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LETTER TO THE EDITOR

New method of analysing self-avoiding walks in four dimensions

S Havlin and D Ben-Avraham

Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

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Abstract. A new method based on the concept of fractal dimensionality is used to study the problem of self-avoiding walks in a four-dimensional lattice. We find from Monte Carlo simulations that the confluent logarithmic exponent related to the end-to-end distance is $\frac{1}{8} \pm 0.01$, in excellent agreement with the prediction derived from the $n \to 0$ vector model.

The solution for the problem of self-avoiding walks (SAW) on a four-dimensional lattice is known through the analogy with the $n = 0$ limit of the ferromagnet vector model (Larkin and Khmelnitskii 1969, Brézin *et al* 1976, de Gennes 1979). Consider for example the theoretical prediction for the correlation length ξ of this model

$$\xi \sim t^{-1/2} |\ln t|^{1/8} \qquad (d = 4) \tag{1}$$

where t is the reduced temperature $t = (T - T_c)/T_c$. In the SAW problem, t is analogous to $1/N_0$ (N_0 being the total number of steps) and ξ is analogous to the end-to-end distance $\langle R_{N_0}^2 \rangle^{1/2}$ (de Gennes 1979), so that

$$\langle R_{N_0}^2 \rangle^{1/2} \sim N_0^{1/2} (\ln N_0)^{1/8} \qquad (d = 4). \tag{2}$$

The logarithmic corrections to scaling laws are of great interest. Series expansions have been performed in order to obtain these corrections for the susceptibility of the $n \to 0$ ferromagnet in $d = 4$ (Domb 1974, Guttmann 1978, McKenzie and Gaunt 1980). However, these methods do not always give good results for the confluent logarithmic exponent (Guttmann and Reeve 1980). Moreover, attempts to obtain logarithmic corrections by Monte Carlo methods have not thus far been successful (Kremer *et al* 1981). Following the ideas of Mandelbrot (1977) about fractal dimensionality, we define for SAWs the concept of local fractal dimensionality (LFD)

$$D(N) = \ln\left(\frac{N+1}{N}\right) \Big/ \ln\left(\frac{\langle R_{N+1}^2 \rangle_{N_0}}{\langle R_N^2 \rangle_{N_0}}\right)^{1/2} \tag{3}$$

where $\langle R_N^2 \rangle_{N_0}$ is the mean square distance of two points separated by N steps in a SAW of N_0 steps. The LFD, $D(N)$, is a measure of how winding is the walk on a length scale corresponding to N. We have discussed elsewhere the physical meaning and the usefulness of this parameter (Havlin and Ben-Avraham 1982). In the present work, we use LFD for SAWs in $d = 4$ in order to analyse the logarithmic corrections to scaling using Monte Carlo simulations. The method provides very precise results for the confluent logarithmic exponent given in (2).

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We may generalise (2) to include intrachain distances by writing

$$\langle R_N^2\rangle_{N_0}^{1/2} \sim N^{1/2}(\ln N)^{1/8}. \qquad (4)$$

Using (3) and (4), we obtain the following prediction for LFD for SAWs in the $d=4$ case

$$D(N) = (\tfrac{1}{2} + 1/8 \ln N)^{-1}. \qquad (5)$$

Equation (5) was investigated numerically for an ensemble of SAWs on a four-dimensional hypercubic lattice. The ensemble consists of 6000 SAWs with $N_0 = 320$. It was generated by the enrichment technique (Wall *et al* 1963) with $p=5$ and $s=80$. In figure 1, we present the numerical results, together with the theoretical curve given by (5). From these results, we conclude that the confluent logarithmic exponent is $\frac{1}{8} \pm 0.01$. This value is in excellent agreement with theory. The accuracy of the present method compares favourably with that obtained using series expansion calculations on other confluent logarithmic exponents (Guttmann 1978, McKenzie 1979).

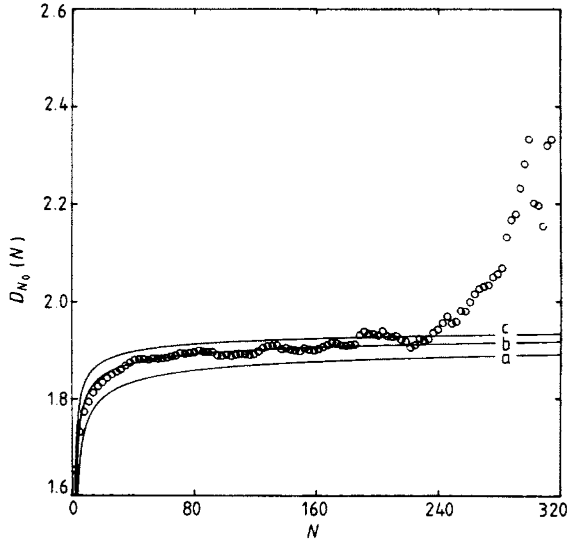

Figure 1. Plot of $D(N)$ as a function of N for 6000 SAWs with $N_0 = 320$ in $d=4$. The circles represent numerical data. The full lines are the theoretical predictions of equation (5) using $\frac{1}{6}$, $\frac{1}{8}$, $\frac{1}{10}$ for the confluent logarithmic exponent in a, b and c, respectively

The generalisation of (2) to intrachain distances is by no means obvious. Consider the case with d lower than 4. In figure 2, we present plots of D as a function of $x = N/N_0$ for $N_0 = 80$, 160, 320 of SAWs traced on a square lattice ($d=2$). It can be seen that the LFD is a function of x but is virtually independent of N_0. For most of the range, the LFD is nearly constant. Its value equals $1/\nu$, where ν is the end-to-end exponent defined by

$$\langle R_{N_0}^2\rangle^{1/2} \sim N_0^{\nu}, \qquad d=2. \qquad (6)$$

These results can be explained if we extend (6) to

$$\langle R_N^2\rangle_{N_0}^{1/2} \sim N^{\nu}\rho(N/N_0). \qquad (7)$$

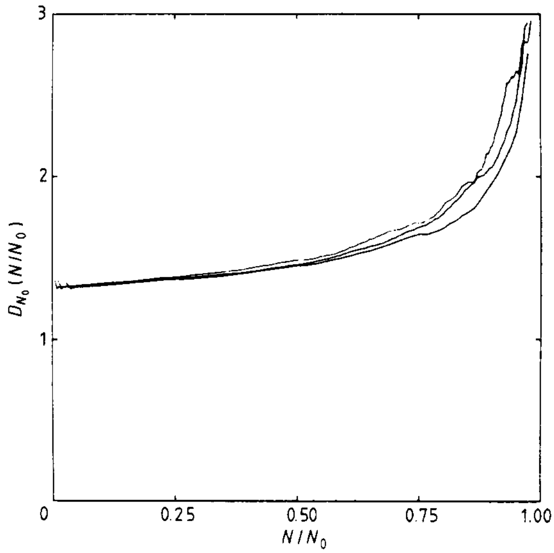

Figure 2. Plot of $D(N)$ as a function of $x = N/N_0$ for 10 000 SAWs with $N_0 = 80$, 160, 320 in $d = 2$ dimensions.

Then, using the definition (3), we obtain

$$D(N) = (\nu + x\rho'(x)/\rho(x))^{-1}, \tag{8}$$

which shows that D is indeed a function of x.

The function $\rho(x)$ is a universal shaping function (for each dimension d). For $x \sim 0$, the value of $\rho(x)$ appears to be nearly constant, whereas $\rho(x)$ decreases slightly near $x \sim 1$ (Havlin and Ben-Avraham 1982). This property of $\rho(x)$ explains why $D = 1/\nu$ over a wide range of x.

In view of the above discussion, it is reasonable to extend (2) in analogy to (7) for $d = 4$

$$\langle R_N^2 \rangle_{N_0}^{1/2} \sim N^{1/2} (\ln N)^{1/8} \rho(N/N_0), \qquad d = 4. \tag{9}$$

Then, using (3), we obtain

$$D(N) = \left(\frac{1}{2} + \frac{1}{8 \ln N} + x\frac{\rho'(x)}{\rho(x)}\right)^{-1}, \qquad x = \frac{N}{N_0}, \qquad d = 4. \tag{10}$$

We see that in this case D is no longer a universal function of x as was the case for $d < 4$, but rather, it also depends on N_0 because of the logarithmic term. It is in this sense that the logarithmic term is a correction to scaling. It can be shown that the corrections for $d = 4$ indeed arise from the logarithm and not from the universal shape function $\rho(x)$. In figure 3, we display plots of D as a function of x for chains of length $N_0 = 40$, 80, 160, 320. The fact that D differs for the different values of N_0 indicates that we indeed measure the logarithmic term (compare with $d = 2$ in figure 2). As to the contribution arising from the shaping functions $\rho(x)$, it is expected to be minor for most values of x. Indeed, for the case $d = 2$ (figure 2), this contribution is negligible over quite a wide range of x, and for $d = 3$, the contribution of $\rho(x)$ is still smaller (Havlin and Ben-Avraham 1982). Therefore, there is reason to believe that for the present case of $d = 4$, the contribution of $\rho(x)$ will have very little effect on D.

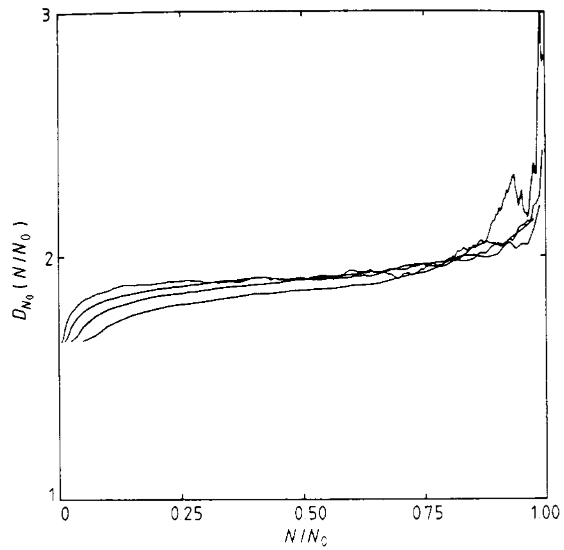

Figure 3. Plot of $D(N)$ as a function of $x = N/N_0$ for 10 000 SAWs with $N_0 = 40$, 80, 160, 320 in $d = 4$ dimensions. The upper curves refer to larger values of N_0.

However, the effect of $\rho(x)$ is important in the vicinity of $x \approx 1$, the end-to-end range (figures 1 and 3). Then, in order to obtain the confluent logarithmic exponent, we made a best fit only up to $x = \frac{1}{2}$.

To summarise, we find that the LFD provides a very useful method for studying SAWs in four-dimensional lattices. The method is very sensitive for determining the confluent logarithmic exponent. It is surprising that the effects of the logarithmic corrections to scaling show even for relatively small values of N.

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