Tests of a scaling theory for self avoiding walks close to a surface

K. De'Bell, N. Jan

J. Phys. France **50** (1989) 769-773 1er AVRIL **1989,** PAGE 769

Classification
Physics Abstracts
05.50

Tests of a scaling theory for self avoiding walks close to a surface

K. De'Bell (1) and N. Jan (2)

(1) Department of Physics, Dalhousie University Halifax, Nova Scotia, Canada B3H 3J5
(2) Department of Physics, Saint Francis Xavier University Antigonish, Nova Scotia, Canada B2G 1C0

(*Reçu le 18 juillet 1988, accepté sous forme définitive le 2 décembre 1988*)

Résumé. — Nous vérifions directement par des techniques de Monte Carlo la loi de puissance qui détermine la variation du nombre de chemins sans intersections en fonction de la distance à la surface du vertex initial. Cette analyse donne à trois dimensions des contraintes très précises sur les valeurs ν de l'exposant de corrélation et Δ de l'exposant de corrections aux lois d'échelles.

Abstract. — The power law which determines the variation in critical amplitude with distance from the surface for self avoiding walks with an initial vertex close to a surface, is tested directly by Monte Carlo techniques. In three dimensions this provides a sensitive consistency check of the correction-to-scaling exponent Δ and the correlation length exponent ν.

1. Introduction.

Self avoiding walks (SAWs) in which the initial vertex lies in the surface of a semi-infinite lattice have been studied in detail, both by Monte Carlo [1] and series expansion analysis [2, 3]. The critical behaviour of SAWs in which the initial vertex is at some distance z from the lattice surface has not, however, (to the best of our knowledge) been studied by numerical methods directly. In particular, if z is small compared with the end to end distance of the walks but large compared with the lattice spacing (taken here to be unity), scaling theory predicts [4]

$$G(p, z) = \sum C_n(z) p^n \sim (p_c - p)^{-\gamma_1} z^{\theta} \tag{1.1}$$

where $C_n(z)$ is the number of self avoiding walks of n steps with initial vertex at a point distance z from the surface. θ may be expressed in terms of conventional bulk and surface critical exponents as

$$\theta = \frac{\gamma - \gamma_1}{\nu}. \tag{1.2}$$

For our present purposes, it is convenient to write the scaling prediction for the variation in the critical amplitude with z as

$$C_n(z) \sim z^{\theta} \mu^n n^{\gamma_1 - 1} \quad (\mu = 1/p_c) \tag{1.3}$$

where (1.3) is expected to be valid in the limit $n \to \infty$. In order to eliminate the n dependence, we consider the ratios

$$C_n(z)/C_n(0) \sim z^{\theta} \tag{1.4a}$$

and

$$C_n(z)/C_n(z-1) \sim [z/(z-1)]^{\theta} . \tag{1.4b}$$

Although we extrapolate these ratios to large n using the correction-to-scaling analysis described below, a remaining difficulty is that equation (1.4) are valid only when z is large compared with the lattice spacing but small compared with the end to end distance of the chains. As a result, we find noticeable deviations from these forms at both small z and « large » (~ 30) z. The range of fit analysis used to overcome these difficulties is described in detail in 2.1.

2. Monte Carlo simulation and analysis.

2.1 THE SQUARE LATTICE SYSTEM. — For the square lattice we have considered walks of length $n = 80$, 100, 200 and 1 000 and, using the wiggle (or pivot) method [5, 6], 200 000, 200 000, 91 000 and 18 100 SAW configurations, respectively, were generated. The number of these configurations allowed if the initial vertex was at a point distance z from the surface was recorded for $0 < z < 30$. The ratios required in (1.4) were then formed for each available value of z and n. Since the forms (1.4) are valid only in the limit $n \to \infty$, we replace (1.4a) by

$$C_n(z)/C_n(0) \sim z^{\theta}(1 + Bn^{-\Delta}) . \tag{2.1}$$

From a previous study of bulk SAWs [7], we expect the effective value of $\Delta = 1$. Using this

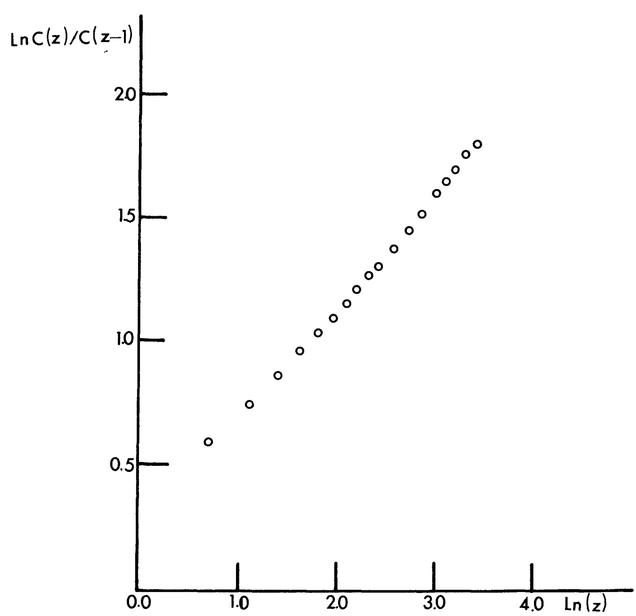

Fig. 1. — ln $(C(z)/C(0))$ *vs.* ln (z) for the square lattice. Deviations from the linear form predicted by scaling theory (1.4) are clearly present at both small and large values of z.

value of Δ in 2.1, we extrapolate the required ratio for each z to the limit $n \to \infty$. The corresponding extrapolation for the ratio in (1.4b) was also performed.

If (1.4a) is valid, a log-log plot of $C_n(z)/C_n(0)$ should be linear. The plot shown in figure 1 clearly deviates from this linear form both at small z and at large z (~ 30). As discussed in the introduction, these deviations from the expected scaling form are a reflection of the restricted range of z in which the scaling form is valid.

To avoid the deviation from scaling at large z, we have restricted our analysis to values of $z \leqq 20$. For data points with $z \leqq 20$, we perform a range of fit test assuming a linear form for $\log [C_n(z)/C_n(0)]$ *vs.* $\log [z]$, in which data points at the smallest values of z are successively removed (Tab. I). We find that the last few entries in table I from this analysis are stable with no significant (relative to the least squares standard error) tendency to higher or lower values. Based on this analysis, we estimate

$$\theta = 0.515 \pm 0.004 .$$

The estimated error given here is based on one standard error in the least squares fit. A similar analysis based on equation (1.4b) gives a value of θ consistent with this, but with larger error bars. Changing the range of z considered to $z \leqq 19$ or $z \leqq 21$ does not significantly (relative to the least squares standard error) change the estimate of θ.

Table I. — *Range of fit analysis for SAWs with initial vertex at distance $z \leqslant 20$ from the surface.*

Number of points	θ ($d = 2$)	θ ($d = 3$)
10	0.500	0.833
9	0.506	0.831
8	0.511	0.828
7	0.516	0.821
6	0.514	0.818
5	0.515	0.819

2.2 THE SIMPLE CUBIC LATTICE SYSTEM. — For the simple cubic lattice, we considered walks of 120, 200, 300 and 1 000 steps and generated 200 000, 73 500, 200 000 and 18 600 configurations, respectively. The ratios required in equations (1.4) were again extrapolated to the $n \to \infty$ limit using a correction-to-scaling analysis as described in 2.1.

The method described in reference [7] was applied to the three dimensional (bulk) walks generated, to determine the effective value of Δ. A difficulty with this method in three dimensions is that the value of the leading exponent ν is not known exactly. The method cannot distinguish between a leading exponent of $\nu = 0.590$, 0.591 and 0.592, but slightly favours $\nu = 0.591$; consequently, we list the corresponding values of Δ in table II. This range of values for ν is consistent with previous studies. However, studies based on both series expansion analysis and Monte Carlo studies result in a central estimate of $\nu = 0.592$ [6, 8, 9], which is slightly higher than the estimate $\nu = 0.5885 \pm 0.0025$ based on the $n \to 0$ limit of R.G. expansion [10].

Initially, adopting a value of $\nu = 0.592$, the analysis described in section 2.1 was repeated for the three dimensional walks. A log-log plot of $C_n(z)/C_n(0)$ *vs.* z again shows a significant deviation form linearity at both small and large values of z. The range of fit analysis described in 2.1 was repeated for this data (Tab. I). Using values of $z \leqq 20$ leads to an estimate of

$$\theta = 0.819 \pm 0.004 .$$

Again changing the values of z used to $z \leqq 19$ or $z \leqq 21$ does not significantly alter the estimate, and a similar analysis based on equation (1.4b) gives a consistent central value but with a much larger standard error. By further decreasing the values of z used to $z \leqq 17$, it is possible, in this case, to obtain central estimates which are somewhat higher (≈ 0.836). However, the standard error is also increased (≈ 0.008), and the stability of the last few entries in the range of fit analysis table is decreased.

The procedure was then repeated, assuming values of $\nu = 0.590$ and 0.591. The resulting estimates of θ based on data points with $z \leqq 20$ and use of equation (1.4a) are quoted in table II.

Table II. — *Estimates of the effective correction to scaling exponent Δ and surface scaling exponent θ for given values of the correlation length exponent ν. The predicted values of θ are obtained from equation* (1.3) *and the estimates of γ and γ_1 given in references* [3, 8]. *(Note the predicted values are not strongly affected by the small changes in ν.)*

ν	Δ	θ	θ (predicted)
0.590	0.52	0.941 ± 0.004	0.82 ± 0.02
0.591	0.60	0.880 ± 0.004	0.82 ± 0.02
0.592	0.71	0.819 ± 0.004	0.82 ± 0.02

3. Summary.

The Monte Carlo simulations described in section 2 are consistent with the scaling laws (1.4) for values of z (the distance of the initial vertex from the surface) large compared with the lattice spacing, but small compared with the end to end distance. In practice, this restriction on the value of z severely limits the number of z values which may be used to determine the exponent θ (1.3).

In two dimensions we estimate

$$\theta = 0.515 \pm 0.004 .$$

For SAWs in two dimensions conformal invariance, theory predicts [10]

$$\gamma = 43/32 \quad \gamma_1 = 61/64 \quad \nu = 3/4$$

and substituting these into (1.2)

$$\theta = 25/48 = 0.5208 .$$

This value lies just outside the error bars of our estimate. However, these error bars represent only the standard error in the least squares fit and make no allowance for systematic errors due to the restricted values of z which may be used. In view of this, we do not believe that this small discrepancy is significant.

In three dimensions, based on $\nu = 0.591 \pm 0.001$ and the corresponding Δ of 0.6 ± 0.1 we would conclude that $\theta = 0.880 \pm 0.065$. The values of γ, γ_1 and ν obtained by series expansion methods [3, 8] may be substituted into (1.3) to obtain a prediction for θ. This is compared with our estimates based on assumed values of Δ (and hence assumed values of ν), in table II. Clearly there is excellent agreement if $\Delta = 0.71$ is adopted, while, if Δ is lowered to 0.60 the value of θ is inconsistent with the series result of 0.82.

Thus if we insist on consistency with the series expansion for the value of θ we find agreement with the recently reported value of ν with the corresponding correction-to-scaling exponent, Δ of 0.71. If the series value for θ in three dimensions is of the same order of accuracy as in two dimensions and is also in keeping with expected accuracy from series analysis in general then our data provides a rather sensitive test of Δ indicating that a value of 0.6 or less can be ruled out.

Acknowledgments.

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada.

References

[1] EISENRIEGLER E., KREMER K. and BINDER K., *J. Chem. Phys.* **77** (1982) 6296.
[2] LOOKMAN T. and DE'BELL K., *J. Phys. A* **20** (1987) 763.
[3] GUTTMANN A. J. and TORRIE G. M., *J. Phys. A* **17** (1984) 3539.
[4] BINDER K., Phase Transitions and Critical Phenomena, Vol. 8, Eds. C. Domb and J. L. Lebowitz (Pub. Academic Press 1983).
[5] MAC DONALD B., JAN N., HUNTER D. L. and STEINITZ M. O., *J. Phys. A* **18** (1985) 2627 ;
MOTI LAL, *Mol. Phys.* **17** (1969) 57.
STELLMAN S. D. and GANS P. J., *Macromolecules* **5** (1972) 516.
STELLMAN S. D. and GANS P. J., *Macromolecules* **5** (1972) 720.
[6] MADRAS N. and SOKAL A. D., *J. Stat. Phys.* **50** (1988) 109.
[7] HUNTER D. L., JAN N. and MAC DONALD B., *J. Phys. A* (1986) L543.
[8] GUTTMANN A. J., *J. Phys. A* **20** (1987) 1839.
[9] RAPPORT D. C., *J. Phys. A* **18** (1985) 113.
[10] LE GUILLOU J. C. and ZINN-JUSTIN J., *J. Phys. Lett. France* **46** (1985) L-137.
[11] CARDY J. L., Phase Transitions and Critical Phenomena, Vol. 11, Eds. C. Domb and J. L. Lebowtiz (Pub. Academic Press) 1987, and references therein ;
DUPLANTIER B. and SALEW H., *Phys. Rev. Lett.* **57** (1986) 3179 ; for predictions of θ for all star vertices with any number of arms near a surface.