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Surface critical exponents for self-avoiding walks on the tetrahedral lattice

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Abstract. Series analysis techniques are used to form estimates of the local (γ_{11}) and layer exponents (γ_1) for self-avoiding walks on the tetrahedral lattice, confined to a half space. The estimates are compared with predictions of surface scaling and with a renormalisation group calculation of Bray and Moore. In addition, a new upper bound on γ_{11} is derived for the self-avoiding walk problem.

1. Introduction

Self-avoiding walks terminally attached to a surface, and confined to lie in or on one side of this surface, have received a good deal of attention because of their importance in the theory of polymer adsorption (Silberberg 1967). Their relationship to critical phenomena in systems with a free surface (de Gennes 1976, Barber *et al* 1978) means both that their properties can be predicted using standard techniques from theory of critical phenomena and also that they can be used as tests of the applicability of these theories to the polymer version of the problem.

Define $c_n^{(1)}$ as the number of n-step self-avoiding walks, weakly embeddable in a lattice, which originate in the plane $z=0$ and have all vertices with non-negative z-coordinate. Let $c_n^{(1,1)}$ be the number of these which also have their last vertex in the plane $z=0$. The only rigorous result on the behaviour of these quantities seems to be that

$$\lim_{n\to\infty} n^{-1} \lg c_n^{(1)} = \lim_{n\to\infty} n^{-1} \lg c_n^{(1,1)} = \lg \mu \tag{1.1}$$

where μ is the 'effective coordination number' of the lattice, i.e. the exponential of the connective constant (Whittington 1975). If we define the generating functions

$$\chi_1(x) = 1 + \sum_{n>0} c_n^{(1)} x^n \tag{1.2}$$

and

$$\chi_{11}(x) = 1 + \sum_{n>0} c_n^{(1,1)} x^n \tag{1.3}$$

then (1.1) implies that $\chi_1(x)$ and $\chi_{11}(x)$ will both diverge at $x = \mu^{-1}$. The behaviour

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close to this singularity is not known but, by analogy with other critical phenomena problems, one would expect that for x close to μ^{-1}

$$\chi_1(x) \sim A_1(1-\mu x)^{-\gamma_1} \tag{1.4}$$

and

$$\chi_{11}(x) \sim A_{11}(1-\mu x)^{-\gamma_{11}}. \tag{1.5}$$

Accepting these assumed functional forms, one can attempt to relate the critical exponents γ_1 and γ_{11} to bulk exponents. Without any additional assumptions, one can show (Whittington 1975, Middlemiss and Whittington 1976) that

$$\alpha - 1 \leqslant \gamma_{11} \leqslant \gamma_1 \leqslant \tfrac{1}{2}(1+\gamma) \tag{1.6}$$

where α and γ are the usual bulk exponents for polygons and walks (see e.g. Guttmann and Whittington (1978) for definitions). In § 2 we show that

$$\gamma_{11} \leqslant 1, \tag{1.7}$$

which is an improvement on (1.6), but this collection of bounds is still not very stringent.

In order to make further progress, additional assumptions are necessary, and perhaps the most interesting predictions come from surface scaling (Barber 1973). This theory predicts that γ_1 and γ_{11} are not independent, but are related to one another and to the bulk exponents γ and ν (the correlation length exponent) through

$$2\gamma_1 = \gamma_{11} + \gamma + \nu. \tag{1.8}$$

Bray and Moore (1977) have argued for a second scaling relation

$$\gamma_{11} = \nu - 1 \tag{1.9}$$

and (1.8) and (1.9) would then imply that these surface exponents can each be expressed in terms of bulk exponents.

For the two-dimensional Ising problem (1.9) is exact (McCoy and Wu 1973) and (1.8) is strongly supported by numerical evidence (Enting and Guttmann 1980). Numerical results on the three-dimensional Ising problem (Whittington *et al* 1979) are also consistent with the value of γ_1 obtained from (1.8) and (1.9).

For the self-avoiding walk problem there have been a number of attempts to estimate γ_1 from series analysis work (Lax 1974, Mark *et al* 1975, Middlemiss and Whittington 1976, Ma *et al* 1977, Barber *et al* 1978). The estimate $\gamma_1 = 0{\cdot}70 \pm 0{\cdot}02$ has been given for the cubic lattice (Barber *et al* 1978), and these error bars would include the central estimates of γ_1 on all other three-dimensional lattices studied. This just includes the scaling prediction. Again for the cubic lattice, γ_{11} has been estimated as $-0{\cdot}35 \pm 0{\cdot}05$, which also just includes the scaling prediction. In two dimensions equation (1.8) appears to agree well with the series data, but there is a clear disagreement between the value of γ_{11} given by (1.9) and the result from series analysis (Barber *et al* 1978).

In this paper we present some further exact enumeration data in an attempt to refine the estimates of γ_1 and γ_{11} in three dimensions. Our experience of estimating the exponent characterising the divergence of the lengths of terminally attached self-avoiding walks led us to concentrate on lattices of low coordination number for which a relatively long series could be derived (Guttmann *et al* 1978). The obvious choice is then the tetrahedral lattice which has, indeed, been examined several times before (e.g. Lax 1974, Middlemiss and Whittington 1976). However, there is a choice available as to which plane is chosen as the surface plane defining the half space. The previous series work chose one such that only alternate vertices of the walk could lie in this surface, which has the disadvantage that alternate members of the sequence $c_n^{(1,1)}$ are zero. To avoid this, we have chosen the surface plane so that the walk can lie entirely in this plane (in a zig-zag or 'all trans' configuration). As far as we are aware, no other exact enumeration work has been carried out for this orientation, although it has been studied by Monte Carlo methods (Clark and Lal 1978).

2. Upper bound on γ_{11}

Let C_n be the set of n-step self-avoiding walks on a d-dimensional hypercubic lattice (with lattice points being the integer points in E^d) and let c_n be the cardinality of C_n. The coordinates of the ith vertex of the walk are $(x_{1i}, x_{2i}, \ldots, x_{di})$ and $x_{10} = x_{20} = \ldots = x_{d0} = 0$. Let A_n be the subset of C_n such that $x_{1n} = 0$, $x_{1j} > 0$, $j = 1, 2, \ldots, n-1$, with cardinality a_n, and let B_n be the subset of C_n such that $x_{1j} > 0\ \forall j > 0$ and $x_{1j} < x_{1n}\ \forall j < n$, with cardinality b_n.

We first note that

$$c_n^{(1,1)} = a_{n+2}. \tag{2.1}$$

Each walk in A_{n+2} has exactly two vertices in the hyperplane $x_{10} = 0$, and these two vertices are of unit degree. By deleting these two vertices and the edges emanating from them, we form an n-step walk starting and ending in the hyperplane $x_{10} = 1$ and having $x_{1j} \geq 1\ \forall j$. Similarly each n-step walk with $x_{10} = x_{1n} = 1$, $x_{1j} \geq 1\ \forall j$ can be converted into a walk in A_{n+2} by adding two edges joining its unit degree vertices to the plane $x_{10} = 0$. (Notice that (2.1) will not be true for *all* lattices but that there will be a lattice-dependent constant, θ, such that $a_{n+2} = \theta c_n^{(1,1)}$.)

For a particular walk in A_n with vertices at $\{x_{1i}, x_{2i}, \ldots, x_{di}; i = 0, 1, \ldots, n\}$ define

$$x_1^{(\mathrm{m})} = \max_j x_{1j} \tag{2.2}$$

and

$$j^{(\mathrm{m})} = \max\{j | x_{1j} = x_1^{(\mathrm{m})}\}. \tag{2.3}$$

Now construct the vertex set with coordinates $\{y_{1i}, y_{2i}, \ldots, y_{di}; i = 0, 1, \ldots, n\}$ given by

$$\begin{aligned} y_{kj} &= x_{kj} \qquad \forall k \neq 1 \quad \text{and} \quad \forall j \\ y_{1j} &= x_{1j} \qquad \forall j \leq j^{(\mathrm{m})} \\ y_{1j} &= x_1^{(\mathrm{m})} + (x_1^{(\mathrm{m})} - x_{1j}) \qquad \forall j > j^{(\mathrm{m})}. \end{aligned} \tag{2.4}$$

This is the vertex set of a walk in B_n since

(i) it is self-avoiding (since the first j steps are self-avoiding, the last $(n-j)$ steps are self-avoiding, all vertices up to and including the jth have $x_{1k} \leq x_1^{(\mathrm{m})}$ and all vertices after the jth have $x_{1k} > x_1^{(\mathrm{m})}$), and

(ii) $x_{10} = 0$, $x_{1n} = 2x_1^{(\mathrm{m})}$, $0 < x_{1j} < 2x_1^{\mathrm{m}}$, $\forall j \neq 0, n$.

Moreover, these walks are distinct members of B_n and this construction therefore defines an injection from $A_n \to B_n$. Hence

$$a_n \leq b_n. \tag{2.5}$$

Now consider an n-step walk $W_n \in B_n$ and an m-step walk $W_m \in B_m$. These walks can be concatenated by translating W_m so that its first vertex coincides with the last vertex of W_n. The resulting graph is a self-avoiding walk and is a member of B_{n+m} and, by concatenating each $W_n \in B_n$ with each $W_m \in B_m$ in turn, the resulting members of B_{n+m} are distinct. However, not all members of B_{n+m} are obtained in this way (since all such walks will have their first n steps on one side of a plane and their last m steps on the other side of this plane). Hence b_n is a supermultiplicative function

$$b_n b_m \leqslant b_{n+m}. \tag{2.6}$$

Since $B_n \subset C_n$, $b_n^{1/n}$ is bounded above and hence (Hille 1948)

$$\sup_{m>0} m^{-1} \lg b_m = \lim_{m\to\infty} m^{-1} \lg b_m < \infty. \tag{2.7}$$

In addition we can identify the value of the limit, since

$$a_n \leqslant b_n \leqslant c_n \tag{2.8}$$

and Whittington (1975) has shown that

$$\lim_{n\to\infty} n^{-1} \lg a_n = \lim_{n\to\infty} n^{-1} \lg c_n \equiv \lg \mu. \tag{2.9}$$

Hence, as $n \to \infty$, $b_n^{1/n} \to \mu$ *from below*. Then (2.5) implies that $a_n^{1/n} \to \mu$ from below and from (1.3), (1.5) and (2.1) we then obtain

$$\gamma_{11} \leqslant 1. \tag{2.10}$$

3. Series analysis for the tetrahedral lattice

We have obtained the first nineteen terms in the $c_n^{(1)}$ series and the first twenty terms in the $c_n^{(1,1)}$ series, and the results are given in table 1. The analysis of the series followed standard lines (see e.g. Gaunt and Guttmann (1974)) and we shall give only a brief account here. We have relied largely on ratio methods with associated Neville tables, and ratios of fourth successive coefficients seem to give most satisfactory convergence for this lattice (Guttmann *et al* 1978). We have therefore formed the ratio estimates

$$\gamma_1(n) = 1 + \tfrac{1}{4}n\{c_n^{(1)}/c_{n-4}^{(1)}\mu^4 - 1\} \tag{3.1}$$

and the linear and quadratic extrapolants

$$\gamma_1^{(r)}(n) = (n\gamma_1^{(r-1)}(n) - (n-4r)\gamma_1^{(r-1)}(n-4))/4r \tag{3.2}$$

for $r = 1$ and 2, with $\gamma_1^{(0)}(n) \equiv \gamma_1(n)$. The behaviour of these extrapolants is shown in figure 1. The value of μ used in these calculations was $\mu = 2{\cdot}8785$ (Watts 1975).

The use of fourth successive coefficients reduces the influence of the expected singularity in χ_1 at $x = -\mu^{-1}$ and also any singularities on the imaginary axis near to $x = \pm i\mu^{-1}$. An alternative approach is to use an Euler transformation such as

$$z = 2x/(1+\mu x) \tag{3.3}$$

which moves the singularity at $-\mu^{-1}$ to infinity and any singularities at $\pm i\mu^{-1}$ to $\mu^{-1}(1 \pm i)$, which are then outside the circle of convergence, though still close to it.

Table 1. Coefficients in the expansion of χ_1 and χ_{11} for self-avoiding walks on the tetrahedral lattice.

n	$c_n^{(1)}$	$c_n^{(1,1)}$
1	3	2
2	7	2
3	19	4
4	53	12
5	147	30
6	401	60
7	1 123	154
8	3 137	404
9	8 793	1 046
10	24 599	2 540
11	69 287	6 720
12	194 967	17 484
13	550 361	46 522
14	1 552 645	120 300
15	4 393 021	323 800
16	12 425 121	856 032
17	35 213 027	2 315 578
18	99 771 855	6 151 080
19	283 162 701	16 745 530
20	—	44 921 984

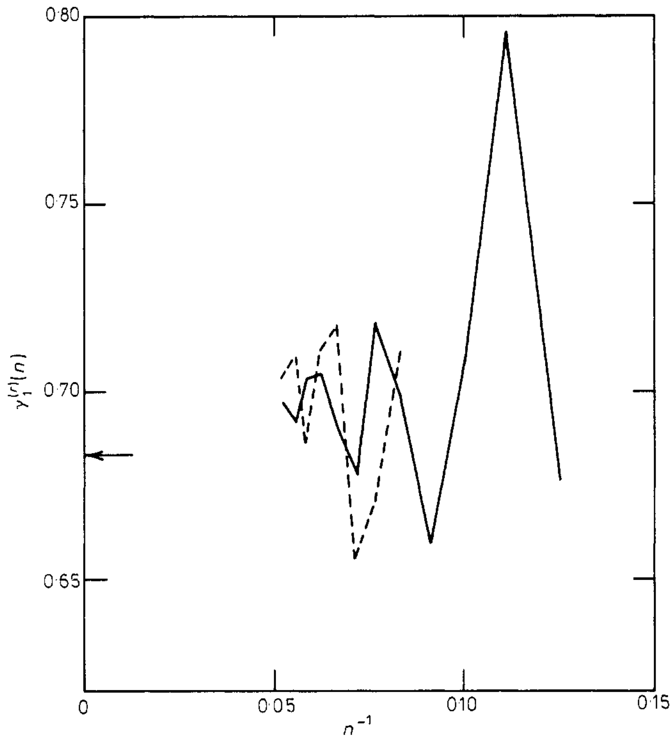

Figure 1. Ratio estimates of γ_1 from fourth successive terms in series: —— $\gamma_1^{(1)}(n)$, the linear extrapolants; - - - $\gamma_1^{(2)}(n)$, the quadratic extrapolants.

Writing

$$\chi_1(z) = \sum b_n^{(1)} z^n, \qquad (3.4)$$

we have also formed ratio estimates using *successive* terms in the sequence $\{b_n^{(1)}\}$ and corresponding linear and quadratic extrapolants. These results are shown in figure 2.

The data in figure 1 suggest that γ_1 is very close to, though possibly just below, 0·7. However, it is more difficult to know how to interpret the trend in figure 2. The Euler transformation seems to have replaced the odd–even alternation by a wave but it is difficult to know if this behaviour will continue. The minimum in the quadratic extrapolant is at about 0·68 while the maximum in the linear extrapolant is at about 0·72, and we believe that it is most unlikely that the value of γ_1 could lie outside this range. In view of this we take as our final estimate

$$\gamma_1 = 0{\cdot}70 \pm 0{\cdot}02 \qquad (3.5)$$

which is identical to the estimate for the cubic lattice (Barber *et al* 1978).

The estimation of γ_{11} is even more difficult since it is small and negative. In table 2 we give some terms in the appropriate Neville table for extrapolating ratio estimates of $\gamma_{11}(n)$ corresponding to the definitions of $\gamma_1(n)$ in equations (3.1) and (3.2). Corresponding results for the estimates from successive ratios of terms in the Euler transformed series are given in table 3.

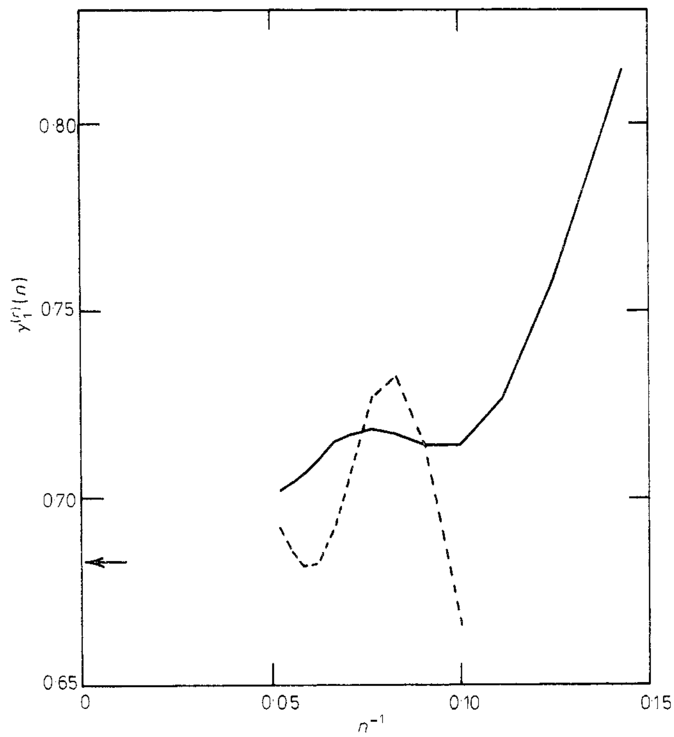

Figure 2. Ratio estimates from successive terms in Euler-transformed series: —— linear extrapolants; – – – quadratic extrapolants.

Table 2. Neville table for estimation of γ_{11} from ratios of fourth successive terms in series expansion.

n	$\gamma_{11}(n)$	$\gamma_{11}^{(1)}(n)$	$\gamma_{11}^{(2)}(n)$
10	0·041 55	−0·129 33	—
11	−0·002 11	−0·410 69	—
12	−0·108 90	−0·288 22	−0·629 02
13	−0·144 55	−0·228 35	−0·202 11
14	−0·085 46	−0·402 98	−0·608 22
15	−0·118 07	−0·436 96	−0·459 95
16	−0·147 38	−0·262 82	−0·237 42
17	−0·168 76	−0·247 43	−0·268 90
18	−0·148 55	−0·369 37	−0·327 36
19	−0·171 91	−0·373 81	−0·286 98
20	−0·178 15	−0·301 22	−0·358 82

Table 3. Neville table for estimation of γ_{11} from ratios of adjacent terms in Euler-transformed series.

n	$\gamma_{11}(n)$	$\gamma_{11}^{(1)}(n)$	$\gamma_{11}^{(2)}(n)$
10	0·145 63	−0·453 20	−1·084 36
11	0·091 28	−0·452 30	−0·448 27
12	0·052 79	−0·370 58	0·038 01
13	0·027 05	−0·281 77	0·206 68
14	0·008 79	−0·228 65	0·090 07
15	−0·006 48	−0·220 21	−0·165 32
16	−0·021 30	−0·243 66	−0·407 85
17	−0·036 51	−0·279 75	−0·550 39
18	−0·051 88	−0·313 19	−0·580 72
19	−0·066 86	−0·336 49	−0·534 53
20	−0·080 95	−0·348 68	−0·458 41

The $\gamma_{11}^{(1)}(n)$ estimates in table 2 show a residual odd–even alternation with a superimposed period-four oscillation. Bearing this in mind, it seems likely that γ_{11} will lie between $\gamma_{11}^{(1)}(19)$ and $\gamma_{11}^{(1)}(17)$. The Euler transformed data has an associated wave which makes table 3 difficult to extrapolate. It is possible that the downward trend in the last few values of $\gamma_{11}^{(1)}(n)$ in table 3 is about to be reversed (compare the reversal at $\gamma_{11}^{(1)}(15)$), but we cannot be sure that the trend will not continue. For this reason we rely largely on table 2 and suggest

$$\gamma_{11} = -0{\cdot}35 \pm 0{\cdot}05.$$

4. Discussion

The bound derived in § 2, $\gamma_{11} \leq 1$, while not a very serious numerical improvement on the previous best bound, $\gamma_{11} \leq \frac{1}{2}(1+\gamma)$, has the advantage that it does not rely on an estimated value for γ. In addition it determines the *direction* from which the limit of $\{c_n^{(1,1)}\}^{1/n}$ is approached.

The numerical data in § 3 confirm our previous estimates (Barber *et al* 1978) for the corresponding exponents on the cubic lattice. The predictions of Bray and Moore (1977) (shown by an arrow in figures 1 and 2) are just on the limits of the estimated uncertainties in our estimates.

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