High precision canonical Monte Carlo determination of the growth constant of square lattice trees

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The number of lattice bond trees in the square lattice (counted modulo translations), t_n, is a basic quantity in lattice statistical mechanical models of branched polymers. This number is believed to have asymptotic behavior given by $t_n \sim A\lambda^n n^{-\theta}$, where A is an amplitude, λ is the growth constant, and θ the entropic exponent. In this paper, we show that λ and θ can be determined to high accuracy by using a canonical Monte Carlo algorithm; we find that $\lambda = 5.1439 \pm 0.0025$, $\theta = 1.014 \pm 0.022$, where the error bars are a combined 95% statistical confidence interval and an estimated systematic error due to uncertainties in modeling corrections to scaling. If one assumes the "exact value" $\theta = 1$ and then determines λ, then the above estimate improves to $\lambda = 5.143\,39 \pm 0.000\,72$. In addition, we also determine the longest path exponent ρ and the metric exponent ν from our data: $\rho = 0.74000 \pm 0.00062$, $\nu = 0.6437 \pm 0.0035$, with error bars similarly a combined 95% statistical confidence interval and an estimate of the systematic error.

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I. INTRODUCTION

Lattice trees are connected and acyclic subgraphs of a lattice (see Fig. 1). These objects have been studied as models of branched polymers [1–4] and they remain an interesting, though intractible, model in lattice statistical mechanics. The most basic quantity in this model is t_n, which is the number of distinct lattice trees of size-n edges counted up to equivalence classes under translations in the square lattice (in other words, these lattice trees are not rooted). The number of edges in a tree is called its size, so that trees counted by t_n have size n. The number of vertices in a tree is its order, and trees counted by t_n have order $n+1$. Very little is known (exactly) about the properties of t_n; the most important general theoretical accomplishment is an asymptotic expression for t_n in high dimensions due to Hara and Slade [5].

A field theoretic description of branched polymers was introduced by Lubensky and Isaacson in Ref. [6]. This development made it possible to study lattice trees from a statistical mechanics point of view, and methods from the theory of phase transitions were used to obtain information about t_n. A number of conjectures were made as a result, most notably with respect to the scaling properties and the critical exponents in this model; obtained by using arguments relying on mean field theory and dimensional reduction [7] in low dimensions. These conjectures have been tested numerically in a variety of numerical studies [7–10], and they motivate the development of Monte Carlo algorithms to sample lattice trees effectively from a given ensemble. Additional algorithms for numerical studies also include the exact enumeration of lattice trees [11].

The asymptotics of t_n is generally accepted to be

$$t_n = An^{-\theta}\lambda^n(1 + Bn^{-\Delta} + Cn^{-1} + \cdots), \qquad (1)$$

where A, B, and C are constants (sometimes referred to as "amplitudes") [7], λ is the *growth constant* of lattice trees, and θ is the *entropic exponent*. The exponent Δ is the *confluent (correction) exponent*, while the term $Bn^{-\Delta}$ is a *confluent correction*. Cn^{-1} is an *analytic correction* to the "pure scaling formula" $An^{-\theta}\lambda^n$. *Rooted trees* are lattice trees with one vertex rooted at the origin. It is apparent that a tree of size n has $n+1$ possible roots, so that the number of lattice trees rooted at the origin is $T_n = (n+1)t_n$. Thus, the asymptotics of T_n is similar to that of t_n:

$$T_n = An^{1-\theta}\lambda^n(1 + Bn^{-\Delta} + Cn^{-1} + \cdots). \qquad (2)$$

The exponents θ and Δ are supplemented by two additional critical exponents, ν and ρ. The *metric exponent* ν characterizes the scaling of lengths; for example, the mean square radius of gyration is believed to scale as a power law with n,

$$\langle R_n^2 \rangle \sim n^{2\nu}, \qquad (3)$$

where "$\sim$" indicates (imprecisely) that $\langle R_n^2 \rangle$ is asymptotic to $n^{2\nu}$ to the leading order. The second exponent describes the scaling of substructures in lattice trees, such as the longest path or the size of a branch (see Fig. 1). For example, the mean longest path $\langle P_n \rangle$ or the mean branch size $\langle b_n \rangle$ should scale with n as

$$\langle P_n \rangle \sim \langle b_n \rangle \sim n^{\rho}, \qquad (4)$$

where ρ is the *longest path* or *branch* exponent [9]. Naturally, there are corrections to scaling in the above asymptotic expressions for $\langle R_n^2 \rangle$, and $\langle P_n \rangle$. To leading order, these corrections include a confluent term with exponent Δ, and an analytic correction [as suggested by Eq. (2)]. Thus, one might guess that

$$\langle R_n^2 \rangle = C_r n^{2\nu}(1 + B_r n^{-\Delta} + D_r n^{-1} + \cdots),$$

$$\langle P_n \rangle \sim \langle b_n \rangle = C_b n^{\rho}(1 + B_b n^{-\Delta} + D_b n^{-1} + \cdots),$$

and analyze data from numerical simulations assuming these asymptotic expressions to obtain statistical estimates for ν and ρ.

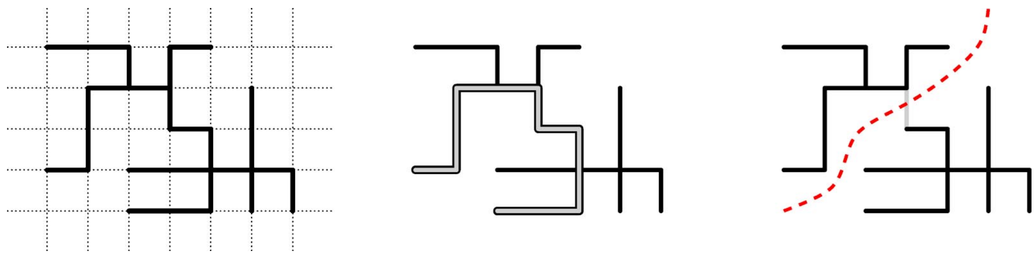

FIG. 1. A square lattice tree. The longest path in this tree is highlighted in the center. If an edge is deleted, then the tree splits into two subtrees on the right; the smaller of which (the top left) is called a branch. This tree has size (number of edges) 24 and order (number of vertices) 25.

The most accurate determinations of λ and θ in two dimensions were obtained by exact series enumeration of T_n for small values of n. The series is analyzed using differential approximants, and the best estimates of λ and θ are extracted. The best value obtained so far is

$$\lambda = 5.140 \pm 0.002, \tag{5}$$

obtained from series analysis [12]. The estimate

$$\nu = 0.641\,15 \pm 0.000\,05 \tag{6}$$

for the metric exponent for branched polymers is also due to series analysis of lattice trees (but in this case for *site trees*) [13].

Grand canonical Monte Carlo simulations of square lattice trees in two dimensions [7] predicted values consistent with those obtained in the exact enumeration studies, namely,

$$\lambda = 5.1431 \pm 0.0017 \pm 0.0057 = 5.1431 \pm 0.0074, \tag{7}$$

$$\theta = 0.994 \pm 0.029 \pm 0.054 = 0.994 \pm 0.083, \tag{8}$$

$$\nu = 0.6402 \pm 0.0040 \pm 0.0044 = 0.6402 \pm 0.0084. \tag{9}$$

The error bars in these estimates are as follows: *best value* $\pm$ *95% statistical confidence interval* $\pm$ *estimated systematic error* [14]. We add the two error terms to find a single combined error bar in the final estimates; these error bars are therefore explicitly comparable to the estimates from this paper given in the abstract above.

Canonical Monte Carlo simulations have also been used to determine ν, ρ, and the confluent exponent Δ [15]. These estimates are

$$\nu = 0.642 \pm 0.010, \tag{10}$$

$$\rho = 0.738 \pm 0.010, \tag{11}$$

$$\Delta = 0.65 \pm 0.20, \tag{12}$$

with error bars as a combined 95% statistical confidence interval and an estimated systematic error. The large uncertainty in the value of Δ is notable; it is generally difficult to determine amplitudes and exponents associated with corrections to scaling.

In this paper, we use canonical Monte Carlo simulations to estimate ν, ρ, and Δ. In the following section, we describe a labeling of trees that allows us to define a statistic that we call the *atmosphere* of a tree. This statistic allows us to estimate μ and θ. In Sec. II, we first consider the atmosphere of trees and show how they may be used to determine the growth constant λ in a canonical Monte Carlo simulation. In Sec. III, we present our numerical data. We give estimates for ρ, ν, θ, and λ, and discuss the numerical confidence in our results. We conclude the paper with some short comments in Sec. IV.

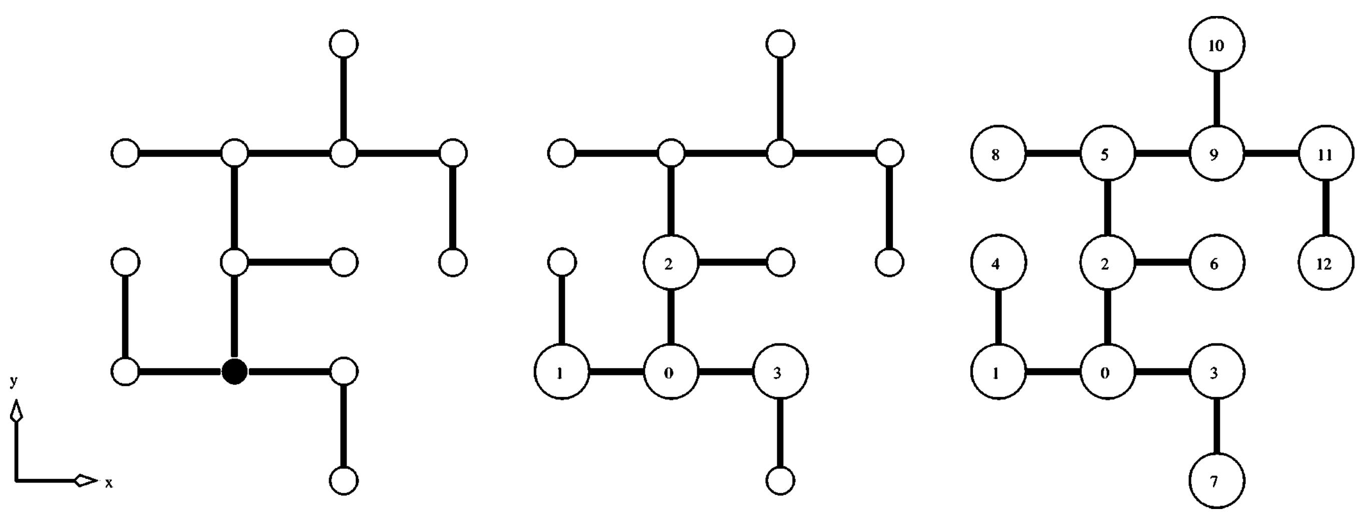

FIG. 2. A rooted tree (left), labeled to depth one (center) and its legal labeling (right).

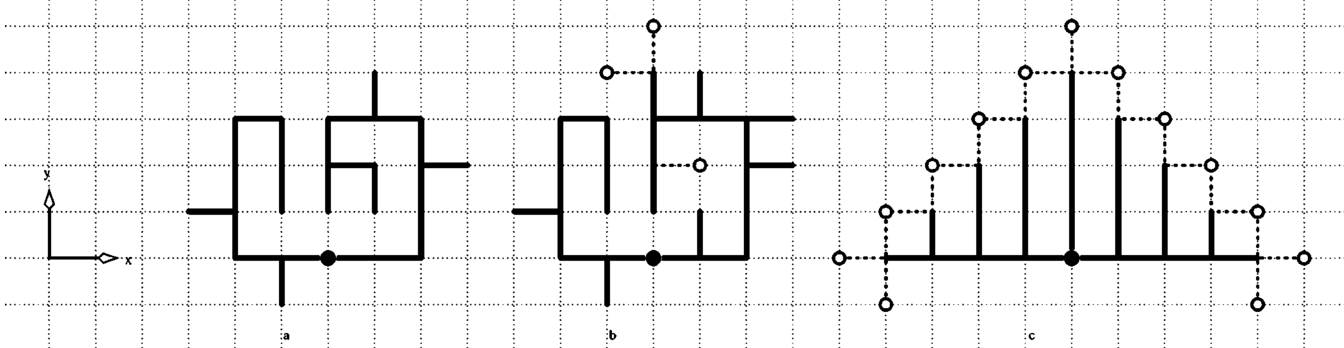

FIG. 3. If a lexicographic breadth-first labeling is put on these trees from the roots denoted by ●, then the atmospheres composed of the dotted edges are obtained. The left-hand tree (a) has no atmosphere, the center tree (b) has an atmosphere of size 3, while the right-hand tree (c) has an atmosphere of size 21.

II. TREES AND THE ATMOSPHERES

Let T be a tree with root vertex labeled 0 located at the origin of the square lattice. The *level* of a vertex v in T is the length of the shortest path from the root to v. Thus, the root has level zero and the immediate children of the root vertex all have level one. Vertices in a rooted unlabeled tree may be systematically labeled, from the root, using two widely used schemes: breadth-first and depth-first labelings (see, for example, Ref. [16]).

The atmosphere of a lattice tree is an intuitive notion (which we shall make precise) of adjacent lattice space into which a tree can grow. The atmosphere is not a unique property of any given tree, but depends on the choice of root and labeling scheme which we use to construct it. On the other hand, we shall collect statistical evidence that the size of the atmosphere of a tree is intrinsic in the sense that some trees will tend to have large atmospheres, and some trees will tend to have small atmospheres, irrespective of the choice of root.

In this paper, we use a breadth-first labeling scheme to define the atmospheres. Such a labeling is not unique and so cannot be used immediately to find a unique atmosphere for any tree. We shall change the labeling scheme so that each lattice tree will be uniquely labeled, in which case we may find a unique atmosphere for each root that we select. The breadth-first labeling is made unique by ordering vertices lexicographically by their coordinates (first in the x direction, then in the y direction), and then labeling the lexicographic least vertex with the next unused label.

Lexicographic breadth-first labeling. This is given as follows.

(1) Label the root of the tree by 0, and let this be the current vertex (in level 0)

(2) Assume that the current vertex v in level r has label k. Search for the children of v in level $r+1$ and label them in lexicographic increasing order with the next unused labels, say $m, m+1, m+2, \ldots$.

(3) When all the children of v (with label k) are labeled, then select the vertex with label $k+1$ as the current vertex (i.e., increment k to find the next vertex and continue the labeling algorithm from there).

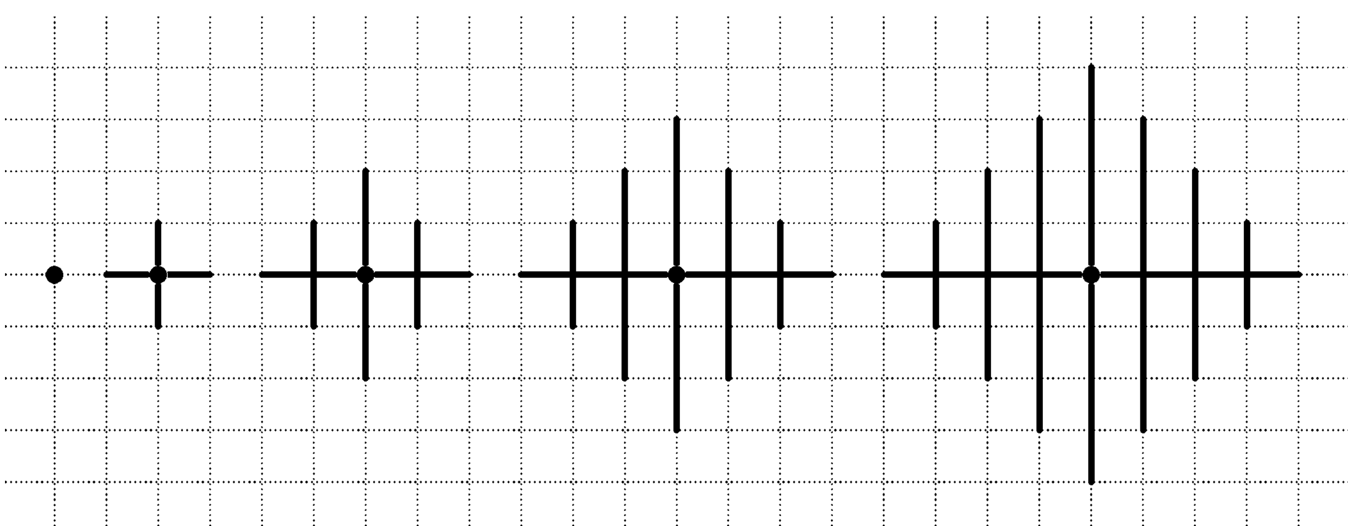

FIG. 4. If the trees in this sequence are labeled by a lexicographic breadth-first labeling from the root denoted by ●, then the atmospheres grow along the sequence in size as $8k+4$, while the size of the trees grow as $n=2k(k+1)$, with $k=0,1,2,\ldots$. In other words, the size of the atmosphere grows proportional to $n^{1/2}$.

(4) Repeat steps (2) and (3) until all the vertices in T are labeled.

This algorithm assigns a unique labeling to each rooted lattice tree. Such a labeling will be called *legal* (see Fig. 2) and all other labelings will be called *illegal*.

A tree T of order n vertices with a legal labeling may grow to a tree of order $n+1$ vertices by adding an edge to T *only* if the resulting tree also has a legal labeling; the new vertex will have label n and will reside in the deepest level of the tree and will be the last vertex to be labeled using the above algorithm.

The set of edges that can be appended to a legally labeled tree of order n, T, to produce a new legally labeled tree of order $n+1$, T', is called the *atmosphere* of T. T' is a *successor* of T and T is the *predecessor* of T'. The predecessor of a legally labeled tree can be obtained simply by deleting the vertex with the highest label. The number of sucessors of a tree T is equal to the size of its atmosphere, and we denote this number by $a(T)$.

There are trees with no atmospheres, and some sequences of trees with atmospheres that increase without bound as $n \to \infty$. In Fig. 3(a), an example of a tree with an empty atmosphere is given, while a tree with a small atmosphere and a tree with a larger atmosphere are illustrated in Figs. 3(b) and 3(c). A sequence of trees of order n and with atmospheres that increase as $O(\sqrt{n})$ is given in Fig. 4.

Assume that $T_n(a)$ is the number of rooted trees of size-n edges and with atmospheres of size-a edges. If T is a tree counted by $T_n(a)$, then there are a trees of size $n+1$ which are descendents of T. Thus, the total number of descendents of trees counted by $T_n(a)$ is $aT_n(a)$, and these are all distinct, since they are labeled uniquely by the lexicographic breadth-first labeling. Since every tree counted by T_{n+1} is a descendent of a tree in $T_n(a)$, for some value of a, it follows that

$$T_{n+1} = \sum_a aT_n(a). \tag{13}$$

Thus, the expected size of the atmosphere is given by

$$\langle a \rangle = \frac{\sum_a aT_n(a)}{T_n} = \frac{T_{n+1}}{T_n}. \tag{14}$$

It is a theorem that $T_{n+1}/T_n \to \lambda$ in high dimensions [5], but this is not known to be the case in dimensions $d \leqslant 8$. However, all numerical evidences suggest that this is indeed the case, and it will be an assumption in this paper.

III. NUMERICAL RESULTS

In this section, we examine numerical data for the mean branch size, mean longest path, mean square radius of gyration, and the mean atmosphere of lattice trees in two dimensions. Lattice trees of size n were sampled from the uniform distribution along a Markov chain using the Metropolis algorithm [17] implemented via a cut-and-paste algorithm for lattice trees [9]. Simulations were performed for values of n starting at $n=4$, and incrementing n in larger leaps to a maximum $n=2048$.[1] At each value of n, a total of 10^9 attempted iterations of the algorithm was performed, with the exception of $n=4$ (8×10^7 attempted iterations) and $n=1448$ (1.5×10^9 iterations), and $n=2048$ (1.8×10^9 iterations) (see Fig. 5). The resulting time series was analyzed for autocorrelations to find sample averages with proper statistical confidence intervals (see, for example, Ref. [18] for an extensive discussion of the techniques for analyzing data from Metropolis Monte Carlo simulations).

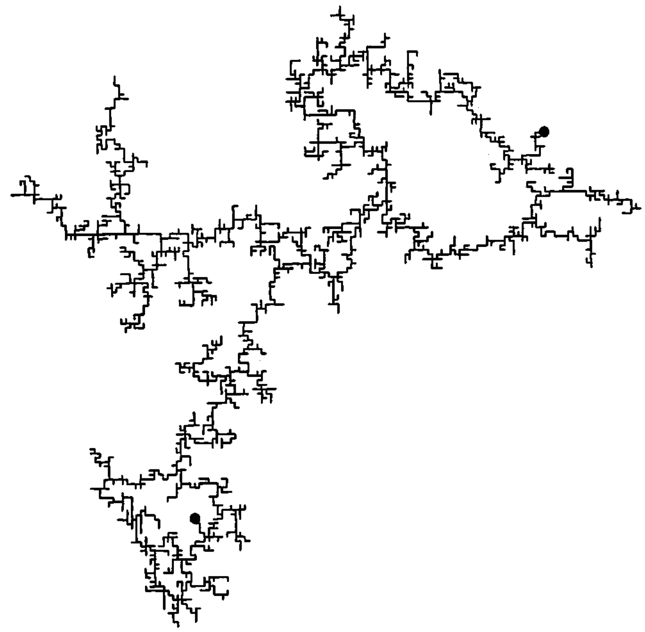

FIG. 5. A lattice tree of size 2048 edges generated by the Monte Carlo routine. The end points of the longest path are indicated by ●.

A. The mean branch size of trees

Select an edge uniformly in a lattice tree and delete it. Since it is a cut edge, this cuts the tree into two subtrees, the smaller of which is called a *branch* [9], see Fig. 1.[2] Let the size of the branch be b_n, and the mean branch size measured uniformly over all the branches in all trees, $\langle b_n \rangle$, is believed to scale with n as described by Eq. (4). Sample averages of b_n over data collected in a Monte Carlo simulation give estimates of $\langle b_n \rangle$, and a suitable scaling ansatz for the mean branch size can be obtained by taking logarithms of Eq. (4) and then expanding the resulting expression (after including confluent and analytic corrections) to obtain

$$\ln\langle b_n \rangle = \ln C_b + \rho \ln n + B_b n^{-\Delta} + D_b n^{-1} + \cdots. \tag{15}$$

[1](The sizes n of the trees were first incremented in steps of 2 from 4 to 22, thereafter in the sequence {26,32,38,46,54,64,78,90,106, 128,180,256,362,512,724,1024,1448,2048}.)

[2]In some cases, two subtrees of the same size may be obtained (if n is odd). In those cases, a random choice is made to identify one as a branch and the other as the remainder of the tree.

TABLE I. Linear regressions for $\langle b_n \rangle$ to determine ρ.

Type of fit	n_{min}	χ^2_d	Acceptable level	ρ
Two parameter linear	390	5.70 (4 df)	78%	0.73768 ± 0.00067
Analytic correction	106	9.11 (7 df)	76%	0.73909 ± 0.00068
Confluent correction	16	27.94 (19 df)	92%	0.74000 ± 0.00016
Both corrections	16	21.45 (18 df)	75%	0.73954 ± 0.00042

Estimates of the exponent ρ can then be made by a weighted least squares fit of a two-parameter linear model $\ln\langle b_n \rangle = \ln C_b + \rho \ln n$ to the data (in which case we ignore the corrections to scaling). The results of this fit are displayed in the first row in Table I. The estimate for the exponent is $\rho = 0.737\,68 \pm 0.000\,67$, where the error bar is a 95% statistical confidence interval. Corrections to scaling may have a potentially important impact on this estimate; since these are most important at small values of n, we discard data at values of $n < n_{min}$, where n_{min} is increased systematically until a statistically acceptable fit is obtained.[3]

The model improves marginally when an analytic correction is included. In this case, a three-parameter model is obtained, and a fit with $n_{min} = 106$ with seven degrees of freedom is acceptable at the 95% level. We notice that the estimate for ρ moves outside its 95% statistical confidence intervals when compared to the estimate previously obtained for the two-parameter fit. However, since this least squares fit has seven degrees of freedom, we accept it as superior to the two-parameter fit that had only four degrees of freedom. The situation is further improved by including a confluent correction instead. Unfortunately, this analysis is nonlinear, and generally may be numerically unstable. Thus, we fix Δ and perform three-parameter linear fits to determine best estimates. The least squares error can be tracked as a function of Δ, and best values for ρ can be chosen at that value of Δ where the error is minimized. This procedure would only give an effective value for Δ, since all other corrections are ignored and probably do contribute to the least square error. For a more careful analysis of Δ, see Ref. [15]. The results of these fits are in Table II; data from values of n less than $n_{min} = 16$ were excluded since no statistically acceptable fits could be found if those are included. Only the two fits with $\Delta = 0.75$ and $\Delta = 0.80$ are statistically acceptable, and we take those to give the best results for ρ . Combining them by taking their average gives a single estimate that we list in Table I.

Yet another model is obtained when the analytic correction is added to the last model, while the confluent exponent is fixed at its effective value. A fit with $\Delta = 0.75$ gives $\rho = 0.739\,54 \pm 0.000\,42$ ($\chi^2_{18} = 21.45$ acceptable at the 75% level), while $\rho = 0.739\,32 \pm 0.000\,40$ if $\Delta = 0.80$ ($\chi^2_{18} = 23.23$ acceptable at the 82% level). The fit at $\Delta = 0.75$ is more acceptable, and we take it as our best estimate in Table I.

Comparing our results in Table I suggests that the models with a confluent correction, and with both a confluent correction and an analytic correction, should be accepted as the most successful in modeling the data. The difference in the best estimates could be viewed as a systematic error. Thus, taking the value of ρ obtained in the model with only a confluent correction as the best estimate, we find

$$\rho = 0.740\,00 \pm 0.000\,16 \pm 0.000\,46, \tag{16}$$

where the error bars are first a 95% confidence interval followed by an estimated systematic error. Previous estimates include $\rho = 0.736 \pm 0.013$ [9] and $\rho = 0.738 \pm 0.010$ [15] (where the error bars are a 95% confidence interval added to an esimated systematic error).

B. The mean longest path of trees

For trees of size n edges, the mean longest path $\langle P_n \rangle$ is believed to scale as in Eq. (4), with the same exponent ρ as the mean branch size [9]. This power law is also corrected by corrections to scaling, and to the leading order one should expect a confluent correction followed by an analytic correction. Thus, a reasonable scaling ansatz for $\langle P_n \rangle$ is

$$\ln\langle P_n \rangle = \ln C_p + \rho \ln n + B_p n^{-\Delta} + D_p n^{-1} + \cdots. \tag{17}$$

The situation is now similar to that of the preceding section. While the constants C_p, B_p, and D_p are presumably different from their values in Eq. (15), the exponents ρ and Δ are expected to be universal.

TABLE II. Linear regressions for $\langle b_n \rangle$ with a confluent correction.

Δ	χ^2_{19}	Level	ρ
0.30	2865.20	>99%	0.76657 ± 0.00032
0.40	1716.42	>99%	0.75569 ± 0.00026
0.50	893.35	>99%	0.74909 ± 0.00021
060	360.32	>99%	0.74463 ± 0.00019
0.65	191.68	>99%	0.74289 ± 0.00017
0.70	82.71	>99%	0.74139 ± 0.00017
0.75	29.49	94%	0.74008 ± 0.00016
0.80	27.94	92%	0.73892 ± 0.00015
0.85	74.67	>99%	0.73789 ± 0.00015
0.90	166.12	>99%	0.73696 ± 0.00014

[3]The least squares error S^2_d in a weighted least squares fit is distributed as a χ^2 statistic on d degrees of freedom, where d is equal to the number of data points minus the number of parameters in the model. We deem the results of a least squares fit to the data statistically acceptable if S^2_d is acceptable at the 95% level. The most succesful model will be taken as the model that maximizes the degrees of freedom while being acceptable at the 95% level.

TABLE III. Linear regressions for $\langle p_n \rangle$ to determine ρ.

Type of fit	n_{min}	χ_d^2	Acceptable level	ν
Two parameter linear	256	9.19 (5 df)	90%	0.73915 ± 0.00046
Analytic correction	106	9.20 (7 df)	76%	0.73951 ± 0.00064
Confluent correction	106	8.66 (7 df)	73%	0.73980 ± 0.00080
Both corrections $\Delta = 0.65$	10	29.78 (21 df)	91%	0.74024 ± 0.00030
Both corrections $\Delta = 0.85$	12	27.30 (20 df)	88%	0.73948 ± 0.00029

A two-parameter least squares fit that ignores the corrections to scaling can be done when only those data with $n < n_{min} = 256$ are excluded; the result is in Table III. In this fit, the number of degrees of freedom is five, which we do not consider to be satisfactory. Including an analytic correction improves the situation somewhat; there are seven degrees of freedom with $n_{min} = 106$. A confluent correction does not improve matters, and we could not find any acceptable model with only a confluent correction and with more than seven degrees of freedom. Assuming, for example, that $\Delta = 0.75$ gives an acceptable fit when $n_{min} = 106$, as seen in Table III. One may also plot $\ln p_n / \ln n$ against $1/\ln n$ in Fig. 6, and extrapolate the data to see that $\rho \approx 0.74$, consistent with the results obtained by examining the mean branch size in the preceding section.

As before, we should ideally attempt to perform a nonlinear fit that includes the confluent exponent Δ as a parameter. Tracking the least squares error as a function of Δ is also not successful: a fit with $\Delta = 0.75$ gives a statistically acceptable fit when $n_{min} = 12$, with $B_p = 0.412 \pm 0.013$ and $D_p = -0.847 \pm 0.018$. These amplitudes are opposite in sign and tend to cancel one another in the range of n. This cancellation has negative effects on the behavior of the least square analysis. A fit with $\Delta = 0.9$ gives instead $B_p = 1.261 \pm 0.040$ and $D_p = -1.738 \pm 0.046$, while $\Delta = 0.99$ gives $B_p = 14.57 \pm 0.46$ and $D_p = -15.08 \pm 0.47$. In other words, with increasing $\Delta < 1$, both B_p and D_p increase in absolute values, but with opposite signs. Thus, the confluent and analytic terms tend to cancel one another over a wide range of n in this case. The fits were all statistically acceptable, but the estimates of ρ depend on the value of Δ, so that no consistent best value for ρ could be found. We therefore proceeded by assuming that $\Delta = 0.65$ or 0.85, two values of Δ suggested in Refs. [15,11], respectively, and then compared the results. The results of these fits are reported in Table III. If $\Delta = 0.65$, then a fit with $n_{min} = 10$ is acceptable at the 91% level, and if $\Delta = 0.85$, then the fit is acceptable with $n_{min} = 12$ at the 88% level.

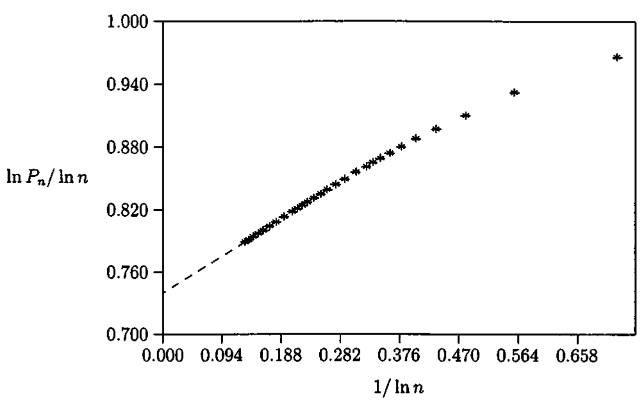

FIG. 6. A plot of $\ln P_n / \ln n$ against $1/\ln n$. Extrapolating the data to $n \to \infty$ suggests that $\rho \approx 0.74$.

Comparing these results shows that they are consistent with those in Table I. The two-parameter fit had only five degrees of freedom, and if only one correction to scaling term is included, it had seven degrees of freedom. These models compare poorly to the last two models with both corrections included and with 20 and 21 degrees of freedom, respectively. We, therefore, take the last two models as our best, and their average as the best value for ρ is

$$\rho = 0.739\,86 \pm 0.000\,30 \pm 0.000\,46. \tag{18}$$

This result is within the error bars of the best value for ρ obtained by considering the mean branch size in Eq. (16).

C. The mean square radius of gyration

It follows from Eq. (3) that a suitable scaling ansatz, which includes a confluent and an analytic term, for the mean square radius of gyration is

$$\ln \langle R_n^2 \rangle = \ln C_r + 2\nu \ln n + B_r n^{-\Delta} + D_r n^{-1} + \cdots, \tag{19}$$

where C_r, B_r, and D_r are constants (amplitudes) and ν is the metric exponent of lattice trees. Least squares fits can be used to estimate ν from estimates of $\langle r_n^2 \rangle$, but again corrections to scaling must be considered. The analysis here is similar to that in the preceding section: Two-parameter statistically acceptable fits could only be done when data with $n < n_{min} = 512$ are excluded. The estimate for the metric exponent in this case is $\nu = 0.640\,14 \pm 0.000\,64$, with a 95% confidence interval and least squares error $\chi_4^2 = 8.0515$ with two degrees of freedom acceptable at the 91% level. One may choose to include only a confluent or an analytic correction to scaling in an attempt to improve the analysis. In those cases, the results are given in Table IV. We fixed Δ at 0.75, its effective value, and obtained an acceptable fit with $n_{min} = 38$ and with 12 degrees of freedom

The best fit (acceptable at the 95% level with the largest number of degrees of freedom) includes both an analytic and a confluent correction. The two-parameter fit has only two degrees of freedom, and so we ignore it here, although its result is not inconsistent with the numerical values of ν determined by the other fits. Comparison of the best fit to the

TABLE IV. Linear regressions for $\langle R_n^2\rangle$ to determine ν.

Type of fit	n_{min}	χ_d^2	Acceptable level	ν
Two parameter linear	512	8.06 (2 df)	91%	0.64014 ± 0.00064
Analytic correction	90	11.85 (10 df)	85%	0.64081 ± 0.00054
Confluent correction	38	14.14 (12 df)	71%	0.64103 ± 0.00028
Both corrections	18	23.66 (17 df)	88%	0.64374 ± 0.00042

remaining fits (including only an analytic or a confluent correction) allows us to determine a systematic error of size 0.0028, so that we state our best estimate for ν as

$$\nu=0.6437\pm0.0005\pm0.0028, \tag{20}$$

where we note that we give ample allowance to a possible systematic error. Comparison with earlier estimates of ν shows that confidence intervals in this estimate of ν is still orders of magnitude larger than the best series estimate of $\nu=0.641\,15\pm0.000\,05$ [13], but is better than Monte Carlo estimates previously obtained [7,15]. The best estimates of lattice tree parameters are listed in Table V.

D. The mean atmosphere of trees

The atmosphere of a lattice tree was defined in Sec. II, and we noted that the mean atmosphere of lattice trees is given by Eq. (14). The asymptotics of T_n is given in Eq. (2), and by substituting this into Eq. (14), we can develop an asymptotic expression for $\langle a_n\rangle$. Keeping only the dominant terms gives

$$\langle a_n\rangle=\lambda+\frac{\lambda(1-\theta)}{n}+\frac{C'}{n^{2\Delta}}+\frac{C''}{n^{1+\Delta}}+\cdots. \tag{21}$$

Thus, we can find both λ and θ from our data, and moreover, the slowest (and thus dominant) correction term to the constant term λ is of the order $1/n$.

Atmospheres were calculated twice for each tree. The tree was rooted at a randomly chosen vertex, and labeled to determine an atmosphere of size $a_n^{(1)}$. This process was repeated to compute a second atmosphere $a_n^{(2)}$, starting again from a randomly selected root. Thus, for each tree, we found two atmospheres, and it follows that

$$\langle a_n^{(1)}\rangle=\langle a_n^{(2)}\rangle=\langle (a_n^{(1)}+a_n^{(2)})/2\rangle. \tag{22}$$

In addition, one may compute the covariance

$$C_n^{aa}=\langle a_n^{(1)}a_n^{(2)}\rangle-\langle a_n^{(1)}\rangle\langle a_n^{(2)}\rangle, \tag{23}$$

TABLE V. Best estimates of parameters for lattice trees.

Parameter	Best value
λ	5.1439 ± 0.0025
θ	1.014 ± 0.082
ρ	0.74000 ± 0.00062
ν	0.6437 ± 0.0035

and when $a_n^{(1)}$ and $a_n^{(2)}$ are independent, this should decay to zero. However, it seems intuitive that the size of the atmosphere of a lattice tree may be an intrinsic property, and is related to the degree of branching in the tree, in which case $C_n^{aa}\to C_\infty^{aa}>0$ as $n\to\infty$.

The first term in Eq. (21) is of the order $O(1/n)$ and is followed by corrections of the orders $O(1/n^{2\Delta})$ and $O(1/n^{1+\Delta})$. Since all evidence we have suggest that Δ is in the range 0.65–0.85 [15], it would be imprudent to include only the $O(1/n)$ term, while ignoring the potentially comparable corrections of the orders $O(1/n^{2\Delta})$ and $O(1/n^{1+\Delta})$. Thus, we attempted linear fits with values of Δ varying from 0.65 to 0.85 and with the further approximation that $1+\Delta=2$, so that the scaling ansatz is

$$\langle a_n\rangle=\lambda+\frac{\lambda(1-\theta)}{n}+\frac{C'}{n^{2\Delta}}+\frac{C''}{n^2}. \tag{24}$$

This ansatz did, in fact, model the data very effectively, with an acceptable fit with $n_{min}=6$, and, moreover, the parameters turned out to be insensitive to (even substantial) changes in Δ. These fits gave best estimates for λ and θ with the 95% statistical confidence intervals as follows:

$$\lambda=5.143\,93\pm0.000\,93 \tag{25}$$

and

$$\theta=1.014\pm0.022, \tag{26}$$

when it is assumed that $\Delta=0.75$, with $n_{min}=6$ and $\chi_{23}^2=21.41$ which is acceptable at the 45% level with 23 degrees of freedom. Changing Δ from 0.65 to 0.85 still gives an acceptable fit at $n_{min}=6$ and does not change the values of either θ or λ outside the 95% confidence intervals stated above. In other words, this is a very successful choice for the model which robustly fits the data and produces λ to at least two decimal places with an uncertainty of atmost 1 in the third decimal place. We attempt to find a systematic error in these results by fitting $\langle a_n\rangle=\lambda(1-\theta)/n$ instead in a two parameter fit. In this case, we obtain $\lambda=5.145\,41\pm0.000\,30$ and $1-\theta=-0.0454\pm0.0020$, in a fit with $n_{min}=20$, with $\chi_{18}^2=28.62$ acceptable at the 95% level. Comparison with Eqs. (25) and (26) then gives our best estimates with the 95% statistical confidence intervals and an estimated systematic error as follows:

$$\lambda=5.143\,93\pm0.000\,93\pm0.001\,48=5.1439\pm0.0025, \tag{27}$$

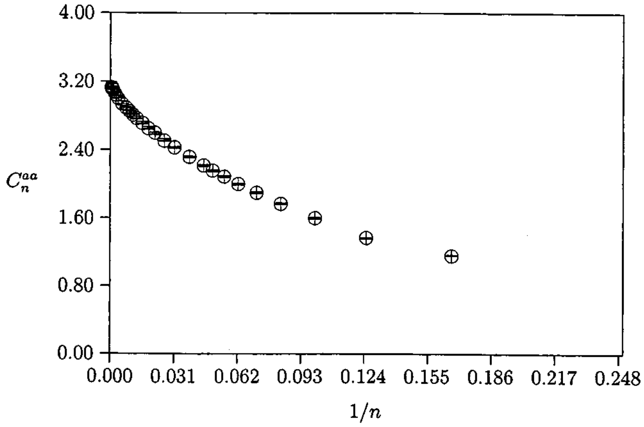

FIG. 7. A plot of C_n^{aa} against $1/n$. This covariance of the atmospheres does not vanish if $n \to \infty$, suggesting that the size of the atmosphere is an intrinsic property of a lattice tree.

$$\theta = 1.014 \pm 0.022 \pm 0.060 = 1.014 \pm 0.082. \tag{28}$$

Adding the statistical and systematic confidence intervals gives the results claimed in the abstract.

We now turn our attention to the covariance $C_n^{aa} = \langle a_n^{(1)} a_n^{(2)} \rangle - \langle a_n^{(1)} \rangle \langle a_n^{(2)} \rangle$. The scaling ansatz in Eq. (24) suggests that

$$C_n^{aa} = C_\infty^{aa} + \frac{\alpha}{n} + O(1/n^2), \tag{29}$$

where C_∞^{aa} and α are constants. The constant C_∞^{aa} should vanish when $a_n^{(1)}$ and $a_n^{(2)}$ becomes uncorrelated quantities as $n \to \infty$ for trees of size n. A plot of C_n^{aa} against $1/n$ is in Fig. 7. Extrapolating the plot to $n = \infty$ by a least squares fit of C_n^{aa} against $1/n$ gives an acceptable $n_{min} = 12$, and $\chi_{21}^2 = 27.04$ acceptable at the 83% level; in which case

$$C_\infty^{aa} = 3.056 \pm 0.018, \tag{30}$$

where the error bar is a 95% confidence interval.

There is strong evidence in Fig. 7 that C_n^{aa} approaches a constant as $n \to \infty$. The atmosphere of a lattice tree is dependent on the choice of root to start the labeling—choosing two roots uniformly in a lattice tree nevertheless gives atmospheres with positively correlated sizes; in other words, it seems that some lattice trees have the intrinsic property of having a large atmosphere, while other lattice trees have a small atmosphere, regardless of the choice of root.

IV. DISCUSSION

The critical exponents of lattice trees are thought to be universal quantities associated with models of branched polymers in a good solvent. Dimensional reduction of branched polymers in $d+2$ dimensions to an Ising model in d dimensions in an imaginary magnetic field relates the exponents of branched polymers to the exponent σ_d (of the Ising model) via the relations

$$\nu_{d+2} = (\sigma_d + 1)/d, \tag{31}$$

$$\theta_{d+2} = \sigma_d + 2, \tag{32}$$

where σ is the exponent that controls the magnetization of the Ising model near the edge singularity [19–21,7]. The Ising model can be solved exactly in $d=0$ and $d=1$ dimensions, in which case $\sigma_0 = -1$ and $\sigma_1 = -1/2$. Thus, the "*exact value*" of θ in two dimensions is $\theta = 1$. This result suggests strongly that λ should be computed by assuming that $\theta = 1$ in Eq. (24). If this is done, then the best estimate for λ is

$$\lambda = 5.143\,39 \pm 0.000\,72, \tag{33}$$

with an error that combines a 95% statistical confidence interval with a systematic error due to uncertainties in the value of Δ (we took fits with $0.65 \leqslant \Delta \leqslant 0.85$). This error bar is roughly a factor of 3 smaller than the error bar obtained in the preceding section. This estimate is also consistent with our previous results, and provides strong evidence that the third decimal digit of λ is a 3.

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