

Critical exponents and universal amplitude ratios in lattice trees

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Lattice trees are generated by a cut-and-paste algorithm to collect data to estimate critical exponents. We are particularly interested in the effects of corrections to scaling on the estimated values of the exponents and we find that a sizable systematic error is introduced if corrections are ignored. Indeed, our final error bars are largely due to systematic errors (which we estimate by using different empirical finite size formulas as models for our data), while statistical error bars contribute only a small fraction. This fact suggests that the estimate of a critical exponent for lattice trees by fitting Monte Carlo data to an empirical finite size formula may ignore a sizable systematic error. The exponents ν and ρ are estimated in dimensions 2–7. In addition, the exponent Δ (associated with confluent corrections) is estimated and the universal amplitude ratios associated with scaling in the mean square radius of gyration and the mean span and with the mean longest path and mean branch size are computed. [S1063-651X(98)05209-X]

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I. INTRODUCTION

The numerical and theoretical study of *lattice trees* provides a natural model for calculating the properties of branched polymers in dilute solution. Lattice trees belong to the same universality class as lattice animals [1–3] and the critical exponents of lattice trees will therefore be the same as for lattice animals. In this same universality class are subcritical percolation clusters [4]. For a description of the phase diagram of interacting lattice trees and animals see the work of Gaunt and Flesia [5], Flesia and Gaunt [6], Flesia *et al.* [7], Janse van Rensburg and Madras [8], and Madras and Janse van Rensburg [9].

Lattice trees are connected acyclic subgraphs of the lattice, with vertices representing monomers and edges the bonds between monomers. There are powerful Metropolis Monte Carlo algorithms for the simulation of lattice trees [8] and these can be used to estimate some observables associated with a uniformly weighted ensemble of lattice trees of fixed number of vertices. In particular, one may wish to estimate the “mean size” of a tree or make estimates of quantities that measure the internal structure of a tree (such as the number of edges in a longest path). The size of a lattice tree can be measured in several ways. We used the following observables to estimate the size of lattice trees (all averages are over uniformly weighted lattice trees with a fixed number of vertices and we assume that the tree contains n vertices).

(i) The mean square radius of gyration of a lattice tree is defined by

$$R_n^2 = \frac{1}{n} \sum_{i=1}^n [\mathbf{r}(v_i) - \mathbf{r}_c]^2,$$

where $\mathbf{r}(v_i)$ is the position vector of the i th vertex of the tree and \mathbf{r}_c is the position vector of the center of mass of the tree. The ensemble average $\langle R_n^2 \rangle$ is the uniform mean of R_n^2 over all trees with n vertices.

(ii) The mean span of a lattice tree is defined by

$$S_n = \frac{1}{d} \sum_{k=1}^d \max_{1 \leq i, j \leq n} |x_k(v_i) - x_k(v_j)|,$$

where $x_k(v_i)$ is the k th coordinate of the i th vertex in the tree.

The intrinsic structure of a lattice tree may be imagined as the longest path (in the tree), decorated with “branches.” The mean sizes of the longest path and branches can also be observed; we define these by the following.

(a) A path P_{ij} with first and last vertices v_i and v_j in a lattice tree is the shortest walk in the tree from vertex v_i to vertex v_j . The longest path is defined by

$$P_n = \max_{i,j} \{|P_{ij}|\},$$

where $|P_{ij}|$ is the number of edges in the shortest walk from vertex i to vertex j [17,18].

(b) Let e be an edge in a tree T ; then $T-e$ consists of two subtrees (one can be a single vertex), the smaller of these is called a branch. The number of edges in the branch is its size, denoted B_n . The ensemble average $\langle B_n \rangle$ is the uniform average over all possible choices of e in T and over all lattice trees.

The end-to-end (Euclidean) distance of the longest path should yet define another quantity that can be used to define a size of the tree; this distance should also define a length scale in the tree and we define it as follows. Let P_{ij} be the longest path in the tree T and let its end vertices be v_i and v_j . The end-to-end distance of the longest path in the tree is the Euclidean distance between v_i and v_j :

$$E_n = \|\mathbf{r}(v_i) - \mathbf{r}(v_j)\|_2.$$

It is commonly accepted that these quantities scale with n as

$$\langle R_n^2 \rangle \sim n^{2\nu}, \quad \langle S_n \rangle \sim \langle E_n \rangle \sim n^\nu, \quad (1)$$

$$\langle P_n \rangle \sim n^\rho, \quad \langle B_n \rangle \sim n^\epsilon, \quad (2)$$

where ν , ρ , and ϵ are critical exponents. It is believed that $\rho = \epsilon$ and we will accept this as fact in this paper [10]. The exponent ν is the *metric exponent*. It has value $\frac{1}{2}$ in three dimensions [11] and its mean field value is $\frac{1}{4}$ [12]. The exponent ρ has the mean field value $\frac{1}{2}$ [10].

II. ESTIMATING THE CRITICAL EXPONENTS

In this paper we examine the above scaling relations in dimensions 2–7 using the Monte Carlo approach for lattice trees developed in the paper by Janse van Rensburg and Madras [10]. In particular, we are interested in obtaining high-quality estimates of ν and ρ from the expressions in Eqs. (1) and (2), as well as estimates of the eigenvalues of the mean square radius of gyration tensor. We will indicate the mean eigenvalues of this tensor by $\langle \lambda_i \rangle$, where $i=1$ will indicate the largest and $i=d$ the smallest in d dimensions. The determinant of this matrix also scales with n : in d dimensions it should scale as $n^{2d\nu}$ and we will collect data on it as well. In the second instance, we will also be interested in the universal amplitude ratios for lattice trees, in particular, we will consider ratios of the general form

$$\left\langle \frac{Z_n}{Y_n} \right\rangle, \quad \left\langle \frac{Z_n}{Y_n} \right\rangle, \quad (3)$$

where Z_n and Y_n will be observables of lattice trees measured by the algorithm with the same scaling exponents. We will be mostly interested in cases where $Z_n = S_n^2$ with $Y_n = R_n^2$ and $Z_n = P_n$ with $Y_n = B_n$. In addition, we will also consider ratios involving other quantities, such as $\langle E_n \rangle$ and the mean largest eigenvalue of the radius of gyration matrix $\langle \lambda_1 \rangle$.

We sampled along a Markov chain in the state space of lattice trees (uniformly weighted) using a cut-and-paste algorithm in two to seven dimensions [10], while we collected data on the mean square radius of gyration, the mean span, the mean end-to-end distance of the longest path, the mean longest path, the mean branch size, the mean square radius of gyration matrix, and its mean largest eigenvalue. Runs were performed on trees of sizes from $n=25$ to 2000 edges, while data were taken every n steps for a sample size of 50 000 (thus a total of 50 000 n attempted iterations of the algorithm was performed for each value of n). Our immediate motivation is to obtain high-quality data for the estimation of the critical exponents ν and ρ in dimensions 2–7. In the case of the exponent ν we will attempt to obtain estimates for comparison with the results from series analysis of animals [13] and Monte Carlo of lattice trees in dimensions 2–4 [10]. In the case of the exponent ρ we hope to improve on the results in two to four dimensions in [10] and to compute the value of this exponent in dimensions 5–7.

Estimates of exponents from data collected by sampling along a Markov chain with a Metropolis Monte Carlo algorithm is usually done by assuming a model that accounts for finite size corrections to scaling (and based on some theoretical insights gained from scaling theory or the renormalization group). Within the reference frame of the assumed model, a least-squares analysis can be used to find best esti-

TABLE I. Estimates of metric exponent $\nu(R^2)$, $\nu(S)$, and $\nu(E)$.

d	$\nu(R^2)$	$\nu(S)$	$\nu(E)$
2	0.6375(10)(64)	0.6500(14)(200)	0.6458(13)(56)
3	0.4932(10)(65)	0.5111(13)(180)	0.4970(10)(35)
4	0.4102(10)(74)	0.4342(12)(240)	0.4101(10)(49)
5	0.3519(10)(29)	0.3851(15)(280)	0.3528(10)(35)
6	0.3124(10)(53)	0.3527(22)(420)	0.3149(10)(110)
7	0.2866(10)(84)	0.3000(10)(16)	0.2897(15)(140)

mators for the parameters in the model, including the exponents, and if the autocorrelation time of the Markov chain is known, then a statistical confidence interval can be assigned (see the appendix in Ref. [19] for details). On the other hand, the results from such an analysis are conditioned on the assumed model and a different model may give a different best estimate. This observation is indicative of the presence of a systematic error in the best estimate and if we knew the correct model, then it would be possible to correct for it. In our case, this is not possible and we had to find a way of estimating a systematic error in our estimates by trying a few related, but different, models (each of which accounts for finite size effects in a different way). The absolute maximum difference in the results from the different models will be assumed to indicate the size of a possible systematic error.

It is known that a ‘‘confluent correction’’ is present in the scaling assumptions in Eqs. (1) and (2) and we will pay particular attention to the effect this confluent correction may have on the values of estimated exponents. The confluent correction modifies Eq. (1) to $\langle R_n^2 \rangle = An^{2\nu}(1 + Bn^{-\Delta})$, where Δ is the confluent exponent. The exponents and amplitudes were estimated using a weighted least-squares analysis: We tracked the least-squares error (which is distributed as a χ^2 statistic) as a measure of goodness of fit, while we discarded data points at the smallest values of n . We accepted a fit as good if the χ^2 statistic is acceptable at the 95% level. We tried this procedure for several models, including

$$\log \langle R_n^2 \rangle = \log A + 2\nu \log n, \quad (4)$$

$$\log \langle R_n^2 \rangle = \log A + 2\nu \log n + Bn^{-0.5}, \quad (5)$$

$$\log \langle R_n^2 \rangle = \log A + 2\nu \log n + Bn^{-\Delta}. \quad (6)$$

The first two models [Eqs. (4) and (5)] are linear models that can be solved using standard numerical procedures (in the

TABLE II. Estimates of metric exponent $\nu(\lambda_1)$ and $\nu(\det)$.

d	$\nu(\lambda_1)$	$\nu(\det)$
2	0.6372(11)(58)	0.6378(12)(52)
3	0.4936(10)(86)	0.4926(10)(55)
4	0.4109(13)(19)	0.4069(10)(21)
5	0.3521(12)(84)	0.3516(10)(23)
6	0.3098(11)(190)	0.3148(10)(99)
7	0.2857(10)(68)	0.2946(10)(180)

TABLE III. Best estimates of metric exponent ν .

d	ν_d
2	0.642 ± 0.010
3	0.498 ± 0.010
4	0.415 ± 0.011
5	0.359 ± 0.011
6	0.321 ± 0.019
7	0.291 ± 0.011

TABLE IV. Estimates of branch exponent ρ .

d	$\rho(P)$	$\rho(B)$	Best estimates
2	0.7391(10)(81)	0.7365(20)(81)	0.738 ± 0.010
3	0.6548(10)(48)	0.6507(10)(50)	0.653 ± 0.006
4	0.6091(10)(70)	0.6054(10)(11)	0.607 ± 0.006
5	0.5793(10)(110)	0.5758(10)(45)	0.578 ± 0.009
6	0.5548(19)(120)	0.5528(10)(140)	0.554 ± 0.015
7	0.5268(10)(31)	0.5338(13)(150)	0.530 ± 0.011

second model we assumed that $\Delta=0.5$). The third model required a nonlinear analysis, which was done using a quasi-Newton procedure, with Δ a parameter of the model. The absolute differences in the estimates of exponents and amplitudes from these analysis were used as estimates of a systematic error in our results (and is presumably due to corrections to scaling that our models could not account for). The best estimates for exponents and amplitudes were taken from successful two-parameter fits, with their associated confidence intervals. Our analysis could not in any case settle on a consistent value for the exponent Δ and we will assume that only an effective exponent is observed (the values of Δ varied between 0.35 and 0.75 in two dimensions, encompassing the estimates in the work by Margolina, Family, and Privman [14], Adler *et al.* [13], Ishinabe [15] and Gonçalves [16]). Our estimates for ν are tabled in Table I. Each entry is presented as the best estimate(statistical error)(systematic error).

The exponent ν can also be obtained by analyzing data obtained from the largest eigenvalue of the radius of gyration matrix or from its determinant. We analyzed these measurements similarly to the data presented in Table I and we list our results in Table II. It turned out to be significantly more difficult to find satisfactory fits to the determinant of the radius of gyration matrix: Indeed, we were generally unable to find satisfactory (acceptable at the 95% level) four-parameter fits to Eq. (6) in this case. [This is perhaps not surprising; the analysis using Eq. (6) is a four-parameter nonlinear model and involves a numerical procedure that

searches a four-dimensional parameter space for a global minimum in the least-squares error. Since the parameter space is so large, one may expect that the procedure may have difficulty converging to a global minimum, especially if there are random statistical uncertainties in the data produced by the the Monte Carlo simulation.]

The three models produced different estimates for ν , as is apparent in Tables I and II. Indeed, this model dependence illustrates the inadequacy of these models in determining ν ; in particular, corrections to scaling *are* important in determining ν and ignoring them introduces a systematic error that often *exceeds* the statistical errors computed from the regressions. We draw attention to this since the standard approach to estimating exponents from numerical data often focuses on only one model for a single quantity (such as the end-to-end length). While this approach is often out of necessity, it is clearly inadequate if a “true” error bar is to be assigned.

The exponent ν was also computed by Gonçalves by the Monte Carlo method ($\nu=0.637 \pm 0.010$) [16]. Our statistical error bars are roughly a factor of 10 better than this, but the systematic errors in Tables I and II are roughly comparable to this error. Estimates of ν in dimensions 2–7 were also made by Adler *et al.* [13] using a series analysis for lattice animals. Our statistical confidence intervals are also roughly a factor of 10 smaller than the results in that paper, and if we combine our 95% confidence intervals with our systematic errors, then we get about the same error as reported there. By combining the data in Tables I and II we list our best esti-

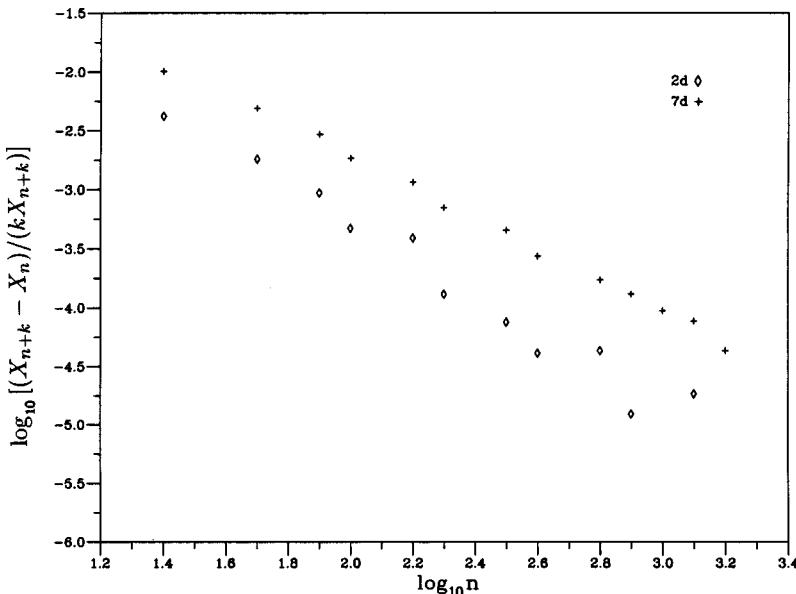


FIG. 1. Plot of $\log_{10}[(X_{n+k}-X_n)/kX_{n+k}]$ against $\log_{10} n$ for $X_n = \langle S_n \rangle^2 / \langle R_n^2 \rangle$ in two and seven dimensions.

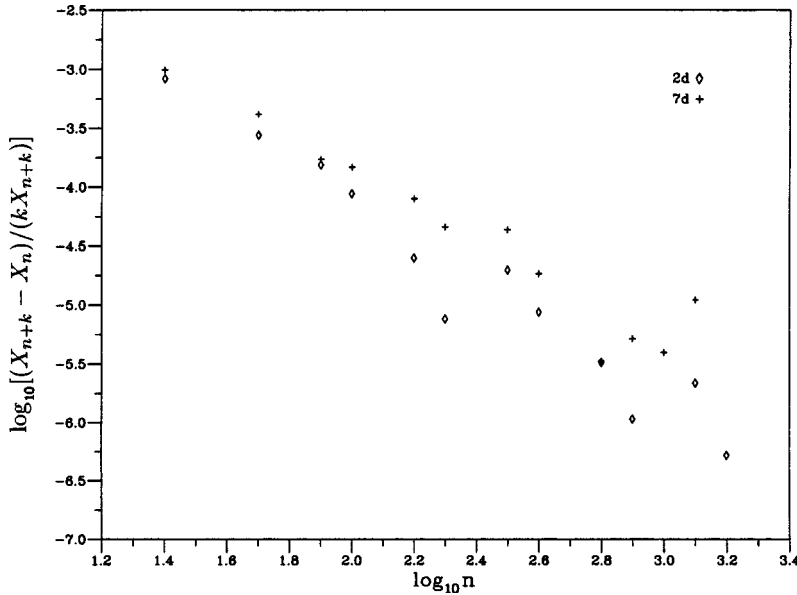


FIG. 2. Plot of $\log_{10}[(X_{n+k}-X_n)/kX_{n+k}]$ against $\log_{10} n$ for $X_n = \langle P_n \rangle / \langle B_n \rangle$ in two and seven dimensions.

mates for ν in Table III (the error bars are taken to be the sum of our statistical and systematic errors). Notice that the error bars in the tables are largely due to systematic errors; the 95%-confidence intervals make only a small contribution.

The data collected for mean longest paths and mean branch sizes were analyzed in a fashion similar to ν above, with models corresponding to those in Eqs. (4)–(6). We list the results in Table IV and our best estimates are stated in the third column of that table. Similarly to the case for ν , we find that regression by the model in Eq. (6) fails to give a consistent value for Δ and we believe that, at best, only an effective exponent is seen. The values of ρ decreases with increasing dimensions to its mean field value of $\frac{1}{2}$ as expected [10], indicating that the degree of branching in the tree increase. Finally, we were unable in two cases to perform a satisfactory two-parameter fit with the model in Eq. (4); these are for the mean span $\langle S \rangle$ and the mean longest path $\langle P \rangle$ in seven dimensions. In those cases we proceeded by considering only the regressions from Eqs. (5) and (6).

III. AMPLITUDE RATIOS AND THE CONFLUENT EXPONENT

We now turn our attention to the amplitude ratios defined in Eq. (3). By assuming that $\langle R_n^2 \rangle = A_R n^{2\nu} (1 + B_R n^{-\Delta})$ and $\langle S \rangle = A_S n^\nu (1 + B_S n^{-\Delta})$, it seems natural to propose that

$$\frac{\langle S_n \rangle^2}{\langle R_n^2 \rangle} \approx \frac{A_S^2 (1 + B_S n^{-\Delta})^2}{A_R (1 + B_R n^{-\Delta})} \approx \frac{A_S^2}{A_R} (1 + C n^{-\Delta} + \dots),$$

where C is a constant. By plotting the ratio $\langle S_n \rangle^2 / \langle R_n^2 \rangle$ against $n^{-\Delta}$, it should be possible to extract an estimate of the ratio A_S^2 / A_R of the amplitudes. Ideally, a nonlinear three-parameter fit of the form

$$\frac{\langle S_n \rangle^2}{\langle R_n^2 \rangle} = \frac{A_S^2}{A_R} + C' n^{-\Delta}, \quad (7)$$

with A_S^2 / A_R , C' , and Δ as parameters, should be performed to find best estimates of the ratio of amplitudes and the exponent Δ . This approach failed to give consistent results and we will first investigate the presence of a confluent term in our data. It is generally difficult to observe Δ in statistical Monte Carlo data. We decided to study a quantity X_n , which will be equal to a dimensionless ratio of our measurements. For example, we will take $X_n = \langle S_n \rangle^2 / \langle R_n^2 \rangle$, $\langle P_n \rangle / \langle B_n \rangle$, $\langle S_n^2 / R_n^2 \rangle, \dots$. In all these cases, our basic assumption is that

$$X_n = C_0 + C_1 n^{-\Delta},$$

where C_0 is the amplitude ratio associated with the dimensionless ratio X_n . If $k \ll n$, then, if higher-order corrections are ignored, it can be shown that

$$\left(\frac{X_{n+k} - X_n}{kX_{n+k}} \right) \approx C'' n^{-\Delta-1}. \quad (8)$$

We test this relation in Figs. 1 and 2, which are graphs of $\log[(X_{n+k} - X_n) / kX_{n+k}]$ against $\log n$ for $X_n = \langle S_n \rangle^2 / \langle R_n^2 \rangle$ (Fig. 1) and $X_n = \langle P_n \rangle / \langle B_n \rangle$ (Fig. 2), where we display the data for only $d=2$ and 7. These graphs support the approximation in Eq. (8) and the slope of the best straight line through the points is an estimate of $-\Delta - 1$.

TABLE V. Estimates of Δ .

d	Δ
2	0.65 ± 0.20
3	0.54 ± 0.12
4	0.46 ± 0.11
5	0.40 ± 0.14
6	0.34 ± 0.13
7	0.35 ± 0.07

TABLE VI. Amplitude ratios.

d	2	3	4	5	6	7
$\frac{\langle S_n \rangle^2}{\langle R_n^2 \rangle}$	7.6203(37)	6.3123(17)	5.7255(20)	5.3020(31)	5.0413(55)	4.7511(65)
$\left\langle \frac{S_n^2}{R_n^2} \right\rangle$	7.8907(83)	6.5050(40)	5.8564(46)	5.3796(76)	5.071(11)	4.780(15)
$\frac{\langle P_n \rangle}{\langle B_n \rangle}$	3.9639(27)	3.9899(19)	4.0216(23)	4.0670(19)	4.1087(18)	4.1588(30)
$\frac{\langle S_n \rangle}{\langle \sqrt{\lambda_1} \rangle}$	3.082(41)	3.017(32)	3.057(32)	3.062(33)	3.088(37)	3.082(38)
$\frac{\langle E_n \rangle}{\langle S_n \rangle}$	0.9428(28)	0.9421(18)	0.9397(20)	0.9493(19)	0.9593(24)	0.9750(21)
$\frac{\langle R_n^2 \rangle}{\langle \lambda_1 \rangle}$	1.2438(48)	1.4398(26)	1.6134(25)	1.7883(31)	1.9493(27)	2.0839(27)

We computed Δ for different amplitude ratios in each dimension (we considered $X_n = \langle S_n \rangle^2 / \langle R_n^2 \rangle, \langle S_n^2 / R_n^2 \rangle, \langle P_n \rangle / \langle B_n \rangle, \langle S_n \rangle / \langle \sqrt{\lambda_1} \rangle, \langle E_n \rangle / \langle S_n \rangle, \langle R_n^2 \rangle / \langle \lambda_1 \rangle$). Our estimates from each of these ratios give values for Δ that are more or less consistent in each dimension. The average over these estimates was taken as our best estimate for Δ ; the stated error bar is equal to one-half the difference between the largest and smallest estimates obtained in the various fits. (We did not measure a statistical error since covariances were not measured.)

Our estimates are generally smaller than those obtained for animals by Adler *et al.* [13] (by using Padé approximations to exact enumeration data). Their data suggest that $\Delta \approx 0.85 \pm 0.10$ in two dimensions, 1.3 ± 0.2 in three dimensions, and 0.8 ± 0.2 in four dimensions, quite different from the results in Table V. On the other hand, their results in five to seven dimensions are more consistent with ours. Figures 1 and 2 clearly signal the presence of Δ in our data. Although we ignored higher-order corrections in Eq. (8), our data also included large trees, where we expect the dominant corrections to be the confluent term (higher-order terms decay more quickly). If we assume the values of Δ in Table V, then we can estimate the amplitude ratios. We report those results in Table VI.

IV. CONCLUSIONS

We have discussed the critical exponents and universal amplitude ratios of lattice trees in dimensions 2–7. The metric exponent ν was computed by analyzing data obtained from the mean square radius of gyration, the mean span, the mean end-to-end distance of the longest path, the largest eigenvalue of the radius of gyration matrix, and its determinant. The data collected from mean longest paths and mean branch sizes were analyzed to estimate the branch exponent ρ . These exponents were estimated using a weighted least-squares analysis for three different models [Eqs. (4)–(6)]. The best estimates for them were taken from successful two-parameter fits, with their associated confidence intervals. In both cases, we found that the regression by the model in Eq.

(6) fails to give a consistent value for Δ and we assume that only an effective exponent is seen. In addition, we found that systematic errors arise in estimates due to inadequate models and that these errors can be larger than statistical errors.

An important observation from our results is that a sizable systematic error could be present in the best estimates of exponents in models of self-avoiding walks, lattice trees, and animals. By estimating an exponent from a number of different models that account for finite size scaling corrections due to a confluent exponent, we found that acceptable fits can be found with a stated statistical confidence interval in more than one model. However, the results from different models are inconsistent. We interpret this as indicative of the presence of a systematic error or, equivalently, that the best estimate obtained in a least-squares analysis is conditioned on the model and that the statistical confidence interval cannot account for this. Indeed, the statistical confidence interval was in many cases much smaller than the change in the value of the best estimate if a different model was assumed; we take this change to be an estimate of an (unknown) systematic error in our estimates and a final error bar was *mostly* due to this error rather than to the statistical error.

We estimated Δ for different amplitude ratios in each dimension using Eq. (8). The average over these were taken as our best estimates for Δ , with a stated error bar that is one-half the difference between the largest and the smallest estimates obtained. Assuming the values of Δ in Table V, we estimated the amplitude ratios from Eq. (7). Our results are very different from previous estimates of the confluent corrections in a number of studies in dimensions 2–4, but in dimensions 5–7 we have estimates that are similar to those in Ref. [13]. The systematic decrease in Δ with increasing dimensions and the graphs in Figs. 1 and 2 support the numerical values in Table V and we view these estimates as a big improvement over previously stated estimates in the literature.

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