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Two-Dimensional Lattice Tree Exponents and Amplitudes: Simulation Algorithms Versus Series

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We use a local Monte Carlo algorithm to simulate lattice trees in two dimensions for the site and bond problem. We investigate the properties of radius of gyration, perimeter-to-site ratio, and vertex degree in a tree, adding some new results in the site problem, compare our results on their noncritical properties with those obtained from earlier reversible and slightly nonreversible algorithms, and combine our determinations with new exact series expansion data. On the controversy surrounding the possible lack of universality for the first confluent singularity for the gyration radius, we feel that conclusions must be guarded.

KEY WORDS: Lattice trees; Monte Carlo radius; perimeter; corrections to scaling.

1. INTRODUCTION

The knowledge of the characteristic parameters of lattice trees and their critical properties has been a specific point of interest, since it has topological similarities with branch polymers in dilute solution (i.e., the vertices act as monomers and the edges as chemical connections). On the other hand, there is clear evidence in favor of the fact that lattice trees share the same universality class as the lattice animals, as demonstrated by several authors.[12,15,6]

In any microcanonical ensemble simulation of a lattice tree by the Monte Carlo method, the mean radius of gyration for a fixed number of s

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sites is the key which expresses common critical parameters with the other systems and is defined for large s as

$$R_g = A's^{\nu}(1 + B's^{-\Delta_1} + \cdots) \tag{1}$$

where ν is the leading exponent, and Δ_1 is the correction-to-scaling exponent, while A' and B' are the specific amplitudes.

Several methods were used to determine ν, and the convergence is toward 0.641, indicated by Derrida and DeSeze[2] and Kertész,[11] in contradiction to the mean-field value given by the Flory approximation of $5/8 = 0.625$.

The value of Δ_1 has not been limited to a narrow band, and remains a bone of contention. From the first value presented by Guttmann and Gaunt[8] of $\Delta_1 \approx 1$ and the evidence of $\Delta_1^{\text{bond}} > \Delta_1^{\text{site}}$, other values presented by several authors (for lattice animals[7,13,1] and for lattice trees[9]) are between 0.635 and 0.87.

In the present work we calculate by a local Monte Carlo algorithm for the bond and site problem in two dimensions all the parameters in the R_g relation (1) for large n, especially the value of Δ_1, to see from this algorithm the extent to which we can get at more solid value.

Besides the mean value of the radius of gyration, we calculated the mean ratio of number of perimeter sites to the number s of occupied sites ($K = \langle t/s \rangle$) (designating the perimeter-to-site ratio, where perimeter is defined in the percolation sense), strongly believed to follow the law

$$K \cong a + bs^{-1} \tag{2}$$

and the vertex degree in a tree, which is the fraction of sites s with v bonds connected to it[15,10]

$$\lim_{s \to \infty} \frac{\langle v_i \rangle}{s} = \zeta_i, \qquad 1 \leqslant i \leqslant z \tag{3}$$

In Section 2 we describe the algorithm, which uses the permanent data structure akin to that used by Duarte[3] and Duarte and Cadilhe,[5] since we need the perimeter information to calculate K. Finally, in Sections 3 and 4 we present the results and conclusions.

2. MONTE CARLO ALGORITHM

The lattice tree is basically an unrestricted branched self-avoiding walk. The simulation procedure we adopted is a local Monte Carlo algorithm and can be identified as the "leaf mover" algorithm used by Seitz and

Klein[15] and Janse van Rensburg and Madras.[10] The whole process consists in the replacement of an extreme site (site with valence equal to one) from its position to a new one. Although, both simulations—site and bond problem—make the same movement, the steps to do so differ from one another. In the site problem, we generate a new tree as follows:

1. Randomly pick one of the s sites of a tree.
2. If it is not an extreme site, we leave the site in its place and return to step 1. Otherwise, we remove the site.
3. Randomly choose one of the $s-1$ remaining sites, and randomly choose one of the z bonds emanating from it.
4. If the other site at the end of that bond is occupied, we return to step 1. Otherwise, we check if it creates a cycle.
5. If a cycle would be created, it is a failure, and we return to step 1. If not, we have a successful transition and we update the old tree before going to step 1 for the next attempt.

This procedure is different from the bond problem in the choice of the removing site and in the absence of cycle checking. If in the site problem it was enough to pick an extreme, in the bond problem it is also necessary to pick, with a probability of $1/z$, the direction to which it is connected. Once we check the state of the site after choosing a bond, the existence of a cycle is totally forbidden.

The algorithm description is reversible, since the probability to move an extreme site and reverse the process is the same:

$$\frac{1}{s}\frac{1}{s-1}\frac{1}{z} \qquad \text{for the site problem} \tag{4}$$

and

$$\frac{1}{s}\frac{1}{s-1}\frac{1}{z^2} \qquad \text{for the bond problem} \tag{5}$$

In either problem and for each run of fixed site, we performed a total of 10^7 iterations. For every thousand iterations, namely N, we took an average, thus obtaining a data point. Hence our results are averages over 10,000 data points. For this total number of iterations, the program structure proved to be efficient; the largest run time, which corresponds to the site problem with $s = 1900$, took a total time of 15.2 hr of computer time on a DEC5000 server (with RISC technology). At each value of s the initial tree was randomly generated. For values of $s \geqslant 500$, we performed ten runs to stabilize the variables.

3. RESULTS

3.1. The Mean Radius of Gyration

The mean radius of gyration is represented in Table I and plotted on a log–log plot in Fig. 1. We used a power law for this value of the form

$$R_g = A' s^{\nu} \tag{6}$$

The results are for the leading exponent $\nu(\text{site}) = 0.639 \pm 0.020$ and $\nu(\text{bond}) = 0.622 \pm 0.020$ with the amplitudes $A'(\text{site}) = 0.449 \pm 0.20$ and $A'(\text{bond}) = 0.389 \pm 0.020$ and our error bars are only statistical. Apart from the fact that the value for the site problem is in good agreement with the value of 0.64, a closer look at the graph shows in this case that the $s = 10$ and $s = 1900$ values are out of the main direction and for the bond problem the values greater than $s = 700$ force a value of ν lower than what might be expected. The analysis without the referenced values indicates for the leading exponents $\nu(\text{site}) = 0.636 \pm 0.010$ and $\nu(\text{bond}) = 0.637 \pm 0.10$, and for the correspondent amplitudes $A'(\text{site}) = 0.469 \pm 0.013$ and $A'(\text{bonds}) = 0.360 \pm 0.020$. Both values of ν are in agreement with the results from the finite-size scaling renormalization value for the site animals problem of $\nu = 0.6408$.[2,11]

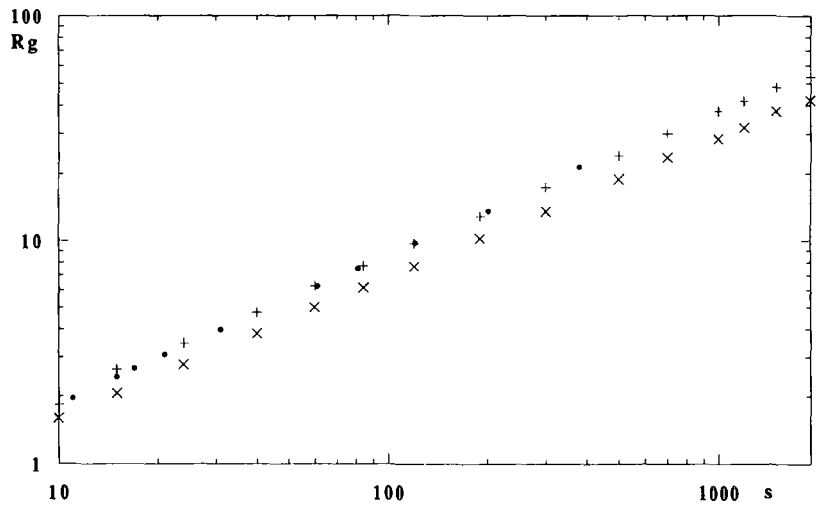

Fig. 1. Log–log plot of R_g versus n for the site (+) and bond (×) problem, and for the site (●) problem of Duarte.[3]

Table I. Mean Radius of Gyration[a]

n	R_g (bond)	R_g (site)
10	1.5950(2)	1.8365(2)
15	2.0627(5)	2.6338(5)
24	2.768(1)	3.441(1)
40	3.811(3)	4.748(3)
60	4.999(5)	6.236(6)
84	6.142(7)	7.697(8)
120	7.64(1)	9.67(1)
190	10.19(1)	12.84(1)
300	13.49(2)	17.32(2)
500	18.82(2)	23.96(3)
700	23.63(3)	30.00(4)
1000	28.51(3)	37.69(5)
1200	31.91(4)	41.73(5)
1500	37.77(5)	48.15(6)
1900	42.09(5)	53.42(5)

[a] Error bars are standard deviations.

Defining $\nu = 0.6408$, we tried to obtain the correction-to-scaling exponent Δ_1, dividing R_g by s^ν, and fitted the values to the law

$$\frac{R_g}{s^\nu} = A' + Cs^{-\Delta_1} \tag{7}$$

A plot of R_g/s^ν versus s is very irregular and any fitting to the Eq. (6) extremely disappointing, even when restricted to lower sizes, where the correction term in Eq. (7) could be expected to slow up.

We tried to obtain Δ_1 by reanalyzing the series of R_g presented by Ishinabe[9] with the finite-size scaling renormalization method[14] to A' and Δ_1 with $\nu = 0.6408$, and through an unbiased Padé method used by Adler *et al.*[1] to ν and Δ_1.

For the bond problem, Fig. 2 represents the $A(\Delta_1)$ curves for $s = 10$–14. We get $\Delta_1 = 0.665 \pm 0.02$ and $(A')^2 = 0.1216 \pm 0.001$, but these values show a dependence on the ν variations. For the second method (Fig. 3), we do not have a definite region, although for the known ν we should expect a Δ_1 between 0.6 and 0.7.

3.2. The Perimeter-to-Site Ratio and Vertex Degree per Site

The perimeter-to-site ratio calculation differs for the site and bond problems. While for the site problem we used the simulation data, in the

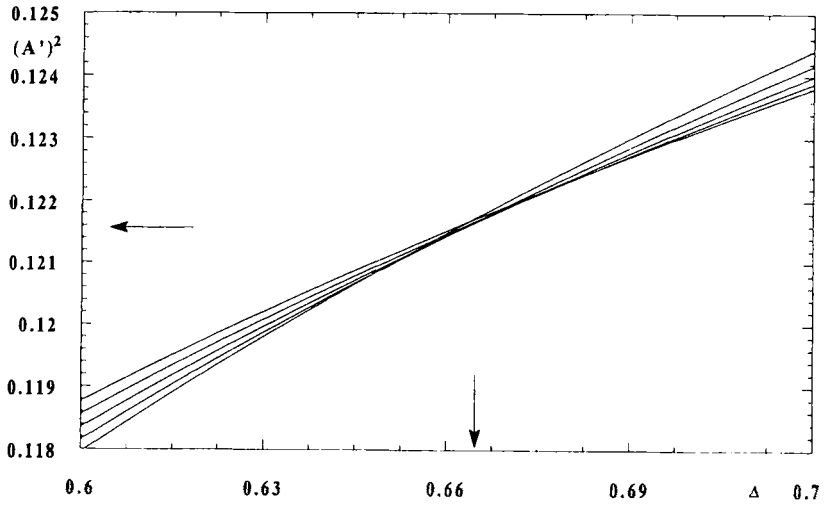

Fig. 2. Curves of $[A'(\Delta_1)]^2$ for input $v = 0.6408$ for the bond problem.

bond problem we used the perimeter polynomials for the site problem[16] to extract the corresponding perimeter polynomials for trees by the dual lattice (we reached $b = 9$ for this previously nonexistent series).[4]

Figure 4 shows the values of the site and bond, and also the results obtained by Duarte[3] for the perimeter-to-site ratio in the site problem.

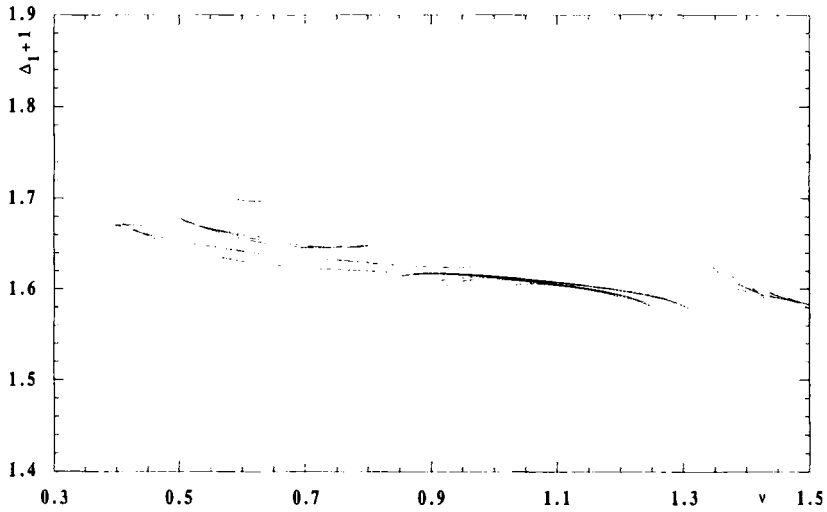

Fig. 3. Plot of Padé approximants to $\Delta_1 + 1$ as a function of v.

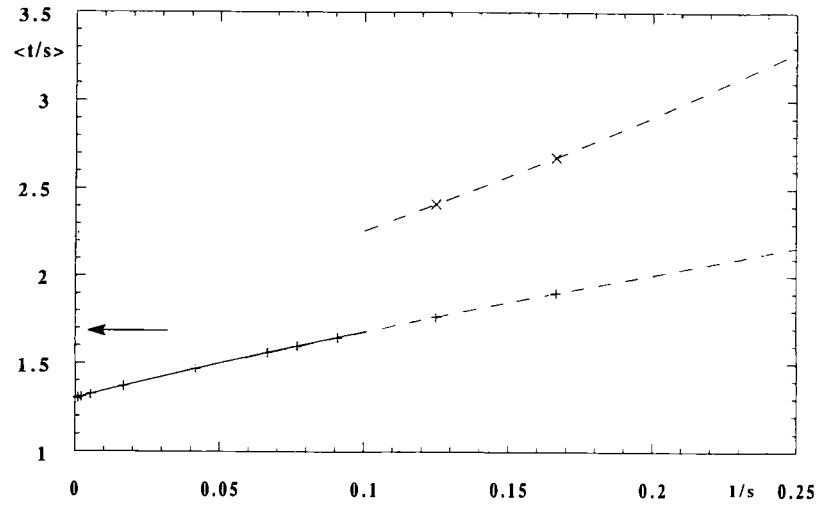

Fig. 4. Plot of $K = \langle t/s \rangle$ versus $1/s$ for site (+) and bond (×) from exact results (dashed line) and Monte Carlo studies (solid line).

The extrapolation to $s \to \infty$ is $K(\text{site}) = 1.303 \pm 0.003$ and Neville tables compounded with fittings leads to a limiting ratio estimate of $K(\text{bond}) = 1.68 \pm 0.02$.

The vertex degree per site results are listed in Table II. The results of the bond problem are in agreement to those presented by Seitz and Klein[15] and van Rensburg and Madras.[10] For the site problem, they have been calculated for the first time.

4. DISCUSSION AND CONCLUSION

The R_g computed for every size with this constant number of iterations has proved to be insufficient for large trees. This constant number divided by the size of a tree can define the mobility degree of a site. In this

Table II. Mean Fraction of Vertices of Degree i[a]

	ζ_1	ζ_2	ζ_3	ζ_4
Bonds	0.2644(2)	0.4965(3)	0.2177(1)	0.02531(6)
Sites	0.2005(2)	0.6097(4)	0.1790(1)	0.01071(5)

[a] Error bars are standard deviations.

context, we say that for a size of 50 sites, each one has a new position for 20 times on average, in contrast to the largest tree used ($s = 1900$), where only half of the tree gets moved around. So, for larger trees each site should have at most one move on average.

The leading exponent of 0.637(10) for site and bond problem estimated in this paper reinforces the value of 0.640 from the best estimates of Derrida and DeSeze[2] and Kertész[11] and the successive Monte Carlo studies.[15,3,10]

In our Monte Carlo results, the amplitude A' for the bond problem stays between the results obtained by Ishinabe,[9] $(A')^2 = 0.1156$, and van Rensburg and Madras,[10] $(A')^2 = 0.1248$, which they calculated with the correction-to-scaling exponent $\Delta_1 = 0.635$ from Ishinabe. However, we can reliably say that we can expect A' to be a value between the Monte Carlo results and the reanalyzed Privman–Fisher estimators from Ishninabe's R_g series, which show a slightly higher value, since the ν used here is lower than 0.644, of $A' = 0.355 \pm 0.010$. For the site problem and to our knowledge, $A' = 0.469 \pm 0.013$ is new.

The Δ_1 in our analyses, not only in the Privman–Fisher estimators with $\nu = 0.6408$, as well as in the Adler unbiased estimators, are in agreement with the value obtained by exact series analyses from Ishinabe[9] of 0.635, against the commonly accepted value $\Delta_1 = 0.87 \pm 0.06$ for lattice animals given by Guttmann.[7] Note in Fig. 3 that $\nu \approx 0.64$ shows no clear confluence (Δ_1 would be, as quoted, 0.6–0.7). Much better convergence occurs in the $\nu = 1.1$–1.3 range at $\Delta_1 = 0.6$.

Finally, if we allow for the need of a permanent perimeter information, the calculation of K leads to a permanent data structure similar to the biased algorithm of Duarte[3] and the estimation of this property in his work as well as in this one does not show any evidence of systematic bias influencing the perimeter-to-site ratio results or ν. Clearly, for these two properties, his Markov evolution, much smaller than either of van Rensburg and Madras[10] or ours (around 10 times larger), does not create a noticeable drift effect on either. Notice, on the other hand, that there is outstanding agreement between our vertex degree partitions and those of Seitz and Klein[15] and van Rensburg and Madras.[10] This is encouraging, particularly in the light of three-dimensional studies that we are currently undertaking, with a much enlarged set of topological variables.

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