Journal of Statistical Physics, Vol. 41, Nos. 1/2, 1985

A New Monte Carlo Simulation for Two Models of Self-Avoiding Lattice Trees in Two Dimensions

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Received February 5, 1985; final May 2, 1985

By means of a new Monte Carlo sampling of a grand canonical ensemble, we verify universality for the critical exponents θ and ν of two models of lattice trees constrained to be self-avoiding on sites or on bonds. The attrition constants are also obtained. This algorithm, a generalization of that recently proposed by Berretti and Sokal for random walks, appears to optimize the critical slowing down in the scaling region. Systematic and statistical errors are carefully estimated.

KEY WORDS: Branched polymers; lattice animals; universality; dimensional reduction.

1. INTRODUCTION

The self-avoiding lattice trees have been considered in physics as models for branched polymers. The repulsive interaction between different polymes and of a polymer with itself is taken into account as an excluded-volume effect. The statistics of polymers is simplified in the limit of large dilution in a good solvent by neglecting the interaction among different polymers and by mimicking the excluded-volume by a self-avoiding constraint.

In the limit in which the dimension D goes to infinity, a mean-field theory, which does not account for the self-avoiding constraint, predicts a critical behavior different from that of random walks.

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0022-4715/85/1000-0095$04.50/0

822/41/1-2-7

In order to take into account fluctuations around the mean-field behavior, which are larger in lower dimensions, a field-theoretic formulation of the model has been introduced by Isaacson and Lubensky.[1] Their analysis shows that 8 is the upper critical dimension and allows to define an expansion in ε for $D = 8 - \varepsilon$ in which the same authors computed the first-order corrections to the critical exponents. They also suggest that the number of cycles is a noncritical quantity so that polymers with and without cycles should have the same exponents in any dimension. Moreover, it is expected that lattice animals belong to the same universality class.

Later, Parisi and Sourlas[2] succeded in establishing a connection between this universality class in D dimensions and the Lee–Yang edge singularity of the Ising model in $D-2$ dimensions. Such a relation allows to express both ν and θ for the branched polymer problem in terms of the critical exponent σ describing the singularity for the magnetization of the Ising model in an imaginary external field:

$$\theta(D) = \sigma(D-2) + 2$$
$$\nu(D) = \frac{\sigma(D-2)+1}{D-2} \tag{1.1}$$

The exponent σ is easily found to be $\sigma = -1$ in 0 dimensions, and $\sigma = -1/2$ in one dimension and (1.1) yields therefore the predictions $\theta = 1$ in two dimensions, and $\theta = 1.5$, $\nu = 0.5$ in three dimensions.

A lot of work has been devoted to estimate these critical exponents in two dimensions, via series analysis (exact-enumeration method), real-space renormalization group, Monte Carlo simulations, and finite-size scaling. In this paper we report estimates for the attrition constant μ and the critical exponents θ and ν for two models of self-avoiding lattice trees in two dimensions. These values were recovered from a new Monte Carlo algorithm sampling the trees in a grand canonical ensemble.

Several reasons led us to undertake such a computation. First, there does not seem to exist any Monte Carlo method which simulates ensembles of the kind that naturally appears in a field-theoretic formulation of the problem. Our algorithm grew out of an attempt to generalize the Monte Carlo method used by Aragão de Carvalho *et. al.*[3] to study the self-avoiding walk in four dimensions. This method allows transitions at any bond within the walk. But, having learned from Sokal[4] that more efficiency in the algorithm combined with a simplification of the programming is achieved by allowing transitions only at the end points of the walks, we decided to follow this suggestion for our simulation. Berretti and Sokal[5] have studied the self-avoiding random walk in two dimensions by

this method, putting great emphasis on how to properly determine systematic and statistical errors in order to obtain Monte Carlo results of at least the same reliability as other numerical techniques. See also the more recent Ref. 6 where Guttmann, Osborn and Sokal tested a conjectured relation between the attrition constants for self-avoiding random walks on the triangular and honeycomb lattices.

Second, we want to test if universality holds for these models and if one recovers the Parisi–Sourlas prediction for the exponent θ. Moreover, since (1.1) does not yield a value for ν in $D=2$, it is interesting to obtain additional information on it.

Third, our aim eventually is to simulate more complicated models, such as random surfaces. We believe that it is essential to gain experience about the efficiency of such simulations by studying comparatively simple models.

In Section 2 we define the models we are concerned with. A detailed description of the algorithm and the data structure is presented in Section 3. Results are collected and analyzed in Section 4. A comparison to previous works is given in Section 5 together with the main conclusions.

2. DEFINITION OF THE MODELS

In order to define the models let us introduce the notion of an *abstract tree*: it is a minimally connected graph, i.e., a collection of points $\{1,..., n\}$ together with an $(n \times n)$ incidence matrix I_{ij} (with elements $I_{i,j}=I_{j,i}=1$ if the points i and j are connected by a *link* and $I_{i,j}=I_{j,i}=0$ otherwise), such that by deleting any one of its nonzero entries the graph is no longer connected. For a given lattice L we define a *labeled lattice tree* as an immersion of an abstract tree into the lattice by means of a correspondence $i \mapsto s_i$ for $i \in \{1,..., n\}$ and $s_i \in L$ such that if $I_{ij}=1$ then s_i and s_j are nearest neighbors. Therefore every link (ij) of the graph must be an elementary bond b_{ij} of the lattice. The *sites* $\{s_i\}$ and *bonds* $\{b_{ij}\}$ are then said to be *occupied*. *(Unlabeled) lattices trees* are equivalence classes of labeled lattice trees with respect to permutations of the indices $i \in \{1,..., n\}$.

The physical effect of self-repulsion of polymers is taken into account as a self-avoiding constraint. We shall deal with (i) *site-self-avoiding lattice trees* (S-SALT) which are lattice imbeddings of abstract trees, i.e., lattice trees that occupy each site at most once; (ii) *bond-self-avoiding lattice trees* (B-SALT), which are lattice trees that occupy each bond at most once.

The S-SALT are often called branched polymers without cycles. Every S-SALT configuration defines a cluster of nearest neighbors sites, also called a site animal (SA). But the inverse is not true: for every SA there are in general many S-SALT which occupy the same sites.

The B-SALT *are not* the branched polymers with no restriction on the number of cycles. The latter are described in the literature as clusters of connected bonds or bond animals (BA). For us, connectedeness is defined on the abstract tree; in particular one knows the images of the end links (ij) of the abstract tree [i.e., of the links (ij) such that either $I_{ik}=0$ or $I_{jk}=0$ for every $k \neq i, j$] which is not always the case for the BA. Notice that, from the definition, it follows that a B-SALT is not an actual tree, it is only the image of an abstract tree. For this reason we shall be concerned for the B-SALT also with quantities like its number of cycles, which should be strictly zero for a tree.

We shall not consider as different ones trees with the same geometrical shape but different location on the lattice and, therefore, we will define a *configuration* $\tilde{T}$ as an equivalence class of SALT which can be mapped onto each other by lattice translations.

If $C_{N,\text{S-SALT}}$ and $C_{N,\text{SA}}$ are the numbers of different configurations with $N+1$ sites of S-SALT and of SA, respectively, one clearly has

$$C_{N,\text{S-SALT}} \geqslant C_{N,\text{SA}} \tag{2.1}$$

Similarly, if $C_{N,\text{B-SALT}}$ and $C_{N,\text{BA}}$ are the numbers of different configurations with N bonds of B-SALT and of BA, respectively, it is true that

$$C_{N,\text{B-SALT}} \geqslant C_{N,\text{BA}} \tag{2.2}$$

For all these models it is expected that for large N

$$C_{N,} \sim \mu^N N^{-\theta} \tag{2.3}$$

If universality holds, then

$$\theta_{\text{S-SALT}} = \theta_{\text{SA}} = \theta_{\text{BA}} = \theta_{\text{B-SALT}} \tag{2.4}$$

and if one counts, for example, the mean number of S-SALT of $N+1$ sites which can be immersed in the corresponding site animal, the power law correction should drop out and asymptotically only an exponential factor should survive.

If T is a SALT, one defines a two point function for the sites x and y in L by

$$G_\beta(x, y) = \sum_{T \ni x,y} \beta^{|T|} \tag{2.5}$$

where $|T|$ is the number of bonds of T and β plays the role of a fugacity.

If $N_s(T)$ is the number of sites of an S-SALT, then

$$N_s(T) = |T| + 1 \tag{2.6}$$

which is not true for a B-SALT, where

$$N_c(T) = |T| + 1 - N_s(T) \tag{2.7}$$

is the number of cycles of T. In both cases $|T| + 1$ is the number of points of the corresponding abstract tree.

The susceptibility is defined by

$$\begin{aligned} \chi_\beta &= \sum_{y \in L} G_\beta(x, y) = \sum_{T \ni x} \beta^{|T|}(|T| + 1) \\ &= \sum_{N=0}^{\infty} C_N \beta^N (N+1)^2 \end{aligned} \tag{2.8}$$

where C_N denotes for both models the number of configurations defined above.

For $\beta \nearrow \beta_c = 1/\mu$, the susceptibility is expected to diverge like

$$\chi_\beta \sim (\beta_c - \beta)^{-\gamma} \tag{2.9}$$

so that using the asymptotic behavior (2.1) one obtains

$$\gamma = 3 - \theta \tag{2.10}$$

Another quantity of interest is the radius of gyration R of a SALT T. We have used the following definition: given an abstract tree with points $\{1,..., n\}$, by the relation

$$i \mapsto s_i = (x_i^1, x_i^2) \tag{2.11}$$

where the superscripts denote the different directions in the lattice, one defines the coordinates $(\bar{x}^1, \bar{x}^2)$ of the barycenter of T such that

$$0 = \sum_{i=1}^{N} (x_i^j - \bar{x}^j) \qquad \text{for} \quad j = 1, 2 \tag{2.12}$$

Then, we introduce, for each T, the mean distance of its sites from its barycenter:

$$R_T^2 = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{2} (x_i^j - \bar{x}^j)^2 \tag{2.13}$$

The mean radius of gyration for all equivalence classes of SALT with N bonds is

$$\overline{R_N} = \frac{1}{C_N} \sum_{\bar{T}: |\bar{T}| = N} R_{\bar{T}} \tag{2.14}$$

It is expected that for large N, $\overline{R_N}$ has a scaling behavior described by an exponent ν:

$$\overline{R_N} \sim N^{\nu} \tag{2.15}$$

Note that (2.3) and (2.15) are only the leading terms in an asymptotic expansion of C_N and R_N for large N; the renormalization group predicts analytic as well nonanalytic subleading correction terms for the actual behavior. In any event, there will be deviations from the asymptotic scaling formulas (2.3) and (2.15) for finite N and we describe in Section 4 how we have treated these in connection with the estimates of the systematic errors.

3. DESCRIPTION OF THE ALGORITHM AND THE DATA STRUCTURE

Our algorithm really generates lattice trees *rooted* at the origin of a square lattice (they are equivalence classes of labeled lattice trees with respect to permutations of the indices $i \in \{2,..., n\}$ and such that the index 1 is mapped onto the origin) in a grand canonical ensemble. Each SALT T rooted at the origin has the probability

$$\Pr(T) = \frac{(1 + |T|)\, \beta^{|T|}}{\sum_{N=0}^{\infty} C_N (N+1)^2 \beta^N} \tag{3.1}$$

of occurring in the ensemble. The normalizing factor is just the susceptibility χ_β of the related field theory. Using mean-field bounds, one can rigorously prove that χ_β diverges for $\beta \nearrow \beta_c = 1/\mu$.

Our algorithm is a Markov process with (3.1) as its unique stationary probability distribution. A Monte Carlo step is defined by the following procedure: an index $i \in \{1,..., |T| + 1\}$ (i.e., a point in the underlying abstract tree) is first chosen at random. A random number $r \in [0, 1)$ is then compared to a constant $p(\beta) < 1$. If $r < p(\beta)$, an attempt is made to remove s_i from T, which is realized if $i \neq 0$ and if i is connected (in the underlying abstract tree) to only one other point. If $r > p(\beta)$, it is attempted to add a bond b at s_i in one of the $2D$ possible directions induced by r lying on one of $2D$ equal sections in the interval $[p(\beta), 1]$. The self-avoidance check is now performed for the site s on the other end of b or on b itself, respectively, for the site and the bond problem. If the transition is not allowed,

then the previous configuration is taken also at the new step. Therefore, the transition probabilities are

$$w(T \to T') = \begin{cases} \dfrac{1}{|T|+1} \dfrac{1}{2D} [1 - p(\beta)] \, \chi_{\text{SALT}}(T'), & \text{if } T \prec T' \\ \dfrac{1}{|T|+1} p(\beta), & \text{if } T' \prec T \\ \dfrac{1}{|T|+1} \left\{ \dfrac{1}{2D} [1 - p(\beta)] \, A(T) + p(\beta) \, B(T) \right\}, & \text{if } T = T' \end{cases} \tag{3.2}$$

Here, the relation $\prec$ means that the tree on the right can be obtained from the tree on the left by adding one bond. χ_{SALT} is the characteristic function on the particular set of SALT (it is not the susceptibility). $A(T)$ is the number of ways a bond can be added to T such that the resulting T' is not self-avoiding. $B(T)$ is the number of indices $i \in \{1,..., |T|+1\}$ (i.e., points in the underlying abstract tree) from which deletion is forbidden: i.e., for which either $i = 1$, or i is connected (in the abstract tree) to more than one point, or both.

The constant $p(\beta)$ is fixed in order that w might satisfy the detailed-balance condition for the probability Pr:

$$\Pr(T) \, w(T \to T') = \Pr(T') \, w(T' \to T) \tag{3.3}$$

inserting (3.1) and (3.2) in (3.3), one finds

$$p(\beta) = \frac{1}{1 + 2D\beta} \tag{3.4}$$

This algorithm is also ergodic: given any trees T and T', bonds can be removed successively from T until the "empty tree" consisting only of the origin is reached, then, by adding bonds, T' can be built up with a finite probability.

The algorithm thus satisfies the detailed balance and is ergodic. This ensures that (3.1) is the unique stationary probability distribution for it.

As in the case of Berretti and Sokal,[5] the observable $|T|$ is executing (crudely speaking) a random walk with drift on the positive integers. It can therefore be expected that the average time for T to return to the "empty tree" is proportional to $|T|^2$. Thus, after a time τ (measured in Monte Carlo steps) of order

$$\tau \sim \langle |T| \rangle^2 \tag{3.5}$$

trees should no longer be significantly correlated. This is actually the case, as reported in Section 4, where a detailed analysis of the autocorrelation time τ is described. The mean number of bonds

$$\langle |T| \rangle = \frac{\sum_{N=0}^{\infty} N(N+1)^2 C_N \beta^N}{\sum_{N=0}^{\infty} (N+1)^2 C_N \beta^N} \sim \frac{\beta\gamma}{\beta_c - \beta} \tag{3.6}$$

can now be adjusted by suitably tuning β.

We shall now describe the data structure we used to represent a tree T in the computer.[4]
Let $\{s_1, \ldots, s_{|T|+1}\}$ be the sites of the tree T, then, to each index i we associate a link field $\{f_{i,l}\}_{l=1}^{2D}$ with $2D$ entries. If the bond $b_{i,l}$ emanating in direction l from s_i is occupied, we set $f_{i,l} = j$, where j is the index of the site s_j at the other end of the bond $b_{i,l}$. Directions are enumerated in such a way that $b_{i,l} = b_{j,2D+1-l}$. Therefore, $f_{i,l} = j$ implies $f_{j,2D+1-l} = i$. We also used an additional array $\{t_i\}$ associated with each site s_i, which contains the number of occupied bonds emanating from s_i. In order to check the self-avoiding constraint for the S-SALT, we assigned one bit to each site of a (512×512)-square lattice. This bit was set to one if the site was occupied and zero otherwise. For the B-SALT, four bits were assigned to each site for the four bonds emanating from it. Although the B-SALT bit map is then redundant by a factor two, the self-avoidance check is greatly speeded up.

Using this data structure, the computer time for a Monte Carlo step does not depend on the number of bonds of T, i.e., is an $O(1)$ operation with respect to $|T|$.

4. RESULTS AND ANALYSIS OF STATISTICAL AND SYSTEMATIC ERRORS

In this section we report the results of our Monte Carlo (MC) simulations for studying the critical behaviour of the SALT models. In the analysis of the statistical and systematic errors, we have relied on the detailed work by Berretti and Sokal[5] and we refer the reader to their paper for further information.

We performed main runs at $\beta = 0.185$ for the S-SALT and $\beta = 0.167$ for the B-SALT. These values correspond to a mean number of bonds $\langle |T| \rangle \approx 40$ for both models. 7×10^9 MC iterations were performed for the S-SALT, which required a total of about 180 hr of CPU time on a CDC-174. One MC iteration therefore takes about 92 μsec. 6×10^9 MC iterations

were performed for the B-SALT, for a total of about 380 hr of CPU time on a VAX 11/780. One MC iteration lasts here more because of the slower computer and the more complex self-avoidance check. The rejection rate, at this value of β, was 65.65%, for the S-SALT, of which 25.35% was due to the self-avoiding constraint and the rest to attempts to remove inner bonds; in the B-SALT case the total rejection rate was the 62.21%, the 21.15% due to the self-avoidance check. In both cases, data were taken every 20 000 MC iterations and stored on tape for the subsequent statistical analysis.

For a correct treatment of the statistical errors, we have estimated the autocorrelation time in MC steps of our stationary stochastic process.

Let $A(T)$ be a real-valued observable; then, successive samples of the sequence $A_t = A(T_t)$ produced by our algorithm are highly correlated, because, in one MC step, at most one point can be added or removed from T_t.

We use the sample mean

$$\langle A \rangle_M^{\text{obs}} \equiv \frac{1}{M} \sum_{t=1}^{M} A_t \tag{4.1}$$

as an estimator of the expectation value

$$\langle A \rangle \equiv \frac{\sum_T A(T) \Pr(T)}{\chi_\beta} \tag{4.2}$$

As $M \nearrow \infty$, $\langle A \rangle_M^{\text{obs}}$ converges with probability 1 to $\langle A \rangle$ (ergodic theorem); and for large but finite M, $\langle A \rangle_M^{\text{obs}}$ is approximately Gaussian distributed with mean $\langle A \rangle$ and variance

$$\begin{aligned} \sigma_A^2 &= \frac{1}{M^2} \sum_{i,j=1}^{M} C_{AA}(i-j) \\ &\approx \frac{1}{M} \sum_{s=-\infty}^{+\infty} C_{AA}(s) \end{aligned} \tag{4.3}$$

where

$$C_{AA}(s) = \langle A_t A_{t+s} \rangle - \langle A \rangle^2 \tag{4.4}$$

is called the autocorrelation function of the process $\{A_t\}$ (central limit theorem). Since $\{A_t\}$ is a function of a reversible Markov process, its

autocorrelation function satisfies the spectral representation (Ref. 5, Appendix B):

$$C_{AA}(s) = \int_0^\infty e^{-a|s|} d\rho(a), \qquad s \text{ even} \tag{4.5}$$

where $d\rho(a)$ is a positive measure. Therefore, we have

$$0 \leqslant C_{AA}(s) \leqslant C_{AA}(0) \exp(-|s|/\tau_{AA}) \tag{4.6}$$

with

$$\tau_{AA} = \lim_{s \to \infty} \frac{|s|}{\log[C_{AA}(s)/C_{AA}(0)]} \equiv \lim_{s \to \infty} \tau(s) \tag{4.7}$$

Hence, inserting (4.6) in (4.3) the variance σ_A^2 can be estimated by

$$\sigma_A^2 \leqslant \frac{1}{M} C_{AA}(0)\, 2\tau_{AA} \tag{4.8}$$

for $M \gg \tau_{AA} \gg 1$. The problem of correctly including the autocorrelation in the evaluation of the statistical error bars is now reduced to estimating the autocorrelation function $C_{AA}(s)$ and thereby the autocorrelation time τ_{AA}. For $C_{AA}(s)$, we use the estimator

$$C_{AA}(s)_M^{\text{obs}} = \frac{1}{M - |s|} \sum_{t=1}^{M-|s|} A_t A_{t+|s|} - (\langle A \rangle_M^{\text{obs}})^2 \tag{4.9}$$

which has a bias of order $1/M$. A crude estimate for the variance of $C_{AA}(s)_M^{\text{obs}}$ is provided by

$$Var(C_{AA}(s)_M^{\text{obs}}) \leqslant \frac{2\tau_{AA}}{M} C_{AA}^2(0) \tag{4.10}$$

In Fig. 1 we have plotted the estimator $\hat{\tau}_{AA}(s)$ of$\tau_{AA}(s)$ for $A = |T|$, obtained by using $C_{AA}(s)_M^{\text{obs}}$ in (4.7). In Table I, we list the sample mean and the autocorrelation times for the number of bonds $|T|$, the square radius of gyration R_T^2, and the number of branches $N_b(T)$ [cycles $N_c(T)$] for the S-SALT (B-SALT). The error bars in Table I were obtained by using the estimated values for τ_{AA} and $C_{AA}(s)$ to obtain the variance of $C_{AA}(s)_M^{\text{obs}}$ from (4.10), which is then used to obtain error bars on $\tau_{AA}(s)$ at $s = 10$ for both models. They are the statistical 95% confidence limits. All these values are consistent with the autocorrelation times

$$\tau = (6.5 \pm 0.6) \times 10^4 \text{ MC steps} \tag{4.11}$$

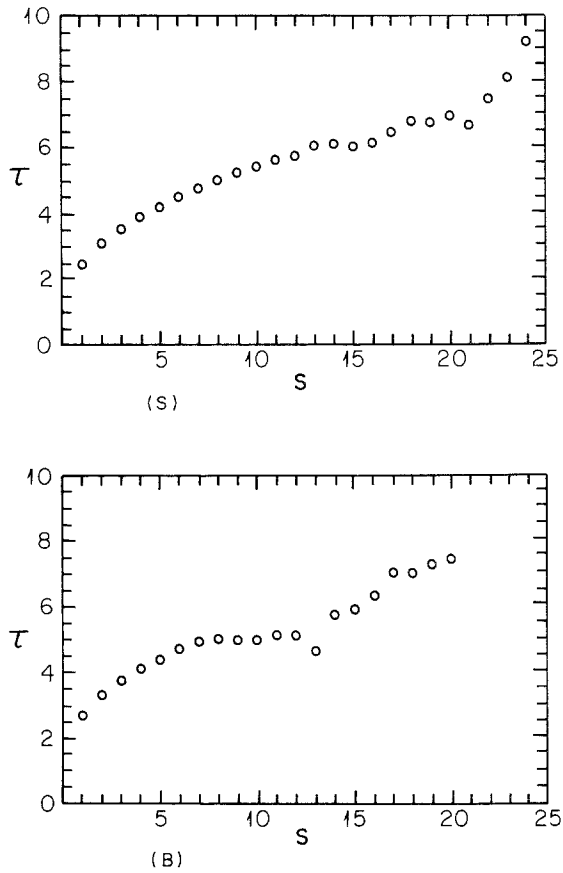

Fig. 1. For the two cases of S-SALT (S) and B-SALT (B) we plot the estimators for the autocorrelation in time of the mean number of bonds in units of 10^4 MC steps, as function of the separation s. After the plateau the signal is already noise.

for the S-SALT, and

$$\tau = (5.0 \pm 0.5) \times 10^4 \text{ MC steps} \tag{4.12}$$

for the B-SALT.

We tested the conjecture

$$\tau = \text{const} \langle |T| \rangle^2 \tag{4.13}$$

empirically by performing additional runs at different values for β. The resulting estimates for τ are consistent with (4.13) with the constant approximately equal to 40 for the S-SALT and 28 for the B-SALT.

Table I. Estimates for the Autocorrelation in Time, Measured in MC Steps, for Various Observables, with Their Statistical Errors.[a]

A	$\langle A \rangle$	$\tau_{AA}/10^4$ MC steps
	I-(S)	
$\lvert T \rvert$	39.41 ± 0.24	6.4 ± 0.6
R_T^2	15.61 ± 0.31	6.7 ± 0.4
$N_b(T)$	10.54 ± 0.06	6.4 ± 0.6
	I-(B)	
$\lvert T \rvert$	43.33 ± 0.23	5.0 ± 0.5
R_T^2	13.35 ± 0.26	4.6 ± 0.6
$N_c(T)$	3.68 ± 0.06	5.0 ± 0.6

[a] The (S) refers to the S-SALT model as the (B) to the B-SALT one. This notation is used also in other tables and in figures.

Our goal will be to measure critical parameters at fixed β. For this purpose we need an ansatz for the asymptotic behaviour in the number of bonds N of the number of configurations C_N and the mean radius of gyration $\overline{R_N}$. This procedure is somehow different from what is usually done in the literature, where measures are taken as a function of β. But, once more following Ref. 5, we could, in this way, keep separated statistical from systematic errors. In order to estimate μ and θ we start from the assumption that for $N \geqslant N_{\min}$ one has *exactly*

$$C_N = a_0 \mu^N N^{-\theta} \left(1 + \frac{a_1}{N}\right) \tag{4.14}$$

for given a_1. Of course this expression does not take into account corrections to scaling as predicted by the renormalization group analysis, but, at the moment, we cannot, within the accuracy of our statistics, disentangle them from the analytic subterms.

In our case, we are actually generating the distribution

$$P_N(\mu, \theta) = \Pr(|T| = N) = \frac{(N+1)^2 C_N \beta^N}{\chi_\beta} \tag{4.15}$$

By (4.14), P_N is—for fixed a_1—an exponential family parametrized by μ and θ. For such a family, the maximum-likelihood estimate for its

parameters amounts to fix them so that the observed (sample) mean values of $|T|$ and $\log |T|$ equal their theoretical mean values. That is, if for an observable $f(|T|)$ one defines the theoretical expectation

$$\langle f(|T|)\rangle_{\mu,\theta} = \frac{\sum_{N=N_{\min}}^{\infty} f(N)\, P_N(\mu, \theta)}{\sum_{N=N_{\min}}^{\infty} P_N(\mu, \theta)} \tag{4.16}$$

and the MC expectation

$$\langle f(|T|)\rangle^{\text{obs}} = \frac{\sum_{t=1}^{M} f(|T_t|)\, \vartheta(|T_t| - N_{\min})}{\sum_{t=1}^{M} \vartheta(|T_t| - N_{\min})} \tag{4.17}$$

with the usual definition of the ϑ function

$$\vartheta(x) = \begin{cases} 1, & \text{if } x \geqslant 0 \\ 0, & \text{otherwise} \end{cases} \tag{4.18}$$

where T_t is the tth SALT in the MC sample; then, one must solve the system of two coupled nonlinear equations

$$\begin{aligned} \langle |T| \rangle_{\hat{\mu},\hat{\theta}} &= \langle |T| \rangle^{\text{obs}} \\ \langle \log |T| \rangle_{\hat{\mu},\hat{\theta}} &= \langle \log |T| \rangle^{\text{obs}} \end{aligned} \tag{4.19}$$

in order to obtain the maximum-likelihood estimates $\hat{\mu}$ and $\hat{\theta}$ as functions of $N_{\min}$ and a_1.

The statistical errors on the values so obtained are known *a priori*, as the statistical distributions of μ and θ become Gaussian, with an explicity known covariance matrix, in the limit of a large sample of independent trees with $N \geqslant N_{\min}$.

In Table II we report the solutions of (4.19) for various $N_{\min}$ and a_1. The underlined values do not exhibit a systematic dependence on $N_{\min}$ for constant a_1. We take the arithmetic mean of these values for μ and θ, respectively, as the central estimates and twice their variance as an estimate of the systematic error.

We find in the case of the S-SALT

$$\begin{aligned} \mu &= 5.1434 \pm 0.0013 \pm 0.0057 \\ \theta &= 1.001 \pm 0.024 \pm 0.054 \end{aligned} \tag{4.20}$$

Table II. Estimators for μ and θ, for the Two Cases, as Function of N_{min} and the Constant a_1 Which Appears in the Ansatz (4.14) to Measure Corrections to Scaling.

N_{min}	10		15		20		25		30	
a_1	μ	θ	μ	θ	μ	θ	μ	θ	μ	θ
					II-(S)					
0	5.1464	1.0533	5.1456	1.0446	5.1443	1.0281	5.1446	1.0321	5.1449	1.0372
0.3	5.1453	1.0349	5.1449	1.0299	5.1437	1.0213	5.1442	1.0213	5.1446	1.0276
0.6	5.1443	1.0171	5.1442	1.0157	5.1432	1.0036	5.1438	1.0107	5.1442	1.0180
0.9	5.1434	1.0000	5.1435	1.0018	5.1427	0.9917	5.1433	1.0003	5.1439	1.0087
1.2	5.1424	0.9834	5.1429	0.9882	5.1422	0.9801	5.1430	0.9901	5.1436	0.9995
1.5	5.1416	0.9673	5.1423	0.9755	5.1417	0.9688	5.1426	0.9800	5.1432	0.9904
1.8	5.1407	0.9518	5.1417	0.9421	5.1413	0.9576	5.1422	0.9701	5.1430	0.9815
2.1	5.1399	0.9367	5.1411	0.9495	5.1408	0.9467	5.1418	0.9605	5.1426	0.9727
					II-(B)					
0.9	5.7357	1.0410	5.7348	1.0298	5.7355	1.0384	5.7346	1.0261	5.7343	1.0229
1.2	5.7349	1.0260	5.7342	1.0174	5.7350	1.0277	5.7342	1.0166	5.7340	1.0143
1.5	5.7341	1.0115	5.7336	1.0053	5.7345	1.0172	5.7338	1.0073	5.7337	1.0058
1.8	5.7334	0.9973	5.7331	0.9934	5.7341	1.0069	5.7335	0.9981	5.7334	0.9975
2.1	5.7	0.9836	5.7325	0.9818	5.7337	0.9968	5.7331	0.9890	5.7331	0.9893
2.4	5.7319	0.9703	5.7320	0.9705	5.7333	0.9868	5.7328	0.9801	5.7328	0.9812
2.7	5.7313	0.9573	5.7315	0.9594	5.7328	0.9771	5.7324	0.9713	5.7326	0.9732
3.0	5.7306	0.9446	5.7310	0.9486	5.7325	0.9675	5.7321	0.9627	5.7323	0.9653

where the first error bars refer to the systematic errors and the second to the statistical ones. Here, as everywhere, the statistical error bars are the classical 95% confidence limits for $N_{min} = 15$.

Furthermore, for the B-SALT

$$\begin{aligned} \mu &= 5.7335 \pm 0.0011 \pm 0.0050 \\ \theta &= 0.999 \pm 0.020 \pm 0.045 \end{aligned} \tag{4.21}$$

Clearly, the Parisi–Sourlas prediction is very well confirmed by both models.

In estimating the critical exponent ν, we replace the definition (2.15) by a more detailed ansatz

$$\overline{\log R^2} = 2\nu \log(N + b_1) + b_0 \tag{4.22}$$

at fixed b_1, which plays the role of a correction to scaling. Here the left-hand side mean is taken at fixed N, greater than or equal to $N_{\min}$. Then the least-squares fit procedure gives rise to the following estimators $\hat{\nu}$ and $\hat{b}_0$ for ν and the constant b_0:

$$\hat{\nu} = \frac{\langle X; Y\rangle^{\text{obs}}}{2\langle X; X\rangle^{\text{obs}}}$$

$$\hat{b}_0 = \frac{\langle X; X\rangle^{\text{obs}}\langle Y\rangle^{\text{obs}} - \langle X; Y\rangle^{\text{obs}}\langle X\rangle^{\text{obs}}}{\langle X; X\rangle^{\text{obs}}} \tag{4.23}$$

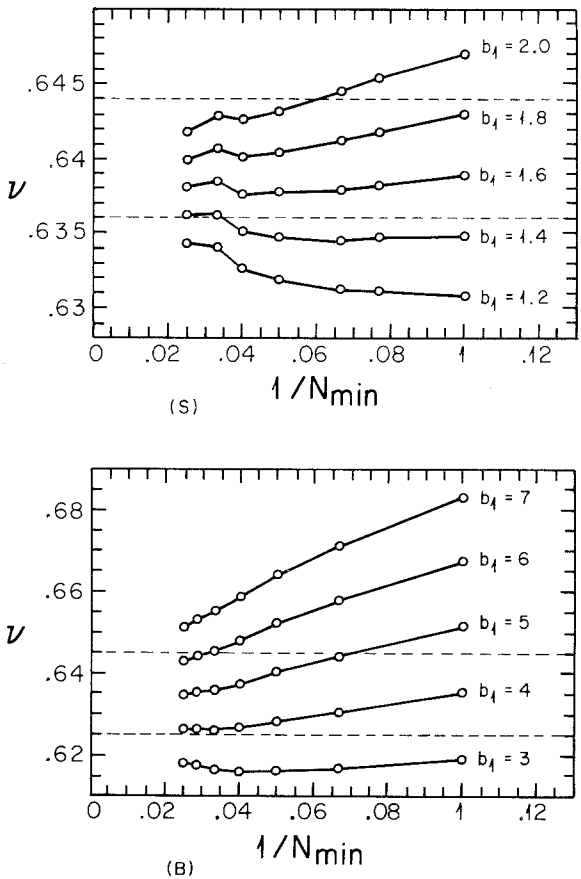

Fig. 2. We plot the estimators for the exponent ν as function of the inverse of the minimum value of bonds allowed in the ensemble and the constant b_1 which appears in the ansatz (4.22). The continuous straight lines are drawn simply to indicate for what b_1 each small circle has been determined. Dotted lines indicate the confidence limits in the analysis of systematic errors.

where $X = \log(|T| + b_1)$, $Y = \log R_T^2 . \langle W; Z \rangle$ denotes the truncated expectation

$$\langle W; Z \rangle = \langle WZ \rangle - \langle W \rangle \langle Z \rangle \tag{4.24}$$

and $\langle . \rangle^{\text{obs}}$ denotes the sample mean (4.17) of all trees T with $|T| \geqslant N_{\min}$.

We found it suggestive to present the resulting estimators $\hat{\nu}(N_{\min}, b_1)$ in form of a plot as function of $1/N_{\min}$ for various values of b_1 in Fig. 2. The lines in Fig. 2 are guides to the eye and we used them to obtain our central estimates

$$\nu = 0.640 \pm 0.004 \pm 0.004 \qquad \text{for the S-SALT} \tag{4.25}$$

$$\nu = 0.635 \pm 0.009 \pm 0.006 \qquad \text{for the B-SALT} \tag{4.26}$$

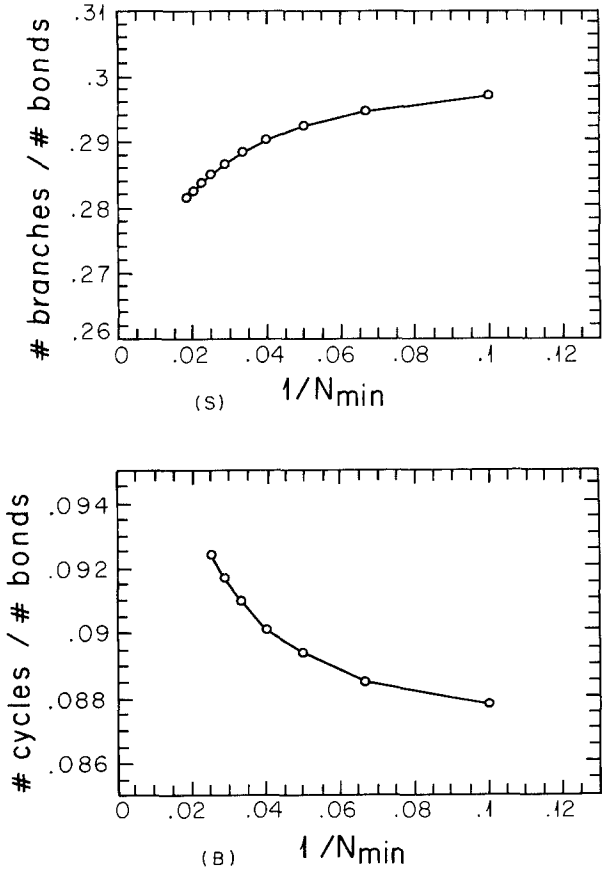

Fig. 3. These are the ratios between the mean number of branches and the mean number of bonds for the S-SALT (S) and the mean number of cycles and the mean number of bonds for the B-SALT (B) as function of the inverse of $N_{\min}$ the minimum value of bonds allowed in the ensemble.

The equations (4.20), (4.21) and (4.25), (4.26) strongly support the conjecture that the two models belong to the same universality class.

Finally, we will report our estimates for the ratio of the mean number of branches $\langle N_b(T) \rangle$ over the mean number of bonds $\langle |T| \rangle$, for the S-SALT. The results are plotted in Fig. 3-(S) as function of $1/N_{\min}$. We can extrapolate

$$\frac{\langle N_b(T) \rangle}{\langle |T| \rangle} = 0.2675 \pm 0.0025 \pm 0.0005 \tag{4.27}$$

In Fig. 3-(B) it is plotted the ratio between the mean number of cycles $\langle N_c(t) \rangle$ and the mean number of bonds $\langle |T| \rangle$ for the B-SALT, as function of $1/N_{\min}$. It is interesting to remark that $N_c(T)$ is increasing with $N_{\min}$ more rapidly than the number of bonds. In the plotted region their ratio is very well described by a function $c_0 + c_1 N_{\min}$ with c_0 and c_1 constants. Presumably, the fact that this ratio is not yet well saturated explains why the errors in (4.26) are larger than those in (4.25).

A word of caution can still be added as far as the evaluation of the systematic errors is concerned. They are obtained only on the basis of internal consistency of the estimate, but, after all, the average radius of gyration of the trees we are simulating is only ≈ 4 lattice spacings, so the corrections to scaling are likely to be fairly large. From this point of view, a simulation of longer trees, at the cost of more computer time, could be used for a more confident discussion of corrections to scaling.

5. COMPARISON WITH PREVIOUS WORK AND CONCLUSIONS

The first observation resulting from a comparative reading of the literature is that there does not seem to exist a study which gives the values for μ, θ, and ν simultaneously.

Gaunt *et al.*[7] have considered the S-SALT problem by series analysis of exact-enumeration data in dimension D, for $2 \leqslant D \leqslant 9$. In $D = 2$ S-SALT are counted up to $N = 11$ and the resulting estimates are

$$\theta = 1.00 \pm 0.02 \tag{5.1}$$

and

$$\mu = 5.14 \pm 0.01 \pm 0.26 \Delta\theta \tag{5.2}$$

where the first error for μ is computed keeping θ fixed at 1 and $\Delta\theta$ is the difference from this central estimate. These estimates agree with ours, but

looking at their plot of θ, we believe that their error bars for θ should be multiplied by at least a factor 5.

S-SALT with a fixed number of bonds, ranging from 20 to 600, have been generated with a Monte Carlo algorithm by Seitz and Klein.[8] Their estimates are

$$\nu = 0.615 \tag{5.3}$$

which is significantly smaller than ours, probably due to the mixing of statistical and systematic errors occurring in their least squares fitting procedure, and the ratio

$$\frac{\langle N_b(T) \rangle}{\langle |T| \rangle} = 0.266 \tag{5.4}$$

which is very close to our value (4.27).

Previously, Redner[9] has measured

$$\nu = 0.57 \pm 0.06 \tag{5.5}$$

for the S-SALT in a static Monte Carlo simulation in which all the vertices were of order four and with a fixed probability of creating a vertex.

By real-space renormalization group recursion relation, Family[10] obtained

$$\nu = 0.637 \tag{5.6}$$

which is surprisingly accurate considered the approximations involved, and the quite different value for the attrition constant

$$\mu = 3.88 \tag{5.7}$$

It seems that the B-SALT had not been considered earlier in the literature and so no direct comparison can be made.

Further information is available for the critical exponents ν and θ since the SALT are believed to belong to the same universality class as lattice animals. We summarize these results in Table III. Some earlier Monte Carlo studies use an algorithm, due to Stauffer,[11] that generates site animals with a fixed number s of occupied sites; each SA with t perimeter sites (i.e., nearest neighbours of occupied sites which are themselves empty) has the probability

$$\Pr(t) = \frac{t(1-p)^t}{\sum_{t=0}^{2(s+1)} t g_{st} (1-p)^t} \tag{5.8}$$

Table III. Summary of the Available Information about the Exponents ν and θ for the Lattice Animals in Two Dimensions

	ν	θ
Monte Carlo	0.66 ± 0.007[11]	
	0.65 ± 0.02[12]	
Exact enumeration	0.64 ± 0.004[13]	1.00 ± 0.02[17]
Real-space Renormalization group	0.649 ± 0.009[14]	
Phenomenological Renormalization group	0.6408 ± 0.0003[15]	

of occurring. The parameter p plays here the same role as the β in (3.1) and g_{st} is the number of SA with given number of s sites and t perimeter sites. It seems that the factor t in (5.8), which is a consequence of choosing perimeter sites at random, has been forgotten in Refs. 11 and 12; fortunately, this does not affect the estimates for ν. In the limit $p \searrow 0$ the desired distribution is then recovered. While the error bars appear to be underestimated in Ref. 11, Ref. 12 gives a very reasonable estimate.

Also the error bars of Derrida and De Seze[15] are very optimistic (see Ref. 16 for a criticism), but their estimate is consistent with ours.

In conclusion, we have obtained by this simulation of two SALT models: (a) estimates of nonuniversal quantities like the attrition constants and the mean number of branches and loops; (b) estimates of the critical exponents ν and θ which support the conjectured universality and the dimensional reduction scheme; (c) a test of validity for this Monte Carlo algorithm and an estimate of the dynamical critical exponent of its autocorrelation; (d) valid statistical error bars and a careful analysis of the systematical errors.

These results are encouraging the application of such methods to more complicated problems, where other methods find more difficulties.

ACKNOWLEDGMENTS

It is a pleasure to thank Jürg Fröhlich for his continuous interest in our work. One of us (S.C.) thanks him also for the warm hospitality in Zürich where the project of this simulation was initiated.

We are also indebted to Alan Sokal whose suggestions helped us at every stage of our study.

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