-step self-avoiding walk in $\mathbf{Z}^d$ is a finite sequence $\omega = (\omega(0), \dots, \omega(N))$ of sites $\omega(i)$ in $\mathbf{Z}^d$ such that $\|\omega(j+1) - \omega(j)\|_1 = 1$ for every j, and $\omega(i) \neq \omega(j)$ whenever $i \neq j$; that is, ω is a path of N nearest-neighbour steps with no repeated sites. Let $\mathcal{S}_N$ be the set of all N-step self-avoiding walks ω such that $\omega(0)$ is the origin. The i-th coordinate of the k-th site of ω is denoted $\omega_i(k)$.

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We shall write P_N to denote the uniform probability distribution on the set $\mathcal{S}_N$, and E_N to denote expectation with respect to P_N. For each dimension d, there should be a *critical exponent* ν such that

$$E_N\left(\|\omega(N)\|_2^2\right) \sim DN^{2\nu} \quad \text{as } N \to \infty \tag{1.1}$$

for some constant D (with logarithmic corrections for $d = 4$); see [6, Section 2.1] for further discussion. Significantly, the value of ν should depend only on d; that is, equation (1.1) should hold with the same value of ν for every d-dimensional lattice. While equation (1.1) is undoubtedly true, it has not yet been proven in every dimension. Hara and Slade [3, 4] proved it for $d \geq 5$ with $\nu = 1/2$, and there is progress towards a proof for $d = 4$ (see Brydges and Slade [1]). For $d = 2$, there is strong theoretical evidence that $\nu = 3/4$, while for $d = 3$ it seems likely that ν is close to 0.588 (see Slade [7] for a current review). However, a proof of equation (1.1) remains frustratingly elusive in low dimensions, namely $d = 2, 3, 4$. Even worse, so far there are no non-trivial rigorous bounds in low dimensions, *i.e.,* known positive numbers D_L, ν_L, D_U, ν_U with $\nu_U < 1$ such that

$$D_L N^{2\nu_L} \leq E_N\left(\|\omega(N)\|_2^2\right) \leq D_U N^{2\nu_U} \quad \text{for all sufficiently large } N. \tag{1.2}$$

The value $\nu_L = 1/2$ would correspond to a "mean-field" bound, based on the intuition that a self-avoiding walk should spread out more quickly than an ordinary classical random walk. However, such a bound has yet to be proved for general dimensions d. Even more simply, one could reasonably expect a lower bound with $\nu_L = 1/d$, since the average distance of all points of an N-step self-avoiding walk from $\omega(0)$ must be at least of order $N^{1/d}$. Alas, no rigorous proof is known even for this bound. The purpose of this note is to prove a lower bound with $\nu_L = 2/(3d)$. The relative weakness of this bound epitomizes the challenges of finding rigorous proofs for low-dimensional self-avoiding walks.

A recent preprint of Duminil-Copin and Hammond [2] proves that in every dimension $d \geq 2$, the self-avoiding walk is sub-ballistic in the sense that $\|\omega(N)\|_2$ is $o(N)$ with high probability. More precisely, they prove that for any $b > 0$, there exists an $\epsilon > 0$ such that $P_N(\|\omega(N)\|_2 > bN) \leq \exp(-\epsilon N)$ for all large N. It follows that $\lim_{N\to\infty} E_N(\|\omega(N)\|_2^2)/N^2 = 0$. Informally this says that $\nu < 1$, but it does not give an upper bound $\nu_U < 1$ for equation (1.2).

The main result of this paper is the following proposition.

Proposition 1.1 *Let N be a positive integer and let p be a real number in $[1, \infty)$. Then*

$$\left(E_N\|\omega(N)\|_p^p\right)^{1/p} \geq \left(E_N\|\omega(N)\|_\infty^p\right)^{1/p} \geq \frac{1}{6}N^{\frac{p}{(p+1)d}}.$$

Setting $p = 2$ shows that we can take $\nu_L = 2/(3d)$ in equation (1.2).

The first inequality in the proposition is clearly trivial.

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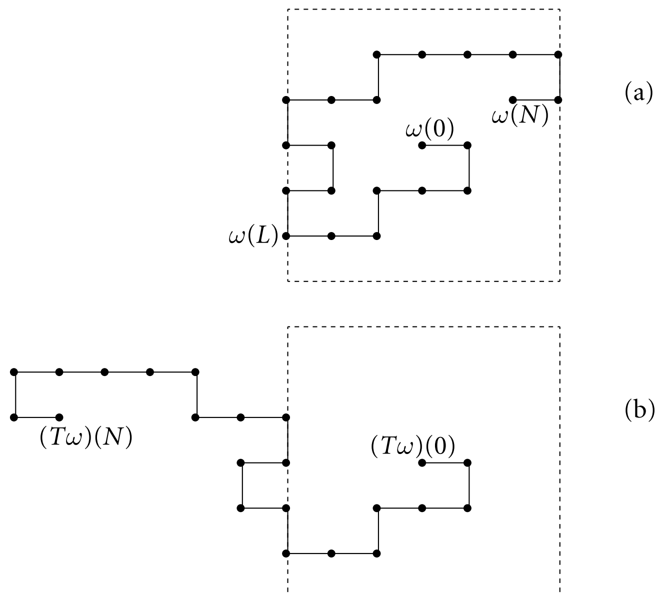

Figure 1: (a) An example of a self-avoiding walk in $\mathbf{Z}^2$ with $|||\omega||| = 3$, $L = 7$, $I = 1$, and $H = -3$. The dashed lines represent the surface of the square $\{x : \|x\|_\infty \le 3\}$. (b) The walk $T\omega$, for the walk ω from (a). In this example, the operator U is reflection through $x_1 = -3$.

2 Proof of Proposition 1.1

Before we prove the proposition, we lay some groundwork. For a self-avoiding walk $\omega \in \mathcal{S}_N$, let

$$|||\omega||| = \max\big\{ \|\omega(k)\|_\infty : k = 0, 1, \dots, N \big\} .$$

Then $|||\omega|||$ is the smallest value of r such that ω is contained in the (hyper)cube $\{x \in \mathbf{R}^d : \|x\|_\infty \le r\}$. We shall now define a transformation T on $\mathcal{S}_N$ that reflects part of each SAW through a face of this minimal hypercube. Given $\omega \in \mathcal{S}_N$, let

$$L = L(\omega) = \min\{k > 0 : \|\omega(k)\|_\infty = |||\omega|||\},$$
$$I = I(\omega) = \min\{i : 1 \le i \le d, |\omega_i(L)| = |||\omega|||\}$$

and

$$H = H(\omega) = \omega_I(L).$$

See Figure 1(a). Observe that

$$|H| = \|\omega(L)\|_\infty = |||\omega\,||| .$$

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Let U be the reflection through the (hyper)plane $x_I = H$, *i.e.*, $U(x)$ is the point y such that

$$y_i = \begin{cases} x_i & \text{if } i \neq I, \\ 2H - x_i & \text{if } i = I. \end{cases}$$

(Our notation suppresses the dependence of the mapping U on ω.) Let $T\omega$ be the SAW $\theta = (\theta(0), \dots, \theta(N))$ such that

$$\theta(k) = \begin{cases} \omega(k) & \text{if } k \leq L, \\ U(\omega(k)) & \text{if } k > L. \end{cases}$$

See Figure 1(b). It is not hard to see that $T\omega$ is indeed a SAW. Likewise, the following lemma is straightforward, and we omit its proof.

Lemma 2.1 *Let $\omega \in \mathcal{S}_N$. Suppose m is an integer such that $\|\omega(N)\|_\infty \leq m \leq |||\omega|||$. Then*

(i) *for each $i \in \{1, \dots, d\}$ with $i \neq I(\omega)$, we have $(T\omega)_i(N) = \omega_i(N) \in [-m, m]$;*
(ii) *$(T\omega)_{I(\omega)}(N)$ has the same sign as $H(\omega)$;*
(iii) *$|H(\omega)| \leq 2|H(\omega)| - m \leq \|(T\omega)(N)\|_\infty \leq 2|H(\omega)| + m$;*
(iv) *$|(T\omega)_{I(\omega)}(N)| = \|(T\omega)(N)\|_\infty$.*

The following lemma is also elementary.

Lemma 2.2 *Let $N > 3^d$. Then $|||\omega||| > \frac{1}{3}N^{1/d}$ for every ω in $\mathcal{S}_N$.*

Proof It suffices to show that the number of sites of $\mathbf{Z}^d$ in the hypercube $\{x \in \mathbf{R}^d : \|x\|_\infty \leq \frac{1}{3}N^{1/d}\}$ is less than the number of sites in ω (which is $N+1$). The number of sites in this hypercube is at most

$$\left(2\left(\frac{1}{3}N^{1/d}\right) + 1\right)^d < \left(\frac{2N^{1/d}}{3} + \frac{N^{1/d}}{3}\right)^d = N. \qquad \blacksquare$$

The next lemma is our key estimate.

Lemma 2.3 *Let m be a real number such that $1 \leq m \leq \frac{1}{3}N^{1/d}$. Then*

$$P_N\left(\|\omega(N)\|_\infty \leq m\right) \leq (m+1)P_N\left(\|\omega(N)\|_\infty \geq \frac{1}{3}N^{1/d}\right). \tag{2.1}$$

Proof We shall assume that m is an integer (the non-integer case follows easily from the integer case). Observe that if $N \leq 3^d$, then the probability on the right-hand side of equation (2.1) equals 1; therefore, we shall assume that $N > 3^d$. By the choice of m and Lemma 2.2, we see that $m \leq |||\omega|||$ for every ω in $\mathcal{S}_N$. Let

$$\mathcal{S}_{N,\leq m} = \left\{\omega \in \mathcal{S}_N : \|\omega(N)\|_\infty \leq m\right\} \quad \text{and}$$
$$\mathcal{S}_{N,+} = \left\{\omega \in \mathcal{S}_N : \|\omega(N)\|_\infty \geq \frac{1}{3}N^{1/d}\right\}.$$

Lemmas 2.1 and 2.2 show that T maps $\mathcal{S}_{N,\leq m}$ into $\mathcal{S}_{N,+}$. Our proof will be finished if we can show that the restriction of T to $\mathcal{S}_{N,\leq m}$ is at most $(m+1)$-to-one.

Assume $\theta, \phi \in \mathcal{S}_{N,\leq m}$ and $T\theta = T\phi = \psi$. By Lemma 2.1(i), (iv), we see that $I(\theta) = I(\phi)$. If $H(\theta)$ also equals $H(\phi)$, then θ must equal ϕ. By Lemma 2.1(iii),

$$\frac{\|\psi(N)\|_\infty - m}{2} \leq |H(\theta)| \leq \frac{\|\psi(N)\|_\infty + m}{2}.$$

Thus, given $\psi = T\theta$, there are at most $m+1$ possible values for $H(\theta)$ (we have also used Lemma 2.1(ii) here). It follows that T is at most $(m+1)$-to-one on $\mathcal{S}_{N,\leq m}$, and the lemma follows. ■

We are now ready to prove Proposition 1.1.

Proof of Proposition 1.1 Observe that $\|\omega(N)\|_\infty \geq 1$ for every SAW ω in $\mathcal{S}_N$; hence the lower bound in the proposition is trivial for $N \leq 6^d$. So it suffices to consider fixed $N > 6^d$.

Let $B = B_N = (E_N\|\omega(N)\|_\infty^p)^{1/p}$. If $B \geq \frac{1}{6}N^{1/d}$, then we are done, so we shall assume that $B < \frac{1}{6}N^{1/d}$. Then

$$\begin{aligned} P_N\big(\|\omega(N)\|_\infty \geq 2B\big) &= P_N\big(\|\omega(N)\|_\infty^p \geq (2B)^p\big) \\ &\leq \frac{E_N\|\omega(N)\|_\infty^p}{(2B)^p} \quad \text{(by Markov's Inequality)} \\ &= \frac{1}{2^p}; \end{aligned}$$

hence we have (since $p \geq 1$)

$$P_N\big(\|\omega(N)\|_\infty < 2B\big) \geq 1 - \frac{1}{2^p} \geq \frac{1}{2}. \tag{2.2}$$

By Markov's Inequality and Lemma 2.3 (recall that we have assumed $2B < \frac{1}{3}N^{1/d}$),

$$\begin{aligned} B^p = E_N\|\omega(N)\|_\infty^p &\geq \Big(\frac{N^{1/d}}{3}\Big)^p P_N\Big(\|\omega(N)\|_\infty \geq \frac{1}{3}N^{1/d}\Big) \\ &\geq \frac{N^{p/d}}{3^p(2B+1)} P_N\big(\|\omega(N)\|_\infty \leq 2B\big) \\ &\geq \frac{N^{p/d}}{3^p 2(3B)} \qquad \text{[by Equation (2.2)]}. \end{aligned}$$

The above inequalities tell us that $B^p \geq N^{p/d}/(3^{p+1}2B)$, which is equivalent to $B^{p+1} \geq N^{p/d}/(3^{p+1}2)$. The proposition follows upon taking $(p+1)$-th roots of both sides of this final inequality. ■

Acknowledgments I constructed this proof several years ago, but did not write it up because the result was disappointingly weak. I was hoping that the argument could be improved, for example, by showing that the restriction of T to $\mathcal{S}_{N,\le m}$ is typically much better than $(m+1)$-to-one. However, no such improvement was apparent, and Gordon Slade was encouraging me to publish the result. In the meantime, Michael Newman independently rediscovered the result and a very similar proof.

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