Correction to scaling for the self-avoiding walk in $d = 2$: Results based on a cell renormalization group

C. M. Chaves and R. Riera
Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro, Caixa Postal 38071, 22452-970 Rio de Janeiro RJ, Brazil
(Received 18 May 1993)

We propose a cell renormalization group for self-avoiding walks (SAW's) in the square lattice based on a new center rule. The results for large cells are obtained by simulation. We calculate the effective fractal dimension $d_f(b)$ for SAW's in cells of size b ($3 \leq b \leq 22$) at criticallity. Small deviations of $d_f(b)$ from the asymptotic value indicate a correction-to-scaling exponent $\Delta = 1$.

Since a few decades ago, many cluster-growth models have been proposed to describe aggregates formed by irreversible kinetic process. Among these, the self-avoiding walk (SAW) is a prototype describing a polymerization process[1] in which excluded volume effects play an essential role.

The main parameter used to describe the scaling properties of the walks is their fractal dimension, defined for sufficiently large walks by $N \sim \langle R \rangle^{d_f}$, where N is the number of steps and $\langle R \rangle$ is the root mean square of the end-to-end distance of the walk. Alternatively, the exponent $\nu = 1/d_f$ is also used.

Using a kind of mean-field argument, Flory, and then Fisher, suggested that $d_f \equiv d_F = \frac{d+2}{3}$ in d dimensions, from which we expect that $d_F = \frac{4}{3} \simeq 1.334$ in $d = 2$. (The basic arguments are reproduced in Ref. 1.)

Later, Nienhuis,[2] using analytical arguments, conjectured that the above result is exact in $d = 2$. (It is not exact in $d = 3$, as de Gennes[3] has demonstrated.)

Many Monte Carlo (MC) simulations[4–7] and position-space renormalization groups[8–10] (PSRG's) have reproduced with great or less accuracy Flory's value in $d = 2$. Some of these methods, however, rely on extrapolation of results for relatively small walks or cells. Because the convergence is rather slow, the question naturally arises about correction to scaling, which is characterized by the leading exponent Δ given by

$$\langle R \rangle^2 \simeq N^{2\nu}(1 + BN^{-\Delta} + \cdots). \tag{1}$$

The value of Δ is still an open question. Nienhuis[2] suggests that $\Delta = 1.5$ while Le Guillou and Zinn-Justin,[12] using the renormalization group, found $\Delta \simeq 1.2$. The latter approach has been subject to some criticism for they also found $\nu = 0.77$, instead of the Flory's value $\nu_F = 0.75$.

Conformal invariance,[13] which often gives exact results in $d = 2$, does not solve completely polymer models. By studying the transfer matrix spectrum, Saleur[14] suggests $\Delta = \frac{11}{16} \approx 0.687$.

The exact enumeration of SAW's on two-dimensional lattices does not give satisfactory results for the exponent Δ. Guttmann,[15] using several series analysis methods, found no evidence of a universal nonanalytical ($\Delta \neq$ integer) correction, at least in the region $\Delta < 1$. For the square lattice, his data are consistent with $\Delta = 1$. For the honeycomb and triangular lattices he obtained $\Delta \approx 0.95$ and $\Delta \approx 0.84$, respectively, but $\Delta = 1$ could not be ruled out for both lattices. The value for the triangular lattice agrees with Wang's[16] result $\Delta = 0.85 \pm 0.05$ from a numerical analysis of an extended 20-term series and disagrees with other previous numerical analysis[17] that gives $\Delta \approx 0.66$ on the same lattice. These widely varying estimates of Δ may be due to the rather small length of the walks. It is not clear if the region of validity of (1), with only one correction term, was reached.

The same statement holds for the Monte Carlo study of Lyklema and Kremer,[4] who found $\Delta \simeq 0.84 \pm 0.04$ from simulations of SAW's on the square lattice up to length $N = 48$.

On the other hand, Rapaport,[5] using an improved MC technique that allowed generation of long walks (up to 2400 steps) on triangular and square lattices, argues that his data are best fitted by $\Delta = 1$. Hunter *et al.*[6] also investigated Eq. (1) for intermediate chain lengths on the square lattice and obtained the extrapolated value $\Delta = 1.0 \pm 0.1$.

These results are in accord with the more recent numerical analysis of Madras and Sokal,[7] which is based on the simulation of fairly large walks (N ranging from 200 to 10 000). Although they did not address specifically the question of correction to scaling, they arrive at values of ν in agreement with Flory's value, using implicitly $\Delta = 1$.

In the context of PSRG's the situation is still less clear.[8–11] This is due to the fact that the main versions of PSRG's proposed so far do not appear to have reached convergence.

The PSRG has been formulated using several rules (or weight functions) to specify the condition of traversing the cell, such as the corner rule of de Queiroz and Chaves,[8] the edge-center rule of Redner and Reynolds,[9] or the center rule of Chao.[10]

In this paper we present a PSRG that allows us to find *monotonic* values of critical exponents and parameters as the cell size varies.

We define a $n_b \times n_b$ cell in a square lattice as made by n_b vertical and n_b horizontal lines [see Fig. 1(a)]. We further choose n_b odd so that the geometrical center of

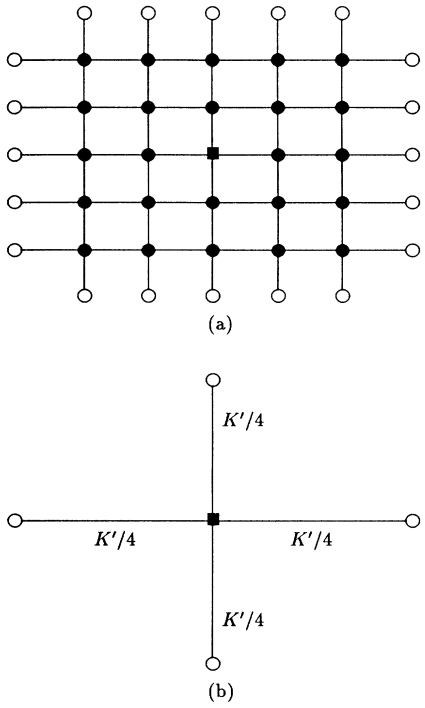

FIG. 1. (a) An $n_b \times n_b$ cell in a square lattice is defined by n_b vertical and n_b horizontal lines. Here $n_b = 5$ and $b = 3$. Internal (external) sites are represented by black (open) dots. Site ■ is the center of the cell. (b) The renormalized cell.

the cell is a lattice site. Upon renormalization (cell-to-bond transformation) the cell is mapped into four bonds, as shown in Fig. 1(b). The rescaling factor is $b = \frac{n_b+1}{2}$.

In order to take advantage of the symmetry of the lattice we do not use the corner rule:[8] The walk starts in the central point of the cell (the origin) and is terminated whenever it reaches, for the first time, an external site or is surrounded by its own previous steps. Our weight function is obtained from the subset of those walks which span the length scale b from the origin in any direction, reaching any external site of the cell.

The advantage of our center-rule scheme is that due to the symmetry, the walk is allowed to twist inside the cell, starting in one quadrant and leaving the cell in another one. In contrast, previous prescriptions[8–10] only consider walks that traverse the cell along one given direction, introducing a bias in the weight function.

To each step is associated a fugacity K and a weight equal to the inverse of the number of allowed steps from a given site. For instance, the first step can be given in any four directions and has accordingly a weight of 1/4. A walk contributes with the product of weight and fugacities of each of its constituent steps. The renormalized fugacity K' is given by the sum of all possible n-step walks starting at the origin and reaching any external site:

$$K' = \sum_{n \geq b} d_n K^n. \tag{2}$$

The nontrivial point K^* of (2) defines the critical fugacity $K_c(b)$ and from it we get $\lambda(b) = \frac{dK'}{dK})_{K^*}$ and $d_f(b) = \ln\lambda / \ln b$. From their definitions, λ measures the average number of steps of the SAW's that span the length scale b at criticality [$\lambda = \langle N(b) \rangle$] and $d_f(b)$ is the effective fractal dimension of these walks at the same scale.

For $b = 2$ the recursion relation (2) can be worked out analytically, giving

$$K' = \frac{K^2}{3} + \frac{4K^3}{9} + \frac{2}{27} K^4 + \frac{4}{81} K^5 + \frac{2}{243} K^6 + \frac{4}{729} K^7 + \frac{2}{2187} K^8 + \frac{4}{6561} K^9. \tag{3}$$

The (nontrivial) fixed point of this relation is $K^* = 1.05$ and thus $d_f = 1.550$.

In order to find the coefficients d_n's in (2) for larger b, a simulation was developed. Let c_n be the probability that an allowed walk of n steps cross the cell from the origin to an external site. The c_n's can be found by generating a large number M_n of walks of n steps and by counting the fraction that crosses the cell.

Given that to reach an external site at the nth step the $n-1$ previous steps must not have left the cell and must not have ended because of the SAW constraint, we can write

$$d_n = c_n \prod_{m=1}^{n-1} [1 - (c_m + e_m)], \tag{4}$$

where e_m is the fraction of walks that ends at mth step due to the SAW constraint.

For $b = 2$ we reproduce Eq. (3) with great accuracy. For b in the range 17–22, a total number of walks as large as 5×10^8 was generated. Table I displays d_f for several values of b. Also shown is the fixed point $K^* \equiv K_c(b)$. Note from Table I that d_f is a monotonic function of b. This represents an improvement over previous treatments, but the convergence (in d_f) is still

TABLE I. Fractal dimension $d_f(b)$ and critical fugacity $K_c(b)$ for several values of the scaling parameter b.

b	$d_f(b)$	$K_c(b)$
3	1.507	1.0700
4	1.483	1.0830
5	1.466	1.0920
6	1.454	1.0990
7	1.445	1.1040
8	1.438	1.1070
9	1.432	1.1100
10	1.428	1.1142
11	1.422	1.1150
12	1.419	1.1170
13	1.413	1.1180
17	1.403	1.1226
18	1.400	1.1235
19	1.397	1.1242
20	1.394	1.1248
21	1.386	1.1253
22	1.384	1.1260

rather slow, an indication that we are not in the asymptotic regime; corrections to scaling are then expected to show up.

To obtain the extrapolated value $K_c(\infty)$, we assume the finite-size scaling form

$$K_c(b) = K_c(\infty) - Ab^{d_F}. \tag{5}$$

With the accepted value[18] of the connectivity $\mu = 2.638$ for the square lattice, we expect that $K_c(\infty) = \frac{3}{\mu} \simeq 1.137$ (note that there is a factor 3 relating the fugacity here and that of Ref. 8). In Fig. 2 we plot $K_c(b)$ against b^{-d_F} with Flory's value $d_F = 4/3$. It extrapolates to $K_c(\infty) = 1.134 \pm 0.004$ in good agreement with the value quoted above (here and throughout this paper, the quoted errors are those associated with linear regression).

We test the following form for $d_f(b)$ to leading order:

$$d_f(b) = d_f^{\infty} + B'b^{-\Delta'} + \cdots. \tag{6}$$

The data in Table I show a change of behavior around $\bar{b} \simeq 15$. For $b > \bar{b}$, law (6) is obeyed and a best fit gives $\Delta' = 1.31 \pm 0.16$. In Fig. 3 we plot $d_f(b)$ against $b^{\Delta'}$; it extrapolates to 1.336 ± 0.007, in good agreement with Flory's value.

Equation (6) states how the effective fractal dimension $d_f(b)$ of spanning SAW's scales with b. We now relate $\nu_{\text{eff}}(b) = [d_f(b)]^{-1}$ with the effective exponent $\nu_{\text{eff}}(N)$ of an N-step SAW. The latter is defined by

$$\langle R \rangle^2 \simeq N^{2\nu_{\text{eff}}(N)}. \tag{7}$$

Expression (7) describes how the mean square end-to-end distance grows locally with increasing N. The deviation of $\nu_{\text{eff}}(N)$ from the asymptotic exponent ν must depend on the correction-to-scaling exponent Δ in (1). Taking the logarithmic derivative of expressions (1) and

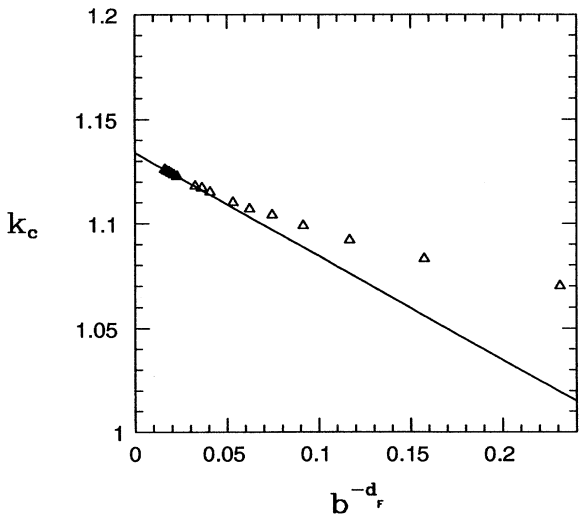

FIG. 2. Plot of $K_c(b)$ as given in Table I vs b^{-d_F}, with $d_F = 4/3$. For large enough b, a straight line is obtained, in agreement with finite-size scaling. It extrapolates to $K_c(\infty) = 1.134 \pm 0.004$.

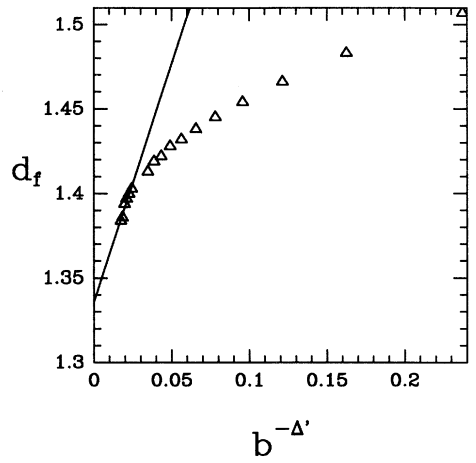

FIG. 3. Plot of $d_f(b)$ as given in Table I vs $b^{-\Delta'}$, with $\Delta' = 1.31$. For large enough b, a straight line that extrapolates to 1.336 ± 0.007 is obtained.

(7) with respect to N and identifying both, leads us to

$$\nu_{\text{eff}}(N) = \nu_F - \frac{\Delta B N^{-\Delta}}{2} + \cdots. \tag{8}$$

On the other hand, from (6), $[d_f(b)]^{-1}$ scales as

$$\nu_{\text{eff}}(b) = \nu_F - \nu_F B' b^{-\Delta'} \ldots \tag{9}$$

using $\nu_F \equiv (d_f^{\infty})^{-1}$ and $\nu_{\text{eff}}(b) = [d_f(b)]^{-1}$.

Identifying expressions (8) and (9) when N and b are related by $N \sim b^{d_f^{\infty}}$, we finally get

$$\Delta' = d_f^{\infty}\, \Delta. \tag{10}$$

Our numerical result is consistent with $\Delta' = d_f^{\infty} = d_F$, thus with $\Delta = 1$; i.e., the leading correction to scaling is analytic, in accord with Guttman[15] and with recent MC simulations.[5–7]

It should be stressed that $\Delta = 1$ is not incompatible with Nienhuis[2] or with Le Guillou and Zinn-Justin.[12] They were basically concerned with nonanalytical corrections coming from the nonanalytic part of the free energy. As they obtained $\Delta > 1$, an analytic correction-to-scaling exponent $\Delta = 1$, coming from the regular part of the free energy, would be the leading correction.

Regarding Saleur's[14] result from the transfer matrix method in connection with conformal invariance, again finite-size effects may explain why his Δ is so small.

In our PSRG, in contrast to others,[8–10] the walks always start at the center of the cell, so that no bias is introduced on the ensemble of contributing SAW's for the renormalized fugacity. For this reason, we were able to obtain the monotonic critical parameters $K_c(b)$ and critical exponent $d_f(b)$. From the analysis of their convergence it was possible to extract the leading correction to scaling. This was achieved using cells of intermediate size, that is, with spanning chains of intermediate length.

Another advantage of the RG technique is that it pro-

vides directly the effective exponent (9), while from MC simulations ν_{eff} is extracted from (1) for an ensemble of SAW's of steps N and N', where $N' - N = 1, 2, \ldots$ is arbitrarily chosen. In the PSRG, the contribution to (9) for each length scale b comes already from a set of chains with a length distribution having an average value $\lambda(b)$. That also explains why the analytical correction manifests in our data.

[1] P.G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, New York, 1979).
[2] B. Nienhuis, Phys. Rev. Lett. **49**, 1062 (1982).
[3] P.G. de Gennes, Phys. Lett. **38A**, 339 (1972).
[4] J. Lyklema and K. Kremer, Phys. Rev. B **31**, 3182 (1985).
[5] D.C. Rapaport, J. Phys. A **18**, L39 (1985).
[6] D.L. Hunter, N. Jan, and B. MacDonald, J. Phys. A **19**, L543 (1986).
[7] N. Madras and A. Sokal, J. Stat. Phys. **50**, 109 (1988).
[8] S.L.A de Queiroz and C.M Chaves, Z. Phys. B **40**, 99 (1980).
[9] S. Redner and P.J. Reynolds, J. Phys. A **14**, 2679 (1981).
[10] N.C. Chao, J. Phys. A **18**, 551 (1985).
[11] F. Lee and H.H. Chen, Int. J. Mod. Phys. B **5**, 3267 (1991).
[12] J. Le Guillou and J. Zinn-Justin, Phys. Rev. B **21**, 3976 (1980).
[13] J. Cardy, in *Phase Transitions and Critical Phenomena*, edited by C. Domby and J.L. Lebowitz (Academic, New York, 1987), Vol. 11.
[14] H. Saleur, J. Phys. A **20**, 455 (1987).
[15] A. Guttmann, J. Phys. A **17**, 455 (1984); **22**, 2807 (1989).
[16] J. Wang, J. Phys. A **22**, L969 (1989).
[17] Z.V. Djordjevic, I. Majid, H.E. Stanley, and R.J. dos Santos, J. Phys. A **16**, L519 (1983); V. Privman, Physica **123A**, 428 (1983).
[18] S. Caracciolo, A. Pelisseto, and A. Sokal, J. Phys. A **23**, 4509 (1990).