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Self-Avoiding Walks with Geometrical Constraints

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We consider self-avoiding walks on a D-dimensional hypercubic lattice, confined to a slab geometry and confined to a half-space. We present a proof of the existence of a "connective constant" for the slab geometry and review some corresponding results for the half-space. We also discuss the way in which scaling arguments can be used to give stronger, but nonrigorous, results.

KEY WORDS: Self-avoiding walks.

1. INTRODUCTION

Self-avoiding walks confined to slabs, or attached (by a unit degree vertex) to a plane and confined to lie on one side of this plane, are of interest in problems such as polymer adsorption, steric stabilization of colloids and surface magnetism. In addition they are interesting as examples of systems in which geometrical constraints are applied so that the self-avoiding walk must also avoid some kind of barrier.

The problem of the asymptotic behavior of the number (c_n) of n-step self-avoiding walks on a lattice is well known. The few rigorous results which are available make use of the theory of functional inequalities[1] and the strongest result[2] is that there exists a constant, k, such that

$$c_n = \exp\left[nk + O(n^{1/2}) \right] \tag{1.1}$$

This result is weak, in that it is widely believed that

$$c_n = \exp\left[nk + O(\log n) \right] \tag{1.2}$$

In Section 2 we prove the existence of the limit

$$\lim_{n\to\infty} n^{-1} \log c_n(L) \equiv k(L) \tag{1.3}$$

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where $c_n(L)$ is the number of self-avoiding walks confined to a slab of $L + 1$ $(D - 1)$-dimensional hyperplanes of a D-dimensional hypercubic lattice, and in Section 3 we discuss the predictions about the behavior of $k(L)$ and related quantities which can be obtained from heuristic scaling arguments. In Section 4 we discuss some corresponding rigorous results for walks in a half-space and describe predictions about critical exponents which follow from considering the self-avoiding walk problem as the zero-spin-component limit of a magnetic problem.

2. SELF-AVOIDING WALKS CONFINED TO A SLAB

We consider a hypercubic lattice whose lattice points are the integer points in R^D, $\mathbf{z} = (x, \ldots, y)$. An n-step self-avoiding walk is a sequence of distinct vertices $w = \{\mathbf{z}_0, \mathbf{z}_1, \ldots, \mathbf{z}_n\}$ such that $\mathbf{z}_i$ and $\mathbf{z}_{i+1}$ differ by unity in exactly one of their coordinates. We shall be concerned with the subset of self-avoiding walks which satisfy the additional constraint

$$0 \leqslant x_i \leqslant L, \qquad i = 0, 1, \ldots, n \tag{2.1}$$

so that the walk is confined to $(L + 1)$ "layers" of the hypercubic lattice. Let $C_n(L, \mathbf{A})$ be the set of n-step self-avoiding walks, subject to (2.1), with $\mathbf{z}_0 = \mathbf{A}$, and let $c_n(L, \mathbf{A})$ be the cardinality of $C_n(L, \mathbf{A})$. Although $c_n(L, \mathbf{A})$ will depend upon the x coordinate of $\mathbf{A}$ it will be independent of the remaining coordinates so we can write $c_n(L, \mathbf{A}) = c_n(L, x_0)$. Summing over all possible values of x_0, we obtain

$$c_n(L) = \sum_{x_0=0}^{L} c_n(L, x_0) \tag{2.2}$$

which is the number of self-avoiding walks, subject to (2.1), per site of the $(D - 1)$-dimensional hypercubic lattice. We shall prove that

$$\lim_{n\to\infty} n^{-1} \log c_n(L) \equiv k(L) \tag{2.3}$$

exists for all L.

In order to do this we consider a subset of $C_n(L, \mathbf{A})$ for which it is easy to prove the existence of the corresponding limit, and then show that the existence of this limit implies (2.3).

Let $C_n^{\ddagger}(L, \mathbf{A})$ be the subset of $C_n(L, \mathbf{A})$ such that

$$y_0 \leqslant y_i \leqslant y_n, \qquad i = 0, 1, 2, \ldots, n \tag{2.4}$$

and let $B_n(L, \mathbf{A})$ be the subset of $C_n^{\ddagger}(L, \mathbf{A})$ such that

$$x_0 = x_n = 0 \tag{2.5}$$

and

$$y_0 < y_i, \qquad i = 1, 2, \ldots, n \tag{2.6}$$

Clearly the cardinality of $C_n^\ddagger(L, \mathbf{A})$ depends only on the x coordinate of $\mathbf{A}$ and we write the cardinality as $c_n^\ddagger(L, x_0)$. The cardinality of $B_n(L, \mathbf{A})$ is independent of $\mathbf{A}$ (since $x_0 = 0$ by definition) and we write the cardinality as $b_n(L)$.

Consider a member of $B_n(L, \mathbf{A})$ whose end point is $\mathbf{A}'$. If we now consider a member of $B_m(L, \mathbf{A}')$ and concatenate these two walks, the resulting walk is a member of $B_{n+m}(L, \mathbf{A})$. However, not all members of $B_{n+m}(L, \mathbf{A})$ are obtained by this construction so that

$$b_n(L) b_m(L) \leqslant b_{n+m}(L) \tag{2.7}$$

and $b_n(L)$ is a supermultiplicative function of n. Moreover, $b_n(L)^{1/n}$ is bounded above [since $b_n(L) \leqslant (2D)^n$]. Hence, by a standard theorem on supermultiplicative functions,[1]

$$0 \leqslant \lim_{n\to\infty} n^{-1} \log b_n(L) = \sup_{n>0} n^{-1} \log b_n(L) \equiv k(L) < \infty \tag{2.8}$$

We now consider the relationship between the sets $C_n^\ddagger(L, \mathbf{A})$ and $B_n(L, \mathbf{A})$. If we define

$$c_n^\ddagger(L) = \sum_{x_0=0}^{L} c_n^\ddagger(L, x_0) \tag{2.9}$$

then clearly

$$b_n(L) \leqslant c_n^\ddagger(L) \tag{2.10}$$

In addition any member of $C_n^\ddagger(L, \mathbf{A})$ can be converted to a member of $B_{n+2L+4}(L, \mathbf{A}')$, where $\mathbf{A}'$ is in the hyperplane $x = 0$. To do this $L + 2$ edges are added to each of the end points of the walk in $C_n^\ddagger(L, \mathbf{A})$ as follows. Suppose that A has coordinates $(x_0, \ldots, y_0)$. Add the edge $(x_0, \ldots, y_0) - (x_0, \ldots, y_0 - 1)$, followed by x_0 edges, $(x_0, \ldots, y_0 - 1) - (x_0 - 1, \ldots, y_0 - 1), \ldots, (1, \ldots, y_0 - 1) - (0, \ldots, y_0 - 1)$, and $L + 1 - x_0$ edges, $(0, \ldots, y_0 - 1) - (0, \ldots, y_0 - 2), \ldots, (0, \ldots, y_0 - L - 1 + x_0) - (0, \ldots, y_0 - L - 2 + x_0)$. Since $x_0 \leqslant L$, $L + 2 - x_0 \geqslant 2$. In a similar way, $L + 2$ edges are added to the other end point of the walk from $C_n^\ddagger(L, \mathbf{A})$ so that the end point of the walk after the addition of these edges is $(0, \ldots, y_n + L + 2 - x_n)$. By this process each walk in $C_n^\ddagger(L, \mathbf{A})$ is converted to a *distinct* walk in $B_{n+2L+4}(L, \mathbf{A}')$ and

$$c_n^\ddagger(L) \leqslant b_{n+2L+4}(L) \tag{2.11}$$

Then from (2.8), (2.10), and (2.11) we have

$$0 \leqslant \lim_{n\to\infty} n^{-1} \log c_n^\ddagger(L) = k(L) < \infty \tag{2.12}$$

To relate $C_n(L, \mathbf{A})$ to $C_n^\ddagger(L, \mathbf{A})$ we make use of an unfolding transformation considered by Hammersley and Welch.[2] For a particular walk in $C_n(L, \mathbf{A})$ let $y_{\min} = \min_i y_i$ and let $y_{\max} = \max_i y_i$. Let p be the smallest integer such that $y_p = y_{\min}$ and let q be the largest integer such that $y_q = y_{\max}$. Now reflect the vertices $i = 0, 1, 2, \ldots, p-1$ in $y = y_{\min}$ and the vertices $i = q+1, q+2, \ldots, n$ in $y = y_{\max}$. By repeated application of these reflections we eventually obtain, apart from the trivial translation, a walk in $C_n^{\ddagger}(L, \mathbf{A})$. In general the same walk in $C_n^{\ddagger}(L, \mathbf{A})$ can be produced from different members of $C_n(L, \mathbf{A})$ but Hammersley and Welch[2] have shown that there exists a constant (a) such that at most $\exp(an^{1/2})$ different members of $C_n(L, \mathbf{A})$ can lead to the same member of $C_n^{\ddagger}(L, \mathbf{A})$. Since $C_n^{\ddagger}(L, \mathbf{A})$ is a subset of $C_n(L, \mathbf{A})$ we have

$$c_n^{\ddagger}(L) \leqslant c_n(L) \leqslant c_n^{\ddagger}(L)\exp(an^{1/2}) \tag{2.13}$$

Then (2.12) and (2.13) imply that

$$\lim_{n\to\infty} n^{-1}\log c_n(L) = k(L) \tag{2.14}$$

It is clear that $c_n(L) < c_n(L+1)$, from which it follows that $k(L) \leqslant k(L+1)$, but the calcualtion of $k(L)$ is, of course, extremely difficult. For the special case $D = 2$, Wall *et al.*[3] have shown that

$$\exp[k(1)] = \tfrac{1}{2}(1 + \sqrt{5}) \tag{2.15}$$

and

$$\exp[k(2)] = 1.914\ldots \tag{2.16}$$

A related quantity of interest is the mean square length of a self-avoiding walk in a slab, $\langle R_n^2(L)\rangle$. Although there are no rigorous results on $\langle R_n^2(L)\rangle$ for general D, Wall *et al.*[4,5] have shown that, for $D = 2$,

$$\langle R_n^2(L)\rangle = O(n^2) \tag{2.17}$$

which implies that the walk has one-dimensional behavior. The L-dependence is more difficult but Wall *et al.*[3] have shown that

$$\lim_{n\to\infty} \langle R_n^2(1)\rangle / n^2 = (3 + \sqrt{5})/10 \tag{2.18}$$

and

$$\lim_{n\to\infty} \langle R_n^2(2)\rangle / n^2 = 0.389\ldots \tag{2.19}$$

for $D = 2$. There are no rigorous results on the L dependence of $\langle R_n^2(L)\rangle$ and no results analogous to (2.17) for $D > 2$.

3. SCALING RESULTS

If we are interested in the L dependence of $k(L)$ and $\langle R_n^2(L)\rangle$ then essentially nothing is known rigorously. However, Daoud and de Gennes[6] have used scaling arguments to investigate these quantities. We describe some of their results below.

We consider a characteristic length $R_n(L)$, which might be $\langle R_n^2(L)\rangle^{1/2}$. For L large, we expect $R_n(L)$ to be determined by the natural dimensions of the walk in the absence of the slab constraints,

$$R_n(L) \sim n^\nu, \qquad L \gg n^\nu \tag{3.1}$$

As L decreases there are two competing length scales, L and n^ν, so we expect $R_n(L)$ to be modified by a function of the ratio of the length scales. If we assume that this function can be written as a power law we have

$$R_n(L) \sim n^\nu \{n^\nu / L\}^\phi \tag{3.2}$$

By analogy with the results of Wall *et al.* discussed in Section 2, we expect that

$$R_n(L) \sim n^{\nu'} \qquad \text{for} \quad L \ll n^\nu \tag{3.3}$$

where ν' is the appropriate exponent for the lower-dimensional situation. For (3.2) and (3.3) to be consistent, we require that

$$\phi = (\nu'/\nu) - 1 \tag{3.4}$$

For $D = 3$, using standard estimates of ν and ν' gives $\phi = \frac{1}{4}$ so that, from (3.2)

$$R_n \sim n^{3/4} L^{-1/4} \tag{3.5}$$

while for $D = 2$ we obtain

$$R_n \sim n L^{-1/3} \tag{3.6}$$

This latter result is in good agreement with series analysis work[7] and Monte Carlo results.[8]

Similar arguments,[6] depending on an Ansatz analogous to (3.2), suggest that

$$k(L) \sim L^{-1/\nu} \tag{3.7}$$

This "entropic repulsion" is one contributor to the steric stabilization of colloidal dispersions by weakly absorbed polymer molecules.[9] Of course, for a random walk $\nu = \frac{1}{2}$ and (3.7) implies that $k(L) \sim L^{-2}$, which agrees nicely with the exact results on this system.

4. SELF-AVOIDING WALKS IN A HALF-SPACE

In this section we review some results on the problem of self-avoiding walk on a D-dimensional hypercubic lattice confined to a half-space defined by a $(D - 1)$-dimensional hyperplane containing either one or both of its vertices of unit degree. That is, we consider the set of self-avoiding walks, $C_n^{(1)}$, with $x_i \geqslant 0\ \forall i$ and $\mathbf{z}_0 = \mathbf{0}$, and the subset $C_n^{(1,1)}$ of $C_n^{(1)}$, with the additional constraint that $x_n = 0$. We write $c_n^{(1)}$ and $c_n^{(1,1)}$ for the cardinalities of these sets. If C_n is the set of n-step self-avoiding walks with $\mathbf{z}_0 = \mathbf{0}$, with cardinality c_n then

$$c_n^{(1,1)} \leqslant c_n^{(1)} \leqslant c_n \tag{4.1}$$

The main rigorous result[10] on these quantities is that

$$\lim_{n\to\infty} n^{-1}\log c_n^{(1,1)} = \lim_{n\to\infty} n^{-1}\log c_n^{(1)} = \lim_{n\to\infty} n^{-1}\log c_n = k \tag{4.2}$$

This follows quite readily from a result due to Hammersley[11] that the number (p_n) of *directed, unrooted* polygons, weakly embeddable in a lattice satisfies the equation

$$\sup_{n>0} n^{-1}\log p_n = \lim_{n\to\infty} n^{-1}\log p_n = \lim_{n\to\infty} n^{-1}\log c_n \tag{4.3}$$

To establish (4.2) we need a relationship between p_n and $c_n^{(1,1)}$. Consider a particular n-step polygon with vertices $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_n$ and let the coordinates of $\mathbf{A}_j$ be $(x_j, \ldots, y_j)$. Define

$$x_{\min} = \min_{1\leqslant j\leqslant n} x_j \tag{4.4}$$

and let q be the smallest value of j such that $x_j = x_{\min}$. Translate the polygon so that $(x_q, \ldots, y_q)$ becomes $(0, \ldots, y_q)$. Then $x_j \geqslant 0\ \forall j$. We now consider three cases:

(i) $x_{q-1} = x_{q+1} = 0$
(ii) $x_{q-1} = 0, \quad x_{q+1} = 1$
(iii) $x_{q-1} = 1, \quad x_{q+1} = 0$, where j is interpreted modulo n

No other possibilities exist. For cases (i) and (ii) delete the edge $\mathbf{A}_{q-1} - \mathbf{A}_q$ and for case (iii) delete the edge $\mathbf{A}_q - \mathbf{A}_{q+1}$. In each case the resulting graph is a member of $C_{n-1}^{(1,1)}$ and this graph is uniquely determined by the polygon from which it is generated. Hence

$$p_{n+1} \leqslant c_n^{(1,1)} \tag{4.5}$$

Because the structure of the hypercubic lattice $p_n \neq 0$ only for n even so that the above construction works for this case. Hence (4.5) has been proved for n odd. One can construct an analogous argument for n even (showing that $p_n \leqslant c_{n+2}^{(1,1)}$). Then (4.1), (4.3), and (4.5) imply (4.2).

If one is interested only in $c_n^{(1)}$, it is possible to prove the existence of the limit (in 4.2) and its equality to k without using Hammersley's result on polygons, but making use of an unfolding transformation, applying successive reflections to only one end of the walk.

By arguments which are an extension of those used above, Ishinabe and Whittington[12] have shown that

$$\sup_{n>0} n^{-1}\log c_n^{(1,1)} = \lim_{n\to\infty} n^{-1}\log c_n^{(1,1)} \tag{4.6}$$

For $c_n^{(1)}$, the direction from which the limit is approached has not been established rigorously.

The subdominant asymptotic behavior has not been established rigorously but there is strong numerical evidence suggesting that

$$c_n \sim n^{\gamma-1}e^{nk} \tag{4.7}$$

$$c_n^{(1)} \sim n^{\gamma_1-1}e^{nk} \tag{4.8}$$

$$c_n^{(1,1)} \sim n^{\gamma_{11}-1}e^{nk} \tag{4.9}$$

The exponents γ_1 and γ_{11} appear in at least one theory of polymer adsorption[13] and in the $N\to 0$ limit of the N-vector model of surface magnetism.[14] From (4.6) and (4.9) we obtain $\gamma_{11} \leqslant 1$, and Middlemiss and Whittington[15] have shown that

$$\gamma_1 \leqslant \tfrac{1}{2}(\gamma+1) \tag{4.10}$$

The exact values of γ_1 and γ_{11} are certainly of interest, for instance as a test of surface scaling theory,[16] which predicts that

$$2\gamma_1 = \gamma_{11} + \gamma + \nu \tag{4.11}$$

where ν is the exponent characterizing the divergence of the length of a self-avoiding walk.

5. DISCUSSION

The two basic techniques which have been used to establish rigorously that limits analogous to (1.3) exist are (i) geomentrical arguments leading to concatenations, followed by results on the theory of super or submultiplicative functions,[1,17,18] and (ii) "squeezing" the set of interest between two sets known to have the same limiting behavior. Essentially all the results on existence of limits for *confined* self-avoiding walks (as well as graphs with other given topologies,[19] lattice animals,[20,21] etc.) have been obtained by variants of one of these approaches.

It is much more difficult to obtain rigorous results on the subdominant asymptotic behavior. A rigorous proof of (1.2) would be a major step forward and would probably lead to the establishment of corresponding subdominant behavior for a variety of related problems. To obtain results on critical exponents characterizing the subdominant asymptotic behavior, currently one is obliged to use nonrigorous arguments such as the scaling methods mentioned in Section 4.

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