Corrections to scaling in self-avoiding walks

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Corrections to scaling, as well as the critical exponent ν , are calculated for self-avoiding walks, with the use of a new highly accurate method based on fractal dimensionality. Numerical results are obtained for 2, 3, 4, and 5 dimensions and are shown to be in excellent agreement with the prediction of the n=0 vector model.

The analogy between self-avoiding walks (SAW's) and critical phenomena through the n=0 vector model¹⁻³ has provided the motivation for extensive investigation of their statistical properties.^{1,4,5} Special effort has been devoted^{6,7} to obtaining the critical exponent ν which is related to the mean-square end-to-end distance. However, there is still no consensus⁶ on the value of ν , and the situation is even worse regarding the corrections to scaling.⁷

In this paper, we present a method for finding the value of the critical exponent ν , as well as its scaling corrections. The method is based on the concept of fractal dimensionality, ⁸ as recently applied ⁹ to polymer chains.

The critical exponent ν for SAW's is related to the end-to-end distance $\langle R_{N_0}^2 \rangle$ through

$$\langle R_{N_0}^2 \rangle^{1/2} \simeq A N_0^{\nu} \quad , \tag{1}$$

where N_0 is the total number of steps. A reasonable assumption is that (1) can be extended to internal distances through the scaling relation

$$(\langle R_N^2 \rangle_{N_0})^{1/2} \simeq N^{\nu} \rho(x), \quad x = N/N_0 ,$$
 (2)

where $\langle R_N^2 \rangle_{N_0}$ is the mean-square distance of all intrachains consisting of N steps in a SAW having a total of N_0 steps.

In order to justify this assumption, we used the concept of local fractal dimensionality (LFD), defined according to the ideas presented by Mandelbrot, 8 as

$$D_{N_0}(N) = \frac{\ln[(N+1)/N]}{\ln(\langle R_{N+1}^2 \rangle_{N_0} / \langle R_N^2 \rangle_{N_0})^{1/2}}$$

$$\simeq \frac{\partial \ln N}{\partial \ln(\langle R_N^2 \rangle_{N_0})^{1/2}} . \tag{3}$$

Applying this definition to (2) yields

$$D_{N_0}(N) = \left[\nu + x \frac{d \ln \rho(x)}{dx} \right]^{-1} . \tag{4}$$

Accordingly, $D_{N_0}(N)$ should scale for SAW's with

different N_0 . Indeed, measurements of SAW's, computer simulated by the Monte Carlo enrichment technique, ¹⁰ traced in a square (d=2) lattice, seem to confirm the scaling assumptions (2) and (4). In Fig. 1, we plot LFD for sets of SAW's with different N_0 as a function of x. It appears from the figure that $D_{N_0}(N)$ is a function of x alone, and results for different N_0 fall on the same curve.

It is also seen from Fig. 1 that for quite a wide range of x, LFD is nearly constant. The value of LFD in this range is defined as the fractal dimensionality (FD) of the SAW's. The FD is a measure of how winding is the walk on most scales of length. Moreover, the mere existence of FD shows that the chain possesses a statistical internal self-similarity.

We now consider a more accurate analysis of LFD by means of more refined measurements of LFD of SAW's traced on two-, three-, four-, and five-dimensional lattices. These more accurate calculations clearly exhibit deviations from scaling. We find that these deviations can be explained by the same

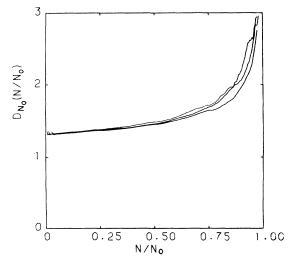


FIG. 1. Plot of $D_{N_0}(N)$ as a function of $x = N/N_0$ for 10 000 SAW's with $N_0 = 80$, 160, and 320 in d = 2 dimensions.

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argument which lead to (2). It is known that there are corrections^{11,12} to the mean-square end-to-end distance law (1) through the analogy with the n=0 vector model. The corrected expression¹³ has the form

$$\langle R_{N_0}^2 \rangle^{1/2} \simeq A N_0^r (1 + b N_0^{-\Delta})$$
 (5)

The generalization of this equation to internal distances yields¹⁴

$$(\langle R_N^2 \rangle_{N_0})^{1/2} \simeq N^{\nu} (1 + bN^{-\Delta}) \rho(x), \quad x = N/N_0 .$$
 (6)

Using the definition of LFD, we obtain

$$[D_{N_0}(N)]^{-1} = \nu - \frac{b\Delta}{N^{\Delta} + b} + x \frac{d \ln \rho(x)}{dx} . \tag{7}$$

The first two terms are in complete analogy with the effective critical exponent $\lambda_{i, \text{ eff}}$ in Ref. 12 when b is neglected compared to N^{Δ} . The last term in (7) stems from the fact that we consider finite SAW's $(N_0 \text{ finite})$. Indeed, for finite N, this term vanishes when $N_0 \rightarrow \infty$ [note that $\rho(x \rightarrow 0)$ must be finite]. Moreover, for $N_0 \rightarrow \infty$ and a finite N >> 1, the second term also vanishes and we regain the fractal dimensionality of the SAW.

The fact that the second term in (7) does not scale with N_0 , whereas the third term does, simplifies the analysis of numerical data. We seek first for the best values of b and Δ such that $[D_{N_0}(N)]^{-1} + b\Delta/(N^{\Delta} + b)$ converges to the scaling function $\nu + xd \ln \rho(x)/dx \equiv f(x)$. Then, extrapolating f(x) to $x \to 0$ gives the value for ν . This kind of analysis yields $\nu = 0.753 \pm 0.004$, $\Delta = 1.2 \pm 0.1$ for SAW's on a square (d = 2) lattice and $\nu = 0.588 \pm 0.003$, $\Delta = 0.50 \pm 0.05$ for SAW's on a simple cubic (d = 3)

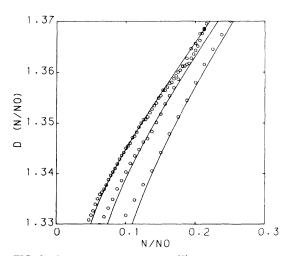


FIG. 2. Comparison between Eq. (7) and numerical data for 10 000 SAW's traced on a two-dimensional lattice, using ν , b, and Δ from Table I, for $N_0=80$, 160, and 320. The circles represent the numerical data.

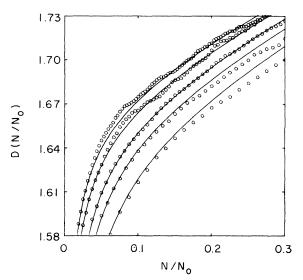


FIG. 3. Comparison between Eq. (7) and numerical data for 10 000 SAW's traced on a three-dimensional cubic lattice, using ν , b, and Δ from Table I, for $N_0 = 80$, 120, 160, 240, and 320.

lattice. Figures 2 and 3 show the excellent agreement between (7) using these numerical values and the numerical data obtained from simulations for d=2 and 3, respectively. In Fig. 4, we plot LFD as obtained from (7) for SAW's in d=3 using different values for ν . The figure shows the high sensitivity obtained in the determination of ν .

For the SAW problem d=4 is the critical dimension¹ and corrections to scaling are logarithmic. From the analogy with the n=0 vector model, ^{15, 16}

$$(\langle R_N^2 \rangle_{N_0})^{1/2} \propto N^{1/2} [\ln(aN)^{1/8}] \rho(x)$$
 (8)

We analyzed, recently, 17 numerical data for SAW's in

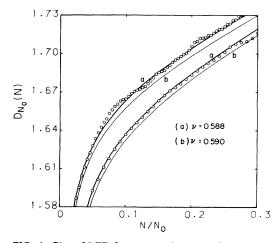


FIG. 4. Plot of LFD from numerical data, for SAW's $(N_0=120, 240)$ traced on a simple-cubic lattice, and b and Δ from Table I but (a) $\nu=0.588$ and (b) $\nu=0.590$.

TABLE I. Numerical results and theoretical predictions for the critical exponent ν and the corrections to scaling parameters for different lattice dimensionalities.

d	ν (numerical)	ν (theory)	Δ (numerical)	Δ (theory)	b (numerical)
2	0.753 ± 0.004	0.75a	1.2 ± 0.1	1.2 ^b	-0.08 ± 0.03
3	0.588 ± 0.003	0.588 ± 0.001^{b}	0.5 ± 0.05	0.47 ± 0.03^{b}	-0.16 ± 0.04
4	0.500 ± 0.002	0.5 ^c	0.123 ± 0.012	$\frac{1}{8}^{c}$	

^aExact result of B. Nienhuis, Phys. Rev. Lett. 49, 1062 (1982).

a four-dimensional hypercubic lattice, assuming a=1, and thus found for the confluent logarithmic exponent $\Delta=0.125\pm0.010$. Working on further data and not assuming anything about a, we have found $a=1.1\pm0.3$ and $\Delta=0.123\pm0.012$. In Table I, we give the numerical results and make comparison to theoretical predictions for the critical exponent ν and the parameters of the corrections b and Δ , for SAW's traced on hypercubic lattices with d=2, 3, and 4. The agreement between our numerical estimates and those of the n=0 vector model is evident from this table.

0.8 N(Z/I-1-10) 0.4

FIG. 5. Plot of $(D^{-1} - \frac{1}{2})N$ against \sqrt{N} for 10 000 SAW's $(N_0 = 240)$ traced on a five-dimensional hypercubic lattice.

For dimensionalities $d \ge 4$, the SAW problem is solved by mean-field methods (through the n = 0 vector model analogy). For d = 5 it is found¹⁸ that

$$D(N)^{-1} = \frac{1}{2} + \frac{b_1}{\sqrt{N}} + \frac{b_2}{N} , \qquad (9)$$

where the effect of $\rho(x)$ is neglected.¹⁹ In order to check Eq. (9) we plotted (Fig. 5) $(D^{-1} - \frac{1}{2})N$ against \sqrt{N} . A linear relation is found as expected, with $b_1 = 0.077 \pm 0.002$, $b_2 = 0.079 \pm 0.003$. In Fig. 6 we show the excellent agreement obtained between Eq. (9) with the above values of b_1 and b_2 , and the nu-

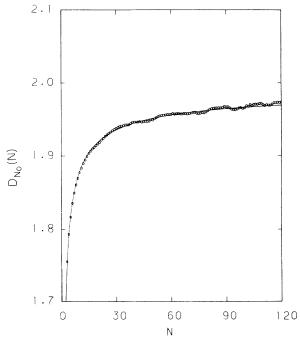


FIG. 6. Comparison between Eq. (9) and numerical data for 10 000 SAW's ($N_0 = 240$) traced on a five-dimensional hypercubic lattice.

bFrom Ref. 11.

^cReferences 15 and 16. The parameter a is estimated numerically (best fit), $a = 1.1 \pm 0.3$.

merical data. It should be noted that there was no need to use the enrichment technique method in the five-dimensional case, and this is since the attrition of samples is very small.

To summarize, we have presented a very accurate method²⁰ for obtaining the critical exponent ν and its corrections to scaling in SAW's. The numerical results presented in Table I are in excellent agreement with theoretical predictions of the n=0 vector model, confirming the analogy between this model and SAW's. We note that $\rho(x)$ seems to have a smaller effect on LFD for higher lattice dimensionalities d, whereas the corrections to scaling increase with d. The universality of the correction parameters

b and Δ for different lattices remains to be checked. Finally, we suggest that a similar kind of analysis may be applied to percolation and spin systems (i.e., Ising ferromagnet) to obtain corrections to scaling.

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thus contributing to an analytical correction to scaling in Eq. (7). For Δ close to 1, it is difficult to separate between this analytical correction and $N^{-\Delta}$.

¹⁴It can be argued that Eq. (6) should be

$$(\langle R_N^2\rangle_{N_0})^{1/2}\!\approx\!N^{\nu}\rho_0(x)+bN^{\nu-\Delta}\rho_2(x)~;$$

however, choosing $\rho_1(x) \neq \rho_0(x)$ yields a second-order correction [in contrast to Δ in Eq. (7) which gives a first-order correction] and may be ignored.

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¹³More generally, in Eq. (5) we should have $N_0 + C$ rather than N_0 . However, C should be small compared to N_0 ,

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¹⁹The effect of $\rho(x)$ becomes smaller as the dimensionality d increases. See also Ref. 17.

²⁰The accuracy of the proposed method is due to the use of all internal intrachain distances of each chain [Eq. (2)], thus increasing the statistics significantly.