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 model[1–3] 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 consensus[6] 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

$$\langle R_{N_0}^2\rangle^{1/2} \simeq A N_0^{\nu} \ , \qquad (1)$$

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

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

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[9] (LFD), defined according to the ideas presented by Mandelbrot,[8] as

$$D_{N_0}(N) = \frac{\ln[(N+1)/N]}{\ln(\langle R_{N+1}^2\rangle_{N_0}/\langle R_N^2\rangle_{N_0})^{1/2}} \simeq \frac{\partial \ln N}{\partial \ln(\langle R_N^2\rangle_{N_0})^{1/2}} \ . \qquad (3)$$

Applying this definition to (2) yields

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

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

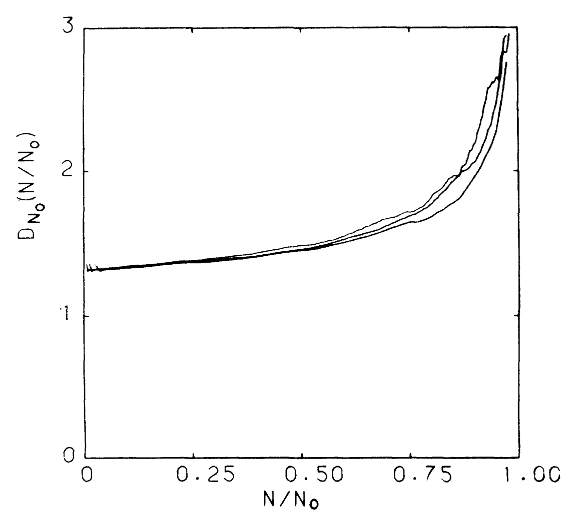

FIG. 1. Plot of $D_{N_0}(N)$ as a function of $x=N/N_0$ for 10000 SAW's with $N_0=80$, 160, and 320 in $d=2$ dimensions.

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 expression[13] has the form

$$\langle R_{N_0}^2\rangle^{1/2} \simeq A N_0^{\nu}(1+bN_0^{-\Delta}) \; . \tag{5}$$

The generalization of this equation to internal distances yields[14]

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

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 $\lambda_{i,\mathrm{eff}}$ 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 finite). Indeed, for finite N, this term vanishes when $N_0 \to \infty$ [note that $\rho(x\to 0)$ must be finite]. Moreover, for $N_0 \to \infty$ and a finite $N \gg 1$, 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 $\nu + x d\ln\rho(x)/dx \equiv f(x)$. 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 ($d=3$) 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 dimension[1] and corrections to scaling are logarithmic. From the analogy with the $n=0$ vector model,[15,16]

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

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

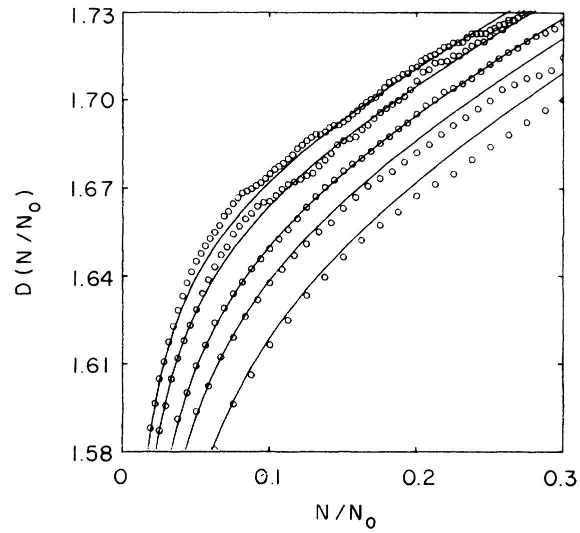

FIG. 3. Comparison between Eq. (7) and numerical data for 10 000 SAW's traced on a three-dimensional cubic lattice, using ν, b, and Δ from Table I, for $N_0 = 80$, 120, 160, 240, and 320.

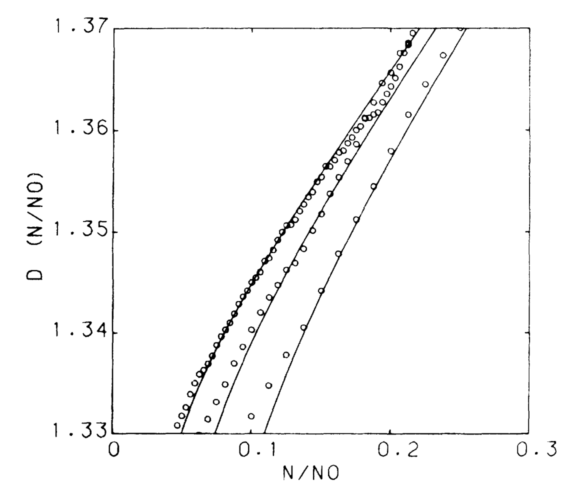

FIG. 2. Comparison between Eq. (7) and numerical data for 10 000 SAW's traced on a two-dimensional lattice, using ν, b, and Δ from Table I, for $N_0 = 80$, 160, and 320. The circles represent the numerical data.

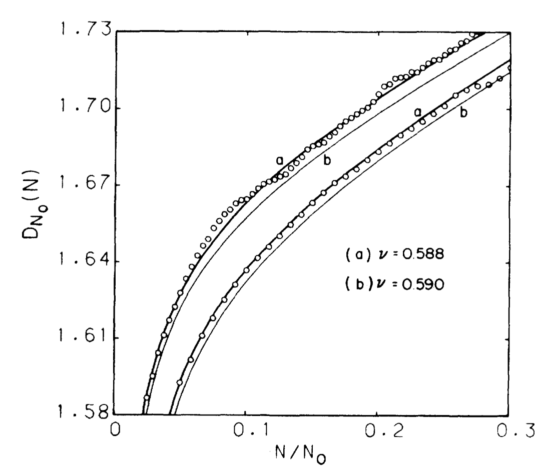

FIG. 4. Plot of LFD from numerical data, for SAW's ($N_0 = 120$, 240) traced on a simple-cubic lattice, and b and Δ from Table I but (a) $\nu = 0.588$ and (b) $\nu = 0.590$.

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	0.75[a]	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]	. . .

[a]Exact result of B. Nienhuis, Phys. Rev. Lett. 49, 1062 (1982).
[b]From Ref. 11.
[c]References 15 and 16. The parameter a is estimated numerically (best fit), $a = 1.1 \pm 0.3$.

a four-dimensional hypercubic lattice, assuming $a = 1$, and thus found for the confluent logarithmic exponent $\Delta = 0.125 \pm 0.010$. Working on further data and not assuming anything about a, we have found $a = 1.1 \pm 0.3$ and $\Delta = 0.123 \pm 0.012$. 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.

For dimensionalities $d \geq 4$, the SAW problem is solved by mean-field methods (through the $n = 0$ vector model analogy). For $d = 5$ it is found[18] 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-

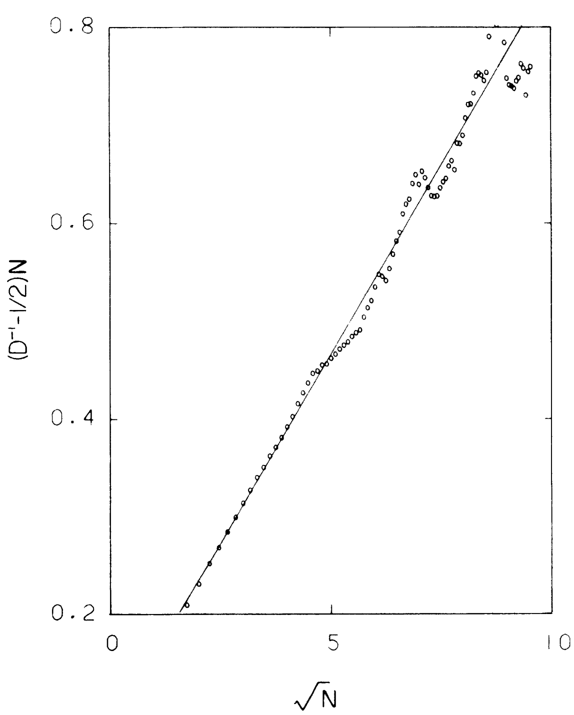

FIG. 5. Plot of $(D^{-1} - \frac{1}{2})N$ against $\sqrt{N}$ for 10 000 SAW's ($N_0 = 240$) traced on a five-dimensional hypercubic lattice.

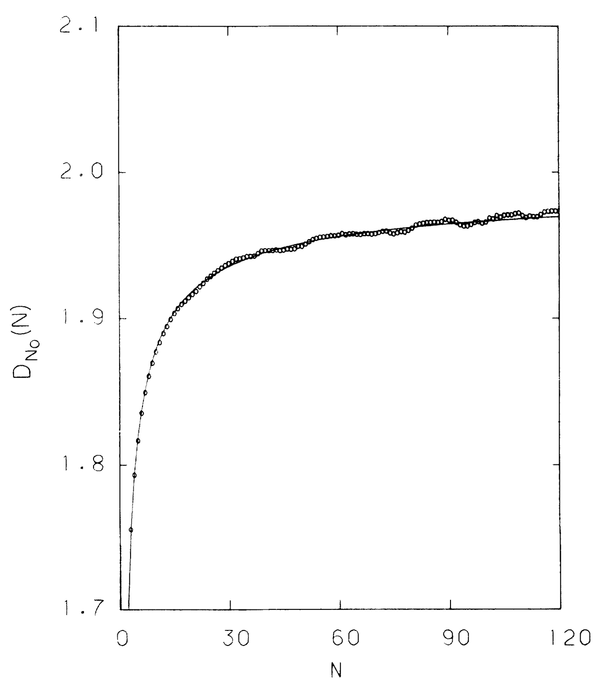

FIG. 6. Comparison between Eq. (9) and numerical data for 10 000 SAW's ($N_0 = 240$) traced on a five-dimensional hypercubic lattice.

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 method[20] 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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[13]More generally, in Eq. (5) we should have N_0+C rather than N_0. However, C should be small compared to N_0, 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 $N^{-\Delta}$.

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

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

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

[20]The 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.