Monte Carlo test of dimensional reduction for branched polymers in three dimensions

1985 J. Phys. A: Math. Gen. 18 L609

(http://iopscience.iop.org/0305-4470/18/10/010)

J. Phys. A: Math. Gen. **18** (1985) L609-L615. Printed in Great Britain

LETTER TO THE EDITOR

Monte Carlo test of dimensional reduction for branched polymers in three dimensions

U Glaus

Theoretical Physics, ETH-Hönggerberg, 8093 Zürich, Switzerland

Received 5 March 1985, in final form 15 April 1985

Abstract. By a Monte Carlo simulation of a grand canonical ensemble for a lattice tree model of branched polymers in three dimensions we obtain the estimates $\theta = 1.501 \pm 0.043$, $\nu = 0.495 \pm 0.013$ for the critical exponents. These estimates strongly support the exact conjecture $\theta = \frac{3}{2}$, $\nu = \frac{1}{2}$ by Parisi and Sourlas obtained using dimensional reduction. The attrition constant μ is also estimated.

The self-avoiding lattice trees are a natural model for isolated branched polymers in a good solvent, since they mimic the repulsive interaction between the monomers of the polymer conformation. The field theoretic formulation of the model suggests that it belongs to the same universality class as the lattice animals (Lubensky and Isaacson 1970). Using this formulation, a connection was found (Parisi and Sourlas 1981) between this universality class in d dimensions and the Lee-Yang edge singularity of the Ising model in $d-2$ dimensions. Since the Ising model can be solved exactly in zero and one dimension, this yielded exact values for the 'critical' exponents θ and ν in two and three dimensions. Namely, $\theta = 1$ in two and $\theta = \frac{3}{2}$, $\nu = \frac{1}{2}$ in three dimensions.

These exponents describe the statistics of the branched polymers in the dilute limit: let $N(n)$ be the number of different configurations of branched polymers made of n monomers (bonds) and R_n the mean radius of gyration. It is then expected that for large n

$$N(n) \sim n^{-\theta} \mu^n \qquad R_n \sim n^{\nu}. \tag{1a, b}$$

An intermediate step of the Parisi-Sourlas dimensional reduction for the branched polymer model is the application of the inverse replica trick, which transforms it into an Ising model in an imaginary random magnetic field. In the approximation of keeping only the leading infrared divergent diagrams, this Ising model is then equivalent to an Ising model with deterministic imaginary magnetic field in two dimensions less. In view of the recent results (Fisher *et al* 1984, Imbrie 1984) concerning the lower critical dimension of the random field Ising model, which strongly indicate that the dimensional reduction is incorrect in the case of a *real* magnetic field, it is interesting to test the Parisi-Sourlas prediction for θ and ν in three dimensions with a highly accurate numerical method. See Bovier *et al* (1985) for a recent review on branched polymers and dimensional reduction.

Although most of the earlier numerical estimates of these exponents are consistent with or close to the predicted exact values, they do not reliably confirm or rule them out. Exact enumerations of lattice animals (Peters *et al* 1979) and lattice trees (Gaunt

0305-4470/85/100609+07$02.25

et al 1982) have only been performed for $\leqslant 11$ sites and are therefore subject to large systematic errors. On the other hand, earlier Monte Carlo studies (Redner 1979, Gould and Holl 1981, Seitz and Klein 1981) have only been concerned with estimating ν and differ considerably from each other in their estimates. This could be due to the method with which the exponent ν is extracted from the Monte Carlo simulation, which produces lattice trees (animals) with a fixed number of bonds (sites) and therefore average radii of gyration R_n for various n. The exponent ν is then obtained by performing a least squares fit to the relation $\ln(R_n) = \nu \ln(n) + c$ following from (1*b*) for large n. However, R_n is not only plagued by a statistical error inherent in any Monte Carlo experiment but also by a systematic error resulting from corrections to scaling at finite n. It seems therefore hard to distinguish these two possible sources for errors on the estimate of the exponent ν by using this method.

In this letter, we report the results of a new Monte Carlo simulation for the self-avoiding lattice trees on the cubic lattice $\mathbb{Z}^3$. This algorithm is very similar to the one used by Beretti and Sokal (1984) to study the self-avoiding walk in two dimensions. It has subsequently been adapted to simulate self-avoiding lattice trees in two dimensions (Caracciolo and Glaus 1984). The only change introduced for the simulation in three dimensions was the usage of hash coding (Knuth 1973) in order to guarantee a quick self-avoiding check.

We define a lattice tree T as an embedding of an abstract tree (i.e. a minimally connected graph) into $\mathbb{Z}^3$, such that the vertices of the graph are mapped onto the lattice sites in a way that two vertices connected by a line are mapped onto nearest-neighbour sites and the line is identified with the elementary bond connecting these two sites. The self-avoiding constraint is imposed by requiring each vertex of the abstract tree to be mapped onto a different point in $\mathbb{Z}^3$. In the polymer language, the elementary bonds are then the monomers.

Our Monte Carlo algorithm generates lattice trees with one point fixed at the origin at a fixed 'bond activity' β. Let $|T|$ be the number of bonds contained in T. Then, each lattice tree T has the probability

$$Pr(T) = (|T|+1)\beta^{|T|}\left(\sum_{n=0}^{\infty}(n+1)^2 N(n)\beta^n\right)^{-1} \tag{2}$$

of occurring in the ensemble.

It follows from (2) that during the simulation, the probability for a tree T to have n bonds is equal to

$$P(|T|=n) = (n+1)^2 N(n)\beta^n\left(\sum_{n=0}^{\infty}(n+1)^2 N(n)\beta^n\right)^{-1}. \tag{3}$$

The extra term $(n+1)$ in the numerator of (3) comes from the fact that the origin is kept fixed and $N(n)$ counts only the configurations, i.e. the equivalence classes of lattice trees with respect to lattice translations.

The algorithm is a Markov process with (2) as its unique equilibrium distribution. A Monte Carlo step is defined by the following procedure: a site s of T is first chosen at random. A random number $r \in [0, 1)$ is then compared to a constant $p(\beta) < 1$. If $r \leqslant p(\beta)$, an attempt is made to remove s from T, which is realised if s is not the origin and it is connected to only one other point. If $r > p(\beta)$, it is attempted to add a bond b at s into one of the $2d$ possible directions induced by r lying on one of the $2d$ equal sections in the interval $[p(\beta), 1]$. The self-avoiding check is now performed for the

site s' on the other end of b. If a transition is not allowed, the previous configuration is taken at the next step.

Caracciolo and Glaus (1984) have verified that by choosing

$$p(\beta) = (1+2d\beta)^{-1} \tag{4}$$

detailed balance is satisfied for (2). The algorithm is also ergodic, any tree T' can be reached from T by removing all bonds from T until only the origin is left and then building up T'.

We tested whether our algorithm actually does produce lattice trees according to the distribution (2) by performing runs at the temperatures $\beta = 0.03, 0.05, 0.07$, which yield primarily trees with a small number of bonds. We then compared the observed distribution for the number of bonds n, conditional on $n \leqslant 10$, and the expected distribution (3), using for $N(n)$ the results of Gaunt *et al* (1982), by the χ^2 test. We found good agreement with theory for all three temperatures.

We have performed a main run at $\beta = 0.091\,98$, which corresponds to a mean number of bonds

$$\langle |T| \rangle \sim \mu\beta(3-\theta)/(1-\mu\beta) = 45. \tag{5}$$

The program was running for 15×10^9 MC steps, requiring about 500 hours of CPU time on a CDC-174. The total rejection rate (null transitions) was 57.1%. Data were taken every 3×10^4 MC steps and stored on tape for the subsequent statistical analysis.

In the determination of the statistical and systematic errors we have relied on the detailed description in the work of Beretti and Sokal (1984) and refer the reader to their paper for further information.

We first estimated the autocorrelation times τ_{AA} for the observables $A = |T|$ and R_T^2, the squared radius of gyration, which we define as

$$R_T^2 = \frac{1}{|T|}\sum_{l=1}^{|T|} x_l^2 - \left(\frac{1}{|T|}\sum_{l=1}^{|T|} x_l\right)^2. \tag{6}$$

Here x_l are the sites of T in $\mathbb{Z}^3$, except the origin. The resulting values are

$$\tau_{R_T^2 R_T^2} = (8.4 \pm 0.8) \times 10^4 \text{ MC steps} \tag{7a}$$

$$\tau_{|T||T|} = (8.7 \pm 0.8) \times 10^4 \text{ MC steps}. \tag{7b}$$

From this, the mean number of bonds in our simulation is estimated to be

$$\langle |T| \rangle = 46.79 \pm 0.27. \tag{8}$$

The error bars above denote the classical statistical 95% confidence limits. For the autocorrelation time τ of our algorithm we take the estimate (7*b*) of $\tau_{|T||T|}$.

In order to estimate μ and θ, we assume that for $n \geqslant n_{\text{MIN}}$, we have exactly

$$N(n) = a_0 \mu^n n^{-\theta}(1 + a_1/n). \tag{9}$$

The term (a_1/n) is introduced to take into account corrections to scaling.

Now, for any observable $A(|T|)$ depending only on the number of bonds $|T|$, we can, using the probability (3) and the theoretical ansatz (9) for $N(n)$, define a theoretical average by

$$\langle A(|T|)\rangle_{\mu,\theta}^{n_{\min}} = \sum_{n=n_{\min}}^{\infty} A(n)(n+1)^2 N(n)\beta^n \left(\sum_{n=n_{\min}}^{\infty} (n+1)^2 N(n)\beta^n\right)^{-1}. \tag{10}$$

Conversely, using our data we obtain the observed average

$$\langle A(|T|)\rangle_{\text{obs}}^{n_{\min}} = \sum_{t=1}^{t_0} A(|T_t|)\chi(|T_t| - n_{\min}) \left(\sum_{t=1}^{t_0} \chi(|T_t| - n_{\min}) \right)^{-1}. \tag{11}$$

T_t are the successive samples of trees stored on tape and t_0 is the sample size, e.g. in our case 5×10^5. χ is the characteristic function for $|T_t|$ to be greater than or equal to $n_{\min}$. Our estimates for μ and θ were obtained by fitting them such that the theoretical averages (10) of $|T|$ and $\log|T|$ agree exactly with their corresponding observed averages (11).

In table 1 we have listed the values for μ and θ for various a_1 and $n_{\min}$. It is seen that for $a_1 = 0$ θ and μ are almost independent of $n_{\min}$! Moreover, the values for $a_1 < 0$ ($a_1 > 0$) show a systematic downwards (upwards) dependence of μ and θ on $n_{\min}$, which seems to converge to the same values as for $a_1 = 0$. From table 1 we obtain the estimates

$$\mu = 10.5439 \pm 0.0016 \pm 0.0063 \tag{12}$$

$$\theta = 1.501 \pm 0.012 \pm 0.031. \tag{13}$$

Here, as later, the format is central estimate ± systematic error ± statistical error. The central estimates are the mean of all values for $a_1 = 0$. The systematic error is twice the difference between the highest and the lowest of these values and the statistical error is twice the variance for $n_{\min} = 20$ obtained from the explicitly known covariance matrix for μ and θ, multiplied by $(2\tau)^{1/2}$. There is complete agreement with the Parisi-Sourlas prediction $\theta = \frac{3}{2}$. For a_1, we estimate $a_1 = 0 \pm 0.2$.

Table 1. (*a*) values for μ and (*b*) values for θ obtained as described in the text.

(*a*)

a_1 \ $n_{\min}$	10	15	20	25	30
−2.0	10.5543	10.5511	10.5493	10.5486	10.5473
−1.0	10.5485	10.5473	10.5464	10.5463	10.5455
−0.5	10.5460	10.5456	10.5451	10.5453	10.5447
0	10.5435	10.5439	10.5439	10.5443	10.5438
0.5	10.5413	10.5423	10.5426	10.5433	10.5430
1.0	10.5391	10.5408	10.5415	10.5424	10.5422
2.0	10.5352	10.5380	10.5393	10.5406	10.5407

(*b*)

a_1 \ $n_{\min}$	10	15	20	25	30
−2.0	1.614	1.591	1.576	1.570	1.558
−1.0	1.553	1.544	1.537	1.536	1.528
−0.5	1.525	1.522	1.519	1.520	1.514
0.0	1.499	1.501	1.501	1.505	1.500
0.5	1.473	1.481	1.484	1.489	1.487
1.0	1.449	1.461	1.467	1.475	1.473
2.0	1.405	1.424	1.435	1.446	1.448

The estimate for ν was obtained by minimising

$$\sum_{t=1}^{t_{max}} [\ln(R_T^2) - 2\hat{\nu}\ln(|T|+b_1) + \hat{b}_0]^2 \chi(|T_t| - n_{min}) \tag{14}$$

with respect to $\hat{\nu}$ and $\hat{b}_0$ for fixed b_1 and n_{min}. Figure 1 shows a plot of the resulting ν's as functions of n_{min}^{-1} for various b_1. From this plot we estimate

$$\nu = 0.495 \pm 0.009 \pm 0.004. \tag{15}$$

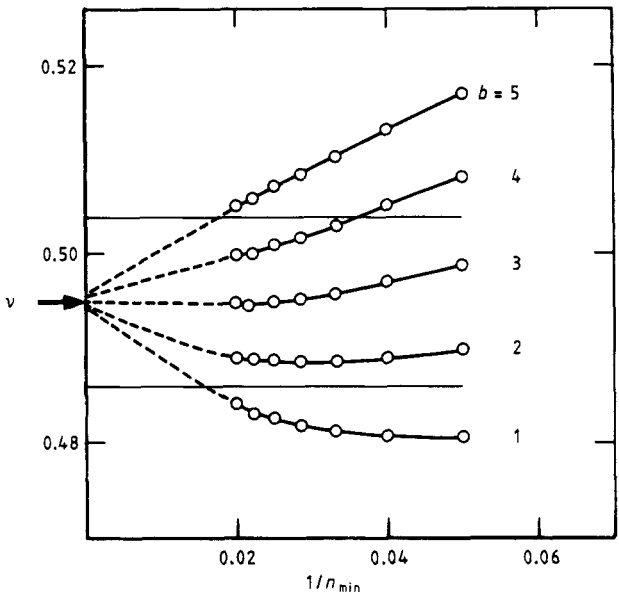

Figure 1. ν as function of $1/n_{min}$ for various b_1. Small circles denote least square values. Lines are guides to the eye. The arrow denotes our central estimate and the thin lines denote our systematic error bars.

The statistical error is twice the variance for $n_{min} = 30$ from least squares theory times $(2\tau)^{1/2}$. Again, we obtain excellent agreement with the Parisi-Sourlas prediction $\nu = \frac{1}{2}$.

Figure 1 indicates that due to corrections to scaling ν depends rather strongly on n_{min}. The decreasing influence of these corrections for increasing n_{min} is reflected by the fact that these curves come closer to each other as n_{min} goes to infinity. It is therefore reasonable to extrapolate each of these curves to $n_{min}^{-1} = 0$ and take the mean of these extrapolated values as our central estimate for ν. The systematic error bars have been chosen large enough to account for the pronounced effect of corrections to scaling for the radius of gyration. Of course, it is assumed in (9) and (14) that these corrections have the form $(1 + cn^{-1})$. For the radius of gyration we have also determined ν assuming

$$R_n = c_0 n^{\nu}(1 + c_1 n^{-\omega}) \tag{16}$$

with a correction-to-scaling exponent $\omega < 1$. Unfortunately, our data do not allow a confident determination of ω and ν at the same time. But the values for ν obtained for various fixed ω and c_1 are all consistent with (15).

Our estimate for the mean ratio of the number of endpoints $N_b(T)$, i.e. the number of points that are connected to only one other point in T, divided by $|T|$ is

$$\langle N_b(T)/|T|\rangle = 0.3134 \pm 0.0050 \pm 0.0005. \tag{17}$$

In table 2 we compare our results to various other theoretical values and numerical estimates for lattice trees and animals.

Table 2. Comparison with previous estimates of θ, ν and μ.

Method		θ	ν	μ
Field theory and dimensional reduction[a]		1.5	0.5	
Flory theory[b]			0.5	
Monte Carlo			0.46[c]	
			0.45 ± 0.06[d]	
			0.53 ± 0.02[e]	
Exact enumeration ($n \leqslant 10$)[f]		1.55 ± 0.05		10.53 ± 0.07
This paper		$1.501 \pm 0.012 \pm 0.031$	$0.495 \pm 0.009 \pm 0.004$	$10.5439 \pm 0.0016 \pm 0.0063$
	trees	$1.001 \pm 0.024 \pm 0.054$	$0.640 \pm 0.004 \pm 0.004$	$5.1434 \pm 0.0013 \pm 0.0057$
2D results[g]	bond SA trees	$0.99 \pm 0.020 \pm 0.045$	$0.635 \pm 0.009 \pm 0.006$	$5.7335 \pm 0.0011 \pm 0.0050$

[a] Parisi and Sourlas 1980, [b] Isaacson and Lubensky 1980, [c] Seitz and Klein 1981, [d] Redner 1979, [e] Gould and Holl 1981, [f] Gaunt *et al* 1982, [g] Caracciolo and Glaus 1984.

The exact enumeration-extrapolation study of Gaunt *et al* (1982) and the pulsating amoeba (at a fixed number of bonds) Monte Carlo study of Seitz and Klein (1981) consider the same model as we do. The ratio (17) has also been estimated by Seitz and Klein (1981) and their value 0.314 agrees well with ours.

In table 2 we have also included the results (Caracciolo and Glaus 1984) of the two-dimensional simulation for the lattice trees and the bond self-avoiding lattice trees, for which the self-avoiding constraint is imposed on the bonds (not on the sites) and therefore loops are allowed to be formed.

In conclusion we have, together with a previous study (Caracciolo and Glaus 1984), given strong support to the Parisi-Sourlas dimensional reduction for branched polymers. It seems therefore worthwhile to try to understand the various approximations involved in this reduction from a more rigorous viewpoint.

It is a pleasure to thank S Caracciolo and A Sokal for stimulating discussions and Jürg Fröhlich for his interest. This work was supported by the Swiss National Science Foundation.

References

Beretti A and Sokal A D 1985 *J. Stat. Phys.* submitted for publication
Bovier A, Fröhlich J and Glaus U 1985 *Lecture Notes of Les Houches Summer School 1984* to appear
Caracciolo S and Glaus U 1984 *J. Stat. Phys.* submitted for publication
Fisher D S, Fröhlich J and Spencer T 1984 *J. Stat. Phys.* **34** 863
Gaunt D S, Sykes M F, Torrie G M and Whittington S G 1982 *J. Phys. A: Math. Gen.* **15** 3209

Gould H and Holl K 1981 *J. Phys. A: Math. Gen.* **14** L443
Imbrie J Z 1984 *Phys. Rev. Lett.* **53** 1747
Isaacson J and Lubensky T C 1980 *J. Physique Lett.* **41** L469
Knuth D E 1973 *The art of computer programming* vol 3 (Reading, MA: Addison Wesley)
Lubensky T C and Isaacson J 1970 *Phys. Rev.* A **20** 2130
Parisi G and Sourlas N 1981 *Phys. Rev. Lett.* **46** 871
Peters H P, Stauffer D, Hölters H P and Loewenich K 1979 *Z. Phys.* B **34** 399
Redner S 1979 *J. Phys. A: Math. Gen.* **12** L239
Seitz W A and Klein D J 1981 *J. Chem. Phys.* **75** 5190