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CRITICAL BEHAVIOUR OF SELF-AVOIDING WALK IN FIVE OR MORE DIMENSIONS

TAKASHI HARA AND GORDON SLADE

ABSTRACT. We use the lace expansion to prove that in five or more dimensions the standard self-avoiding walk on the hypercubic (integer) lattice behaves in many respects like the simple random walk. In particular, it is shown that the leading asymptotic behaviour of the number of n-step self-avoiding walks is purely exponential, that the mean square displacement is asymptotically linear in the number of steps, and that the scaling limit is Gaussian, in the sense of convergence in distribution to Brownian motion. Some related facts are also proved. These results are optimal, according to the widely believed conjecture that the self-avoiding walk behaves unlike the simple random walk in dimensions two, three and four.

1. INTRODUCTION

The self-avoiding walk is a simply defined mathematical model with important applications in polymer chemistry and statistical physics. It serves as a basic example of a non-Markovian stochastic process, but lies beyond the reach of current methods of probability theory. In addition, it poses simply stated combinatorial problems which have not yet met a mathematically satisfactory resolution.

The basic definitions are as follows. An n-step self-avoiding walk ω on the d-dimensional integer lattice $\mathbf{Z}^d$ is an ordered set $\omega = (\omega(0), \omega(1), \dots, \omega(n))$, with each $\omega(i) \in \mathbf{Z}^d$, $|\omega(i+1) - \omega(i)| = 1$ (Euclidean distance), and $\omega(i) \neq \omega(j)$ for $i \neq j$. We always take $\omega(0) = 0$. Thus a self-avoiding walk can be considered as the path of a simple random walk, beginning at the origin, which contains no closed loops. We denote by c_n the number of n-step self-avoiding walks, and for $x \in \mathbf{Z}^d$ we denote by $c_n(x)$ the number of n-step self-avoiding walks for which $\omega(n) = x$. By convention, $c_0 = 1$ and $c_0(x) = \delta_{x,0}$. When x is a nearest

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neighbour of the origin $c_n(x)$ yields the number of self-avoiding polygons. The mean square displacement $\langle|\omega(n)|^2\rangle_n$ is by definition the average value of the square of the distance from the origin after n steps, i.e.,

$$\langle|\omega(n)|^2\rangle_n = \frac{1}{c_n} \sum_{\omega:|\omega|=n} |\omega(n)|^2, \tag{1.1}$$

where the sum is over all n-step self-avoiding walks.

We use the notation $a_n \sim b_n$ to mean $\lim_{n\to\infty} a_n/b_n = 1$. The conjectured asymptotic behaviour of the above quantities is

$$c_n \sim A\mu^n n^{\gamma-1}, \tag{1.2}$$

$$\langle|\omega(n)|^2\rangle_n \sim Dn^{2\nu}, \tag{1.3}$$

and

$$c_n(x) \sim B\mu^n n^{\alpha_{\text{sing}}-2}, \tag{1.4}$$

where in (1.4) n and $\|x\|_1$ have the same parity. Here A, B, and D are dimension dependent constants, and μ is a dimension dependent constant known as the *connective constant.* The *critical exponents* γ, ν, α_{sing} are introduced in (1.2)–(1.4) to conform with analogues in other statistical mechanical systems, such as the Ising model. In all dimensions it is believed that the hyperscaling relation $\alpha_{\text{sing}} - 2 = -d\nu$ is satisfied. The critical exponent γ is believed to take the values $43/32$ for $d = 2$, $1.162\ldots$ for $d = 3$, and 1 for $d \geq 4$, with a logarithmic correction when $d = 4$. The conjectured values for ν are $3/4$ for $d = 2$, $0.59\ldots$ for $d = 3$, and $1/2$ for $d \geq 4$, again with a logarithmic correction in four dimensions. These conjectures are based on nonrigorous renormalization group arguments and numerical work (see e.g., [12, 11]).

Few rigorous results concerning (1.2)–(1.4) have been obtained. It is known that $\mu \equiv \lim_{n\to\infty} c_n^{1/n}$ exists and that $c_n \geq \mu^n$ [4]. The best general upper bounds on c_n are of the form $c_n \leq \mu^{n+O[n^{2/(d+2)}\log n]}$ (the factor $\log n$ can be omitted from the exponent for $d = 2$) [5, 9]. There is no proof that in every dimension $\nu \geq 1/2$ or that $\nu \leq 1-\varepsilon$ for some $\varepsilon > 0$. In high dimensions, it has been proved that for $d \geq d_0$, for some undetermined dimension d_0, that (1.2) holds with $\gamma = 1$ [15] and (1.3) holds with $\nu = 1/2$ [13]. This announcement concerns the further development and extension of these high d results to $d \geq 5$. The method is based on the lace expansion, which was introduced by Brydges and Spencer [1] to study the *weakly* self-avoiding walk above four dimensions. (In the weakly self-avoiding walk, intersections are suppressed but not forbidden.)

We require the generating function for c_n (the *susceptibility*):

$$\chi(z) = \sum_{n=0}^{\infty} c_n z^n , \tag{1.5}$$

and for $c_n(x)$ (the *two-point function*):

$$G_z(x) = \sum_{n=0}^{\infty} c_n(x) z^n . \tag{1.6}$$

It is known that for $z \in (0, \mu^{-1})$ the two-point function decays exponentially as $|x| \to \infty$, and that the limit

$$\xi(z)^{-1} = - \lim_{n\to\infty} n^{-1} \log G_z((n, 0, \ldots, 0)) \tag{1.7}$$

exists and decreases to zero as $z \nearrow \mu^{-1}$ [2]. It is widely believed that $\xi(z)$ is asymptotic to a multiple of $(\mu^{-1} - z)^{-\nu}$ as $z \nearrow \mu^{-1}$, with the same critical exponent ν as that governing the mean square displacement in (1.3).

2. Main results

The purpose of this article is to announce the following theorems.

Theorem 2.1. *For $d \geq 5$, there are constants A, D, $C > 0$ such that the following hold.*

(a) $c_n = A\mu^n[1 + O(n^{-\varepsilon})]$ *as* $n \to \infty$, *for any* $\varepsilon < 1/2$.

(b) $\langle |\omega(n)|^2 \rangle_n = Dn[1 + O(n^{-\varepsilon})]$ *as* $n \to \infty$, *for any* $\varepsilon < 1/4$.

(c) $\sup_x \sum_{n=0}^{\infty} n^a c_n(x) \mu^{-n} < \infty$ *for all* $a < (d-2)/2$.

(d) $\xi(z) \sim C(\mu^{-1} - z)^{-1/2}$, *as* $z \nearrow \mu^{-1}$.

In (d), $f(z) \sim g(z)$ means $\lim_{z \nearrow \mu^{-1}} f(z)/g(z) = 1$. A corollary of (a) is that $\lim_{n\to\infty} c_{n+1}/c_n = \mu$. This is believed to be true in all dimensions, but remains unproved for $d = 2, 3, 4$. We have not succeeded in obtaining a bound $c_n(x) \leq O(\mu^n n^{-d/2})$ for $d = 5$, although such a bound can be obtained for d moderately larger than $5 (d \geq 10$ is likely more than enough, although this has not been checked). Part (c) of the above theorem is a statement for the generating function which is consistent with such a bound on $c_n(x)$, for $d \geq 5$.

The two-point function at the critical point $z_c = \mu^{-1}$ is conjectured to decay like $|x|^{-(d-2+\eta)}$ for large $|x|$, with η determined by Fisher's relation $(2-\eta)\nu = \gamma$. This corresponds formally to behaviour of the form $k^{\eta-2}$ near $k=0$ for the Fourier transform

$$\widehat{G}_z(k) = \sum_{x\in\mathbf{Z}^d} G_z(x)e^{ik\cdot x}, \qquad k \in [-\pi, \pi]^d$$

at $z = z_c$. For $d \geq 5$, inserting the values $\nu = 1/2$ and $\gamma = 1$ from Theorem 2.1 into Fisher's relation gives $\eta = 0$. The analogue of $\widehat{G}_z(k)$ for simple random walk is $[1 - 2dzD(k)]^{-1}$, where $D(k) = d^{-1}\sum_{j=1}^{d} \cos k_j$. Our results for the two-point function are as follows.

Theorem 2.2. *For $d \geq 5$ and $p < (d-2)/2$ or $p \leq 2$, there is a constant $C(p)$ such that for all $x \in \mathbf{Z}^d$, $G_{z_c}(x) \leq C(p)|x|^{-p}$. The Fourier transform satisfies the two-sided "infrared bound" $C_1[1 - D(k)]^{-1} \leq \widehat{G}_{z_c}(k) \leq C_2[1 - D(k)]^{-1}$, for some C_1, $C_2 > 0$; in this sense $\eta = 0$.*

To discuss the scaling limit we first introduce some notation. Let $C_d[0, 1]$ denote the continuous $\mathbf{R}^d$-valued functions on $[0, 1]$. Given an n-step self-avoiding walk ω, we define $X_n \in C_d[0, 1]$ by taking $X_n(t)$ to be the linear interpolation of $n^{-1/2}\omega([nt])$, where $[nt]$ denotes the integer part of nt. We denote by dW the Wiener measure on $C_d[0, 1]$, normalized so that $\int e^{ik\cdot B_t}\,dW = \exp[-Dk^2t/2d]$, where D is the diffusion constant of Theorem 2.1(b). Expectation with respect to the uniform measure on the n-step self-avoiding walks is denoted by $\langle\cdot\rangle_n$. The following theorem states that the scaling limit of the self-avoiding walk is Gaussian, for $d \geq 5$.

Theorem 2.3. *For $d \geq 5$, the self-avoiding walk converges in distribution to Brownian motion. More precisely, for any bounded continuous function f on $C_d[0, 1]$,*

$$\lim_{n\to\infty} \langle f(X_n)\rangle_n = \int f\,dW.$$

All of the above results rely on the lace expansion. As a further application of the method, combined with the method used in [10] for very high dimensions, the infinite self-avoiding walk can be constructed in dimensions $d \geq 5$.

In the course of the proof of Theorem 2.1, good bounds on the value of μ were required. An elementary method of obtaining a lower bound on μ was developed, which does not use the lace expansion, and which is valid above two dimensions. The resulting bound in three dimensions slightly improves the previous best rigorous lower bound 4.352 of [3]. Our results for $d = 3, 4, 5$ are as follows.

Theorem 2.4. *Let $\mu(d)$ denote the connective constant for $\mathbf{Z}^d$. Then $\mu(3) \geq 4.43733$, $\mu(4) \geq 6.71800$, and $\mu(5) \geq 8.82128$.*

3. Discussion of the proof

The proofs will appear in [7,8]. The basic tool used in the proofs of Theorems 2.1–2.3 is the lace expansion. The lace expansion is an expansion for $\widehat{G}_z(k)^{-1}$, which can be derived either using the inclusion-exclusion relation or by a kind of cluster expansion. Convergence of the lace expansion requires a small parameter, which previously has been taken to be the weakness of the interaction for the weakly self-avoiding walk, and the inverse dimension for the standard self-avoiding walk on $\mathbf{Z}^d$, for $d \gg 1$. For $d \geq 5$ the small parameter responsible for convergence of the lace expansion is the critical "bubble diagram" $B(z_c) = \sum_{x \neq 0} G_{z_c}(x)^2$. For $d = 5$ we show $B(z_c) \leq 0.5$. Thus our small parameter is not terribly small, and proving convergence of the expansion poses considerable new difficulties. Convergence was obtained by following the basic method of [13], with substantial elaboration. Very careful estimation of the Feynman diagrams arising in the expansion was required. Computer calculations played an important role in the analysis as an experimental tool, and also in allowing numerical evaluation of the simple random walk two-point function and some related Gaussian quantities (whose precise values were needed in the convergence proof). Rigorous error bounds were obtained for these numerical calculations.

As $d \to 4^+$, we expect $B(z_c) \to \infty$, and hence our method will fail for d fractionally larger than 4. In this sense our proof is unnatural. An ideal proof would have the condition $B(z_c) < \infty$, rather than $B(z_c)$ small, as its driving force, and would not require the very detailed numerical estimates used in our proof. Unfortunately such a proof has not materialized.

Convergence of the lace expansion yields good control over the two-point function (1.6), the susceptibility (1.5) and the *correla-*

tion length of order two $\xi_2(z) = [\chi(z)^{-1}\sum_x |x|^2 G_z(x)]^{1/2}$, in the vicinity of the critical point $z_c = \mu^{-1}$. The more detailed information contained in the asymptotics of c_n and the mean square displacement is extracted using contour integration. In contrast to [1, 13], we work directly with the self-avoiding walk in this analysis and need not consider walks which are self-avoiding with finite memory. To bound the error terms in the contour integration we use a new method to control "fractional" z-derivatives of the two-point function at the critical point, using the following identity. Let $f(z) = \sum_{n=0}^{\infty} a_n z^n$ have radius of convergence R. Then for any z with $|z| < R$, and for any $\varepsilon \in (0, 1)$,

$$\delta_z^\varepsilon f(z) \equiv \sum_{n=1}^{\infty} n^\varepsilon a_n z^n = C_\varepsilon z \int_0^\infty f'(ze^{-\lambda^{\frac{1}{1-\varepsilon}}} e^{-\lambda^{\frac{1}{1-\varepsilon}}}\, d\lambda,$$

where $C_\varepsilon = [(1-\varepsilon)\Gamma(1-\varepsilon)]^{-1}$. With $f(z) = G_z(x)$, the integral on the right side can be estimated using the lace expansion.

The proof of Theorem 2.1(d) follows the approach used to study the analogous problem for percolation in [6]. Theorem 2.3 is proved using the method of [15, 14]. Fractional derivatives play a simplifying role in the proof of Theorem 2.1(d), and an essential role in Theorem 2.3.

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Department of Physics, Gakushuin University, Toshima-ku, Tokyo 171, Japan

E-mail address: hara@tkyux.phys.s.u-tokyo.ac.jp

Department of Mathematics and Statistics, McMaster University, Hamilton, Ontario, Canada L8S 4K1

E-mail address: slade@sscvax.mcmaster.ca