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Relaxation Monte Carlo for 3D Branched Polymers: The Leading Confluence Exponent

J. A. M. S. Duarte[1,2] **and Antonio M. R. Cadilhe**[1]

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A relaxation study of simple-cubic site trees taking 18 months of CDC Cyber computer time is used to estimate the radius-of-gyration dependence on the size, both as regards the correlation exponent and the confluent correction. The latter is found to be compatible with an analytic term within the uncertainty limits. The radius prefactor is estimated as 0.542 ± 0.005 and the limiting site perimeter-to-size ratio as 2.905 ± 0.005.

KEY WORDS: Branched polymers; relaxation; Monte Carlo; correction to scaling.

1. INTRODUCTION

Among branched lattice polymers, trees (i.e., polymers with no closed loops) have been a favored model for the study of the corresponding universality class which they share in common with unrestricted polymers (i.e., polymers with or without loops).[1-3]

For that purpose specific simulation techniques have grown in sophistication[4-6] and now the critical fugacity and the critical exponent Θ for the total number of trees can also be obtained from Monte Carlo studies through very detailed procedures.

By extending to three dimensions the relaxation method described in a previous pilot paper on two-dimensional square trees,[4] we have attempted to achieve sufficiently long runs to study the radius-of-gyration evolution in detail. The correlation exponent ν is 0.5[7] and this enables us to write

$$Rg(n)/n^{\nu} = A + Bn^{-\phi} + \cdots \tag{1}$$

[1] CIUP and CFUP Faculdade de Ciencias, 4000 Porto, Portugal.
[2] Institut für Teoretische Physik, 5000 Cologne 41, Federal Republic of Germany.

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where Rg is the average radius of gyration and ϕ the confluent correction exponent.

The values for this exponent, mostly ranging well below 1 and due exclusively to unrestricted polymers, are summarized in ref. 8, where a value $\phi = 1.10 \pm 0.01$ for simple cubic bond polymers and a global estimate of $\phi = 1.3 \pm 0.2$ have been found. The Monte Carlo tree studies, on the other hand, have always assumed $\phi = 1$ for both Θ and ν, even in two dimensions.[5,6]

The relaxation procedure for trees,[4] adopted from earlier looped polymer simulations,[9,10] randomly chooses an endpoint of a tree, deletes it, and adds a perimeter site if this operation does not close a loop. Starting from an initial configuration chosen at random, the process is then iterated.

2. DATA ANALYSIS

For the present simulation, tree sizes varied from 7 to 151 with between 15 and 30 million iterations in an average of 130 runs for each size. By labeling the perimeter and end sites, we compressed their arrays without the use of any hash procedure, so that the time spent per million iterations increased by only 10% between sizes 7 and 51, for example. Even so, we had to rely on extensive use of a Cyber 830 for the 540 CPU days of this simulation (the speed would be 20 times faster on a Cyber 855).

The average perimeter-to-size ratio was a quantity that seemed appropriate to monitor the accuracy of the method. For size values 7, 9, and 11 the difference between the exact series expansions (J. A. M. S. Duarte, unpublished) and the Monte Carlo values was 0.2%.

The evolution of the Monte Carlo values, however, is a definite improvement over the series, which do not extrapolate in agreement with the overall behavior of two- and three-dimensional polymers.[4,11,12] On the contrary, Monte Carlo results converge smoothly to a linear dependence on the inverse size with

$$\langle t/s \rangle \approx 2.905 \pm 0.005 \tag{2}$$

as shown in Fig. 1.

Once again, as for site square trees,[4] this ratio falls closer to the unrestricted animal value (2.78 ± 0.04[11]) than to the upper limit ratio 4.

For the radius of gyration, the leading dependence on ν is well satisfied and the confluent factor can be isolated according to Eq. (1). We have fitted the sequence of values extensively, trying to determine the asymptotic behavior of ϕ. Figure 2, where the data are plotted against, respectively, $\phi = 1.2$, 1.0, and 0.8, is a good graphic summary of our conclu-

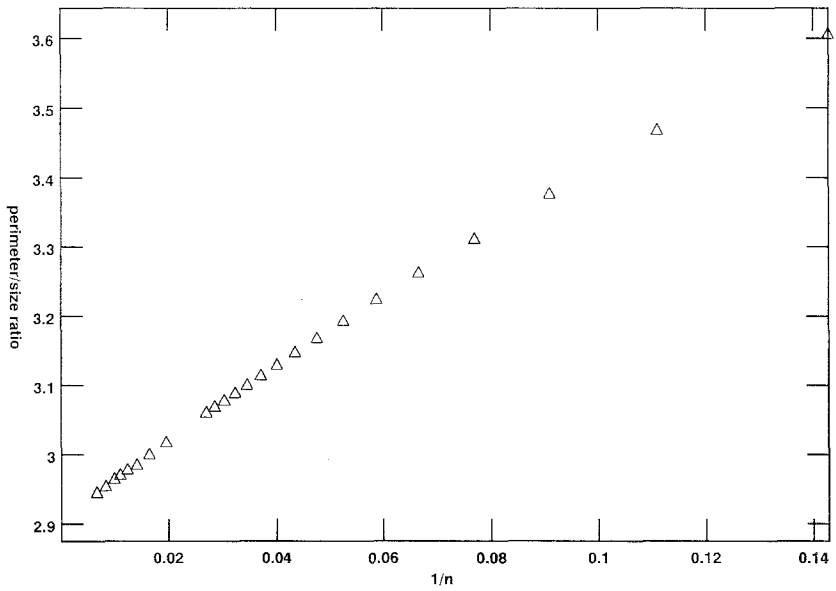


Fig. 1. Average perimeter-to-size ratio for cubic site trees plotted against the inverse size.

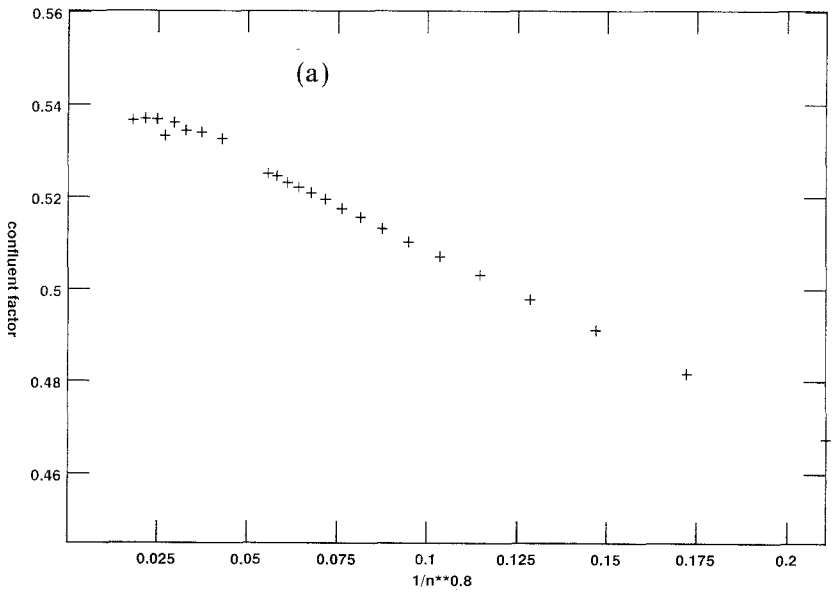
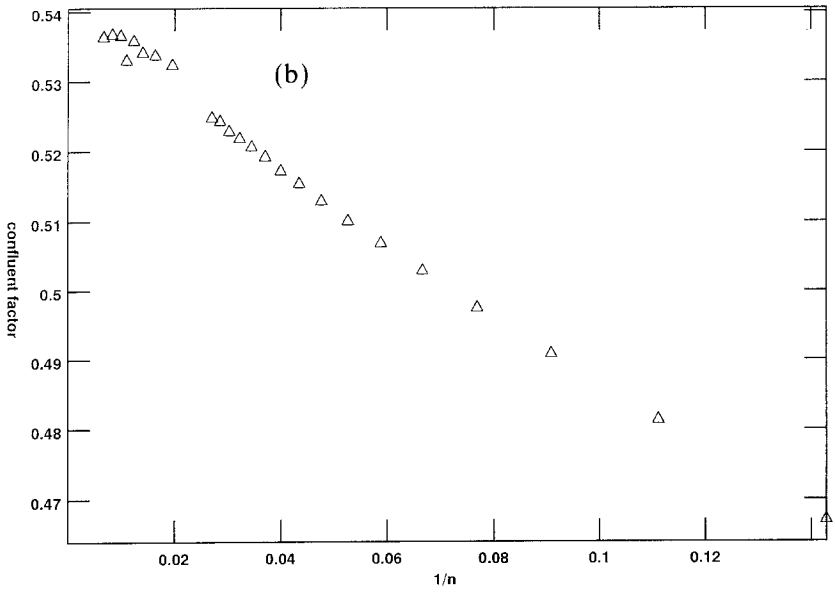


Fig. 2. Confluent factor, Eq. (1), plotted against (a) $(1/n)^{**}0.8$ (†), (b) $1/n$ (△), (c) $(1/n)^{**}1.2$ (○).



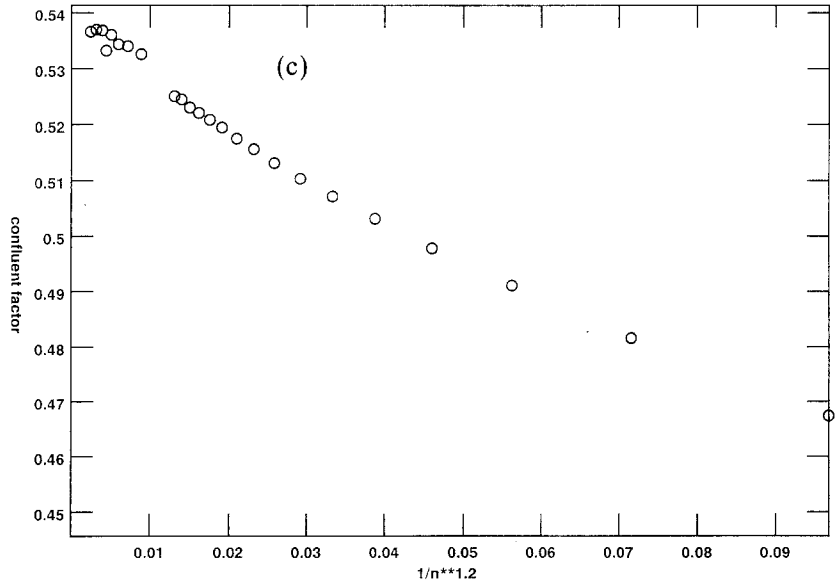


Fig. 2 (*continued*)

sions. The first section of values is well fitted to an exponent around 0.8, which increases steadily to 1.0 toward the end of it. The second set of points, for size values over 51, is very scattered and would bring the value of ϕ close to 1.1. Higher values, however, are in poor agreement with the initial section (as can be seen from the noticeable curvature in their plots in Fig. 2).

We believe that this attempt at a Monte Carlo 3D confluent correction is in broad agreement with an exponent ϕ around 1.0 that might include both 0.8 and 1.1. The last value was found for cubic bond polymers with loops in ref. 8 and therefore it seems plausible that the identity of exponents between trees and unrestricted polymers should extend to the confluent terms also.

In fact, since the set of critical exponents corresponds to those of the Yang–Lee edge singularity in one dimension,[7,8] our result can be seen to be in good, unforced agreement with the analytic correction obtained for that case. Our estimated value of $A = 0.542 \pm 0.005$ tries cautiously to reflect the consequences of this range of possible ϕ values.

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