

## Polymers with restricted branching

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We use exact enumeration and series analysis methods to study how restricting the degree of branching of lattice trees and animals affects their growth constants. In addition to trees with only nearest neighbor steps, we enumerate trees involving next nearest neighbor steps on the triangular and square lattices, allowing us to study the influence of lattice coordination number on the growth constant. We also study the asymptotics of the number of subtrees of the Bethe lattice with the same branching restrictions as above and compare the results with those for lattice trees. [S1063-651X(96)10505-5]

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### I. INTRODUCTION

The configurational properties of linear polymers in dilute solution in a good solvent are now well understood [1]. Self-avoiding walks are a simple model of linear polymers and have been important in developing our current level of understanding [2]. Branched polymers are less well understood although there is considerable recent work in this area [3–6]. Experimentally branched polymers can be formed when a large number of polyfunctional monomers react [3]. There are two important lattice models for studying branched polymers. These are lattice trees and lattice animals. Each of these is a connected cluster of vertices of a lattice, but with different technical restrictions. A lattice animal can have cycles, so that an edge can be deleted without disconnecting the animal, while a lattice tree has no cycles so that every edge is a cut edge. This means that upon deleting any edge the tree becomes disconnected. There are at least two versions of each of these models. A tree is *strongly embeddable* if every pair of vertices in the tree that are a unit distance apart in the lattice have an edge of the tree joining them. That is, a strongly embeddable tree is a connected section graph of the lattice, having no cycles. If two vertices, a unit distance apart, are not necessarily joined by an edge then the tree is *weakly embeddable*. That is, a weakly embeddable tree is a connected subgraph of the lattice, having no cycles. Strongly and weakly embeddable animals are defined in a similar way.

Lattice trees also appear in a related problem, *planar vesicles*, discussed in more detail in [7]. Planar vesicles are closed self-avoiding walks or polygons embedded in a two-dimensional plane and subject to a pressure differential between the interior and the exterior. When the external pressure is much larger than the interior one, and the rigidity of the vesicle is small, the system is found to exhibit *treelike* configurations, i.e., the object dual to the planar vesicle has few large cycles.

From the point of view of critical phenomena, problems with fixed topology (i.e., fixed homeomorphism type), such as self-avoiding walks, stars, combs, etc. [8,9], are relatively well understood. In particular, for a given fixed topology  $\tau$  the asymptotic behavior of the number of embeddings, with

$N$  vertices or bonds, is conjectured to be

$$C_N(\tau) \sim \mu^N N^{\gamma(\tau)-1}, \quad (1)$$

where  $\mu$  is independent of the topology under a wide range of conditions [9] and scaling theory arguments suggest that the exponent  $\gamma(\tau)$  may be written in terms of the exponents for  $f$  stars [8].

Lattice trees are perhaps the simplest model for which the exponential rate of growth of the number of embeddings is larger than for self-avoiding walks. The number of rooted trees (i.e., with one vertex labeled and called the root),  $t_N$ , with  $N$  vertices is thought to increase as

$$t_N = A_0 \lambda_0^N N^{1-\theta} (1 + B_0 N^{-\Delta} + \dots), \quad (2)$$

with  $\lambda_0 > \mu$ . As  $N$  increases more topologies (homeomorphism types) can occur and this is responsible for the increased exponential growth rate. However, the relationship between the value of the growth constant ( $\lambda_0$ ) and the rate at which new topologies appear is not well understood. The work reported here is an empirical study of this problem in which the rate of appearance of new topologies is limited by restrictions placed on the branch vertices. In this sense, the present work is complementary to the work in [7], where the appearance of topologies is controlled by a fugacity.

Renormalization group arguments suggest that lattice trees and animals are in the same universality class [10,11]. Thus, for animals and trees, the number  $a_N$  of rooted clusters with  $N$  elements is expected to behave asymptotically as

$$a_N = A \lambda^N N^{1-\theta} (1 + B N^{-\Delta} + \dots). \quad (3)$$

This generalizes Eq. (2).  $\lambda$  is the growth constant,  $\theta$  is the scaling exponent, and  $\Delta$  the correction-to-scaling exponent. The growth constant is dependent on the lattice, and also on the restrictions imposed on the degree of branching of a vertex. In addition  $\lambda$  is different for trees and animals [12], different for strong and weak embeddings [13], and, in the case of animals, depends on whether the animal is counted by vertices or bonds [14]. However, the exponent  $\theta$  is believed to be universal [15] and equal to 1 in two dimensions and to 3/2 in three dimensions.

In a reaction to synthesize branched polymers, the monomers have a maximum value for their functionality, so that no monomer can be directly connected to more than say  $v$  other monomers. Similarly, steric hindrance can effectively limit the maximum number of monomers to which a given monomer can be directly connected [3,16]. These effects can be modeled by imposing a restriction on the maximum valence of a vertex of a tree or animal. Here, the valence ( $v$ ) (or functionality or degree of branching of a vertex) is the number of bonds incident on a vertex. One can investigate both the effect of changing this maximum valence and also changing the lattice coordination number. In this work, our primary aim is to study the detailed effects of valence restrictions and lattice coordination number  $z$  on growth constants for trees on lattices including Bethe lattices. As pointed out in [17], the dependence of growth constants on the lattice coordination number is of fundamental interest in trying to understand the relationship between geometrical structure and critical phenomena. In addition, polymers containing vertices of high functionality can be synthesized and are of considerable interest. In this context, stars on lattices with high coordination number have previously been studied [18].

We consider bond trees (i.e., weak embeddings) on square (sq), triangular (tr), simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices. In order to obtain larger coordination numbers in two dimensions, we generate series of trees that include next nearest neighbor (nnn) steps on sq and tr lattices [17], and from now on these series will be denoted sqnnn and trnnn. For the sq lattice this amounts to increasing  $z$  from 4 to 8, and, for the tr lattice, the increase is from 6 to 12. In addition to the above, we also study existing series for strongly embeddable animals on the triangular [19], simple cubic [20], and body-centered cubic [21] lattices.

The rest of the paper is organized as follows: In the next section, we discuss rooted lattice trees in two and three dimensions under various branching restrictions, and estimate  $\lambda$  in each case by means of standard methods of series analysis. In addition to studying the original series [see Eq. (4) below] in each case, we also perform a *a ratio of coefficients* analysis with some interesting consequences. In Sec. III, the asymptotic analysis of trees on Bethe lattices is discussed. Finally, in Sec. IV, we present an overall discussion and a summary of our results.

## II. LATTICE TREES WITH RESTRICTED BRANCHING

Consider the generating function of the rooted tree series

$$G(x) = \sum_{n \geq 1} r_n(v) x^n, \quad (4)$$

where we have suppressed the  $z$  dependence. In this equation,  $r_n(v)$  is the number of trees with  $n$  vertices, and  $v$  refers to the restriction imposed on the valence of the branch points. In our work, we impose only the following restrictions on the valence ( $v$ ) of the branch points:  $v=3$ ,  $v=4$ ,  $v=5$ ,  $v=6$ ,  $v \leq 4$ ,  $v \leq 5$ , and  $v \leq 6$  for all lattices including those with  $z > 6$ . The reason, as will be demonstrated later, is that the growth constant does not change noticeably when

the restriction is relaxed from  $v \leq 5$  to  $v \leq 6$ , and so allowing branchings with  $v > 6$  is not likely to change our conclusions noticeably.

We have enumerated rooted trees on the sq, tr, sc, bcc, and fcc lattices using the Martin algorithm [22]. Note that on the triangular lattice, in addition to trees involving the usual nearest neighbor steps, we have enumerated trees that include next nearest neighbor (nnn) steps. In the case of the sq lattice, only the nnn case was considered, since in the nearest neighbor case  $z = v_{\max} = 4$  and the number of possible valence restrictions is too small to provide a meaningful comparison. In most cases, the number of terms in the series was less than 15, owing to computational limitations. The series corresponding to the larger coordination numbers were especially short: in fact, for fcc and trnnn with  $z=12$ , we were able to obtain only 11 terms. Copies of the series coefficients are available from the authors upon request. As mentioned earlier, the animal series used in this work were taken from published sources [19–21].

The series were studied using standard methods of analysis including Neville table extrapolation, D-Log Padé approximation, and the Baker-Hunter method [23]. In addition to the above *direct* analysis, we have also used a method based on the ratios of coefficients of each restricted series and an appropriate reference series. For a given lattice, the series with  $v \leq 6$  has been used as the reference series in each case. To demonstrate the advantages of this approach, consider the generating function of the series of ratios of coefficients, namely,

$$g(x) = \sum_{n \geq 1} \frac{r_n}{r_n(v)} x^n. \quad (5)$$

Here  $r_n \equiv r_n(v \leq 6)$  is the  $n$ th coefficient of the reference series, and  $r_n(v)$  is the  $n$ th coefficient of one of the restricted series using the same lattice. Substitution of Eq. (3) immediately yields (to lowest order)

$$g(x) \sim \sum_{n=0} \left( \frac{\lambda x}{\lambda(v)} \right)^n \approx \left( 1 - \frac{\lambda x}{\lambda(v)} \right)^{-1}, \quad (6)$$

where the dependence on  $\theta$  has canceled out.  $\lambda(v)$  and  $\lambda$  are the restricted and reference growth constants, respectively. The critical point of  $g(x)$  is located at  $x_c = \lambda(v)/\lambda$ . Because of the simple pole structure,  $g(x)$  is amenable to a straightforward Padé analysis, in addition to all of the methods cited above.

The results of the *direct* analysis of the series are shown in Tables I and II. The values shown are overall estimates consistent with the Parisi-Sourlas [15] predictions for  $\theta$  in two and three dimensions. While the shortness of the series does not seem to affect the accuracy of our results for  $v \leq 6$ , 5, 4, and 3 (shown in Table I), this is not the case for  $v=4$ , 5, and 6 (Table II). For the latter group, the number of trees for a given number of vertices  $r_n(v)$  is relatively small. Now, it is important to note that  $r_n(v)$  includes the number of walks as well as the number of trees. Since the asymptotic behavior of the number of walks is quite different from that of trees (in that both  $\lambda$  and  $\theta$  are different), it is not surprising that in these cases our analysis is not very accurate. That is, the self-avoiding walk contribution to these low order

TABLE I. Estimates of the growth constant  $\lambda$  for lattice trees and animals for  $v \leq 6$ , 5, 4, and  $v \leq 3$ .

	$z$	$v \leq 6$	$v \leq 5$	$v \leq 4$	$v \leq 3$
Trees					
fcc	12	23.585 $\pm 0.020$	23.575 $\pm 0.010$	23.4 $\pm 0.2$	21.5 $\pm 0.8$
bcc	8	15.17 $\pm 0.01$	15.160 $\pm 0.006$	15.10 $\pm 0.05$	13.7 $\pm 0.4$
sc	6	10.549 $\pm 0.002$	10.550 $\pm 0.002$	10.504 $\pm 0.005$	9.95 $\pm 0.05$
trnnn	12	21.19 $\pm 0.02$	21.166 $\pm 0.020$	21.00 $\pm 0.03$	19.735 $\pm 0.011$
sqnnn	8	12.4290 $\pm 0.0006$	12.4246 $\pm 0.008$	12.3655 $\pm 0.0006$	11.737 $\pm 0.007$
tr	6	8.396 $\pm 0.007$	8.396 $\pm 0.007$	8.374 $\pm 0.004$	8.06 $\pm 0.05$
Animals					
bcc	8	11.161 $\pm 0.007$	11.142 $\pm 0.007$	10.9685 $\pm 0.0015$	10.5 $\pm 0.1$
sc	6	8.343 $\pm 0.001$	8.340 $\pm 0.007$	8.265 $\pm 0.010$	7.8 $\pm 0.5$
tr	6	5.183 $\pm 0.001$	5.181 $\pm 0.003$	5.1 $\pm 0.3$	4.7 $\pm 0.2$

terms is still large, and new topologies appear relatively slowly because of the restrictions; we therefore expect the analysis to be affected by crossover effects. In particular, the Baker-Hunter method was not successful in the analysis of  $v = 5$  and trees, and the values quoted in Table II are largely based on Neville table extrapolation and D-Log Padé methods. It is also worth noting that, in almost all cases, working with the first and second moments of the series rather than the zeroth moment was found to improve considerably the precision of the results of the D-Log Padé and the Baker-Hunter analyses.

It is seen from Tables I and II that in all cases  $\lambda$  seems (almost) to *saturate* once the least restrictive branching,  $v \leq 6$ , is reached. In fact, the values of  $\lambda$  for  $v \leq 5$  and

TABLE II. Estimates of the growth constant  $\lambda$  of lattice trees for  $v = 3, 4, 5$ , and 6.

	$z$	$v = 3$	$v = 4$	$v = 5$	$v = 6$
fcc	12	21.5 $\pm 0.8$	17.3 $\pm 0.1$	14 $\pm 1$	12 $\pm 1$
bcc	8	13.7 $\pm 0.4$	11.3 $\pm 0.3$	9 $\pm 2$	8.2 $\pm 0.7$
sc	6	9.95 $\pm 0.05$	7.7 $\pm 0.1$	7.45 $\pm 0.30$	5.25 $\pm 0.80$
trnnn	12	19.735 $\pm 0.011$	15.7 $\pm 0.7$	14 $\pm 1$	10 $\pm 1$
sqnnn	8	11.737 $\pm 0.007$	9.3 $\pm 0.3$	7.8 $\pm 0.3$	6.8 $\pm 0.5$
tr	6	8.06 $\pm 0.05$	6.20 $\pm 0.05$	5.2 $\pm 0.1$	4.55 $\pm 0.01$

TABLE III. Estimates of the ratio  $q(v) = \lambda/\lambda(v)$  for trees and animals using the method of ratios of coefficients.

	$z$	$q(v \leq 5)$	$q(v \leq 4)$	$q(v \leq 3)$
Trees				
fcc	12	1.009 $\pm 0.005$	1.009 $\pm 0.005$	1.085 $\pm 0.010$
bcc	8	1.0005 $\pm 0.0005$	1.014 $\pm 0.008$	1.08 $\pm 0.01$
sc	6	1.0002 $\pm 0.0001$	1.0047 $\pm 0.0003$	1.065 $\pm 0.004$
trnnn	12	1.005 $\pm 0.005$	1.010 $\pm 0.005$	1.07 $\pm 0.02$
sqnnn	8	1.0003 $\pm 0.0003$	1.0050 $\pm 0.0005$	1.060 $\pm 0.002$
tr	6	1.0001 $\pm 0.0001$	1.002 $\pm 0.001$	1.044 $\pm 0.002$
Animals				
bcc	8	1.0004 $\pm 0.0002$	1.009 $\pm 0.001$	1.08 $\pm 0.01$
sc	6	1.00015 $\pm 0.00010$	1.005 $\pm 0.001$	1.06 $\pm 0.01$
tr	6	1.0005 $\pm 0.0005$	1.0007 $\pm 0.0005$	1.075 $\pm 0.005$

$v \leq 6$  are not distinguishable, given the limited length of the series used in the analysis. It is then reasonable to suppose that relaxing the branching restriction any further, say to  $v \leq 7$ , even on a lattice with  $z = 12$ , is unlikely to produce any increase in  $\lambda$  detectable by series analysis. However, pattern theorem arguments similar to those used in [13] show rigorously that  $\lambda(v \leq z) > \lambda(v \leq z - 1)$ . For a given valence restriction, a plot of  $\lambda$  against  $z$  approximately follows a straight line with only slight scatter in both two and three dimensions.

The results from the ratio of coefficients analysis are shown in Tables III and IV. Note that the ratios  $q(v) = \lambda/\lambda(v)$ , where  $\lambda = \lambda(v \leq 6)$ , depend much more strongly on the valence restrictions than on the lattice. In-

TABLE IV. Estimates of  $q(v) = \lambda/\lambda(v)$  for lattice trees using ratios of coefficients.

	$z$	$q(v = 3)$	$q(v = 4)$	$q(v = 5)$	$q(v = 6)$
fcc	12	1.085 $\pm 0.010$	1.37 $\pm 0.05$	1.80 $\pm 0.15$	1.94 $\pm 0.06$
bcc	8	1.08 $\pm 0.01$	1.38 $\pm 0.05$	1.6 $\pm 0.1$	1.9 $\pm 0.1$
sc	6	1.065 $\pm 0.004$	1.35 $\pm 0.01$	1.5 $\pm 0.1$	2.00 $\pm 0.06$
trnnn	12	1.07 $\pm 0.02$	1.35 $\pm 0.02$	1.6 $\pm 0.1$	1.9 $\pm 0.1$
sqnnn	8	1.060 $\pm 0.002$	1.35 $\pm 0.02$	1.5 $\pm 0.1$	1.87 $\pm 0.03$
tr	6	1.044 $\pm 0.002$	1.36 $\pm 0.01$	1.57 $\pm 0.06$	1.85 $\pm 0.05$

TABLE V. Estimates of  $\lambda(v)$  and  $q(v)=\lambda/\lambda(v)$  for free trees.

	$\lambda(v)$	$q(v)$
$v \leq 6$	$2.943 \pm 0.004$	
$v \leq 5$	$2.91 \pm 0.01$	$1.0100 \pm 0.0006$
$v \leq 4$	$2.81 \pm 0.01$	$1.0460 \pm 0.035$
$v \leq 3$	$2.480 \pm 0.005$	$1.183 \pm 0.005$
$v = 4$	$2.20 \pm 0.01$	$1.341 \pm 0.001$
$v = 5$	$2.00 \pm 0.05$	$1.51 \pm 0.06$
$v = 6$	$1.85 \pm 0.06$	$1.555 \pm 0.020$

deed, the ratios are almost independent of the lattice chosen and also, within error bounds, independent of whether the clusters are trees or animals.

As a means of testing our series analysis methods, especially the Baker-Hunter method, we have also studied planted free trees (i.e., abstract trees, with no reference to their embeddings) with the same branching restrictions as for the lattice trees. The term *planted tree* refers to trees that are rooted at a vertex of degree one. We obtain exact results for the numbers  $t_N$  of planted free trees containing  $N$  vertices using recursion relations derived from Polyá theory (see [24] for a more detailed discussion). The resulting recursion relations obeyed by  $t_N$  are easily solved using Maple. Series expansions for  $t_N$  may be obtained to any desired order in this way. The asymptotic behavior of  $t_N$  is analogous to that of lattice trees [see Eq. (2)]:

$$t_N \sim \lambda^N N^{-\alpha}, \quad (7)$$

where the exponent  $\alpha$  equals  $1/2$ , and  $\lambda$  depends on the valence restriction imposed.

The free tree series were analyzed using the methods described above for lattice trees. We used terms up to  $t_{15}$  in order to make a fair comparison with the lattice tree results. In all cases, the second moment series seems to yield the best results, as borne out by the value of  $\alpha$  extracted from the Baker-Hunter method for  $v \leq 3, 4, 5, 6$  and  $v = 4$ . For  $v = 5$  and  $6$ , however, the convergence of the Baker-Hunter method and the D-Log Padé methods was poor. The results, however, showed marked improvement when the series were enlarged to 30 terms.

Table V displays our results. It is seen that the  $\lambda$ 's shown compare favorably with the following exact values [24]:

$$\lambda(\text{unrestricted}) = 2.9558,$$

$$\lambda(v \leq 4) = 2.815,$$

$$\lambda(v \leq 3) = 2.4833.$$

### III. TREES ON BETHE LATTICES

In the preceding section, we discussed the behavior of the growth constant for rooted trees embedded in different lattices in two and three dimensions. In an attempt to separate the influence of the branching restrictions from those of the lattice and the dimension of the space in which it is embedded, we now consider trees in a Bethe lattice with the same valence restrictions as before. A rooted Bethe lattice is an

infinite uniform Cayley tree rooted at a distinguished vertex labeled the origin. Initially we focus on subtrees of the Bethe lattice planted at the root of the lattice, with the first bond specified. We refer to these as planted subtrees. In this section we show that the generating function for planted subtrees of the Bethe lattice determines the generating function for rooted subtrees of the Bethe lattice. Furthermore, the number of rooted subtrees for the Bethe lattice of coordination number  $z$  is an upper bound for the corresponding numbers of rooted trees on regular lattices, embeddable in  $R^d$ , with coordination number  $z$ . For convenience, in the remainder of this section the term regular lattice will imply embeddable in  $R^d$ .

We denote the rooted Bethe lattice with coordination number  $z$  by  $\mathcal{T}_z$ . Define  $P_n(v)$  to be the number of  $n$ -vertex planted subtrees of  $\mathcal{T}_z$  where  $v$  refers to the restriction imposed on the valences of the vertices as in Sec. II. Note that  $P_0(v) = 0$ ,  $P_1(v) = 0$ , and  $P_2(v) = 1$ . Define  $R_n(v)$  to be the number of  $n$ -vertex rooted subtrees of  $\mathcal{T}_z$  (rooted at the origin) where  $v$  refers to the restriction imposed on the valences of the vertices. We will show that the asymptotic behavior of either  $R_n$  or  $P_n$  is analogous to that of lattice trees [see Eq. (3)]:

$$R_n \sim P_n \sim \lambda^n n^{-\alpha}, \quad (8)$$

where the exponent  $\alpha$  equals  $3/2$ , and  $\lambda$  depends on the valence restriction imposed.

We first show that the numbers of planted and rooted subtrees of the Bethe lattice with coordination number  $z$  are upper bounds on the corresponding numbers on a regular lattice with the same coordination number. Given any regular lattice with coordination number  $z$ , just as we defined  $r_n(v)$  in Sec. II to be the number of  $n$ -vertex rooted lattice trees with vertex valences restricted according to  $v$ , we now define  $p_n(v)$  to be the corresponding number of planted lattice trees. For each vertex of the regular lattice we can define a single *in bond* in  $z$  ways and then for each in bond of the vertex we can define a unique ordering of the remaining  $z-1$  *out bonds*. For each vertex (except the root) on the rooted Bethe lattice there is a unique in bond, i.e., the bond connecting that vertex to the root, and we can fix an ordering of the remaining  $z-1$  out bonds. Since for every vertex (except the root) in a rooted subtree of a regular lattice there is a unique in bond (i.e., the bond of the tree connecting that vertex to the root), one can define an injection from the set of rooted subtrees of a regular lattice with coordination number  $z$  to the set of rooted subtrees of  $\mathcal{T}_z$  using the out-bond orderings specified above for each lattice. Hence

$$r_n(v) \leq R_n(v) \quad (9)$$

and

$$p_n(v) \leq P_n(v). \quad (10)$$

Let  $P(x) \equiv P^{(v,z)}(x) = \sum_{n=0}^{\infty} P_n(v) x^n$  be the ordinary generating function for the sequence of  $P_n(v)$ 's. Let  $S$  be the set of possible numbers of children for a vertex under the branch point restriction  $v$ . We can derive a functional equation for the generating function  $P(x)$  by constructing a recurrence relation for the sequence of  $P_n$ 's as follows. Start with any

$n$ -vertex planted subtree of  $\mathcal{F}_z$  for  $n \geq 3$ . First remove from the subtree the root  $v_0$  and its adjacent vertex  $v_1$  (and all bonds of the subtree incident on either of these vertices). We are then left with  $j$  rooted trees where  $j$  is the number of children of  $v_1$  ( $1 \leq j \leq z-1, j \in S$ ) and the roots of these trees are the children of  $v_1$ . Now we can add a new bond and vertex (which will become the new root) to the root of each of these trees to obtain  $j$  planted subtrees of  $\mathcal{F}_z$ . Let  $m_i$  be the number of vertices in the  $i$ th planted tree. Note that  $\sum_{i=1}^j m_i = n-2+j$ . This implies the following recurrence relation for  $P_n, n \geq 3$ :

$$P_n = \sum_{j \in S, j > 0} \binom{z-1}{j} \times \sum_{\{m_i, i=1, \dots, j; \sum_{i=1}^j m_i = n-2+j\}} P_{m_1} P_{m_2} \cdots P_{m_j} \quad (11)$$

Multiplying both sides by  $x^n$ , summing from  $n=3, \dots, \infty$  and then using the fact that  $P_0=P_1=0, P_2=1$  leads to the following functional equation:

$$P(x) = x^2 \sum_{j \in S} \binom{z-1}{j} \left[ \frac{P(x)}{x} \right]^j \quad (12)$$

Note that if  $v \leq 2$  ( $S = \{0,1\}$ ) then the solution of the resulting equation for  $P$  yields the expected result that  $P_n(v) = (z-1)^{n-2}$  (i.e., the number of planted self-avoiding walks on  $\mathcal{F}_z$ ). Since Eq. (12) is a polynomial equation in  $P(x)/x$  of degree  $k = \min\{j | j \in S\}$ , one could solve this to find  $P(x)/x$  and hence  $P_n(v)$  for at least  $k \leq 3$ . However, we are primarily interested in the asymptotic behavior of  $P_n(v)$ , and in larger values of  $k$ , so we take a different approach. In particular we follow Theorem 5 of Bender [25] (p. 502, see also Harary *et al.* [26] and Meir and Moon [27]), replace  $P(x)/x$  by  $w$ , and rewrite the functional equation above as

$$F(x,w) \equiv \left[ \sum_{j \in S} x \binom{z-1}{j} w^j \right] - w = 0. \quad (13)$$

Note that since  $P_0(v) = 0$  and  $P_1(v) = 0$ ,  $P(x)/x$  is a power series in  $x$ , which is 0 for  $x=0$  and the radius of convergence for  $P(x)/x$  is equal to the radius of convergence for  $P(x)$ .  $F(x,w)$  is a polynomial in  $x$  and  $w$  and hence it is analytic for all  $x$  and  $w$ . The coefficients of  $F(x,w) + w$  are all non-negative so that Theorem 1, p. 82, of Meir and Moon [27] guarantees that Bender's result is valid for this problem. Thus the growth constant  $\lambda(v)$  can be determined by first solving the two simultaneous equations  $F(r,s) = 0$  and  $F_w(r,s) = 0$  for  $r$  and  $s$ , where  $F_w$  is the partial derivative of  $F$  with respect to  $w$ . Then, according to Bender's result,  $r$  is the radius of convergence of  $P(x)/x$  and hence  $\lambda(v) = 1/r$  and  $s = P(r)/r$ . From Eq. (13) one can solve for  $r$  and  $s$  to obtain

$$\lambda(v) = \frac{1}{r} = \sum_{j \in S} j \binom{z-1}{j} s^{j-1} = \sum_{j \in S} \binom{z-1}{j} s^{j-1} \quad (14)$$

and where  $s$  is the unique positive real solution of

$$\sum_{j \in S} (j-1) \binom{z-1}{j} s^j = 0. \quad (15)$$

Given valence restriction  $v$  with corresponding set  $S$ , such that  $1 \in S$ , there is a corresponding homeomorphically irreducible case  $\bar{v}$  with corresponding set  $\bar{S} = S - \{1\}$ . We note that the term  $j=1$  does not contribute to the left-hand side of Eq. (15) so  $s$  is the same for both  $v$  and  $\bar{v}$ . Hence  $\lambda(v) = \lambda(\bar{v}) + (z-1)$ .

The general asymptotic behavior of  $P_n$  is then as follows:

$$P_{n+1} \sim \left[ \frac{F_x}{2\pi\lambda F_{ww}} \right]^{1/2} n^{-3/2} \lambda^n, \quad (16)$$

where  $F_x$  and  $F_{ww}$  are evaluated at  $(r,s)$ . Using Eqs. (14) and (15) we get

$$\frac{F_x}{F_{ww}} = \frac{s^2 \lambda^2}{\left[ \sum_{j \in S} \binom{z-1}{j} j^2 s^{j-1} \right] - \lambda}. \quad (17)$$

Three cases can be solved fairly easily, and the results can be summarized as follows.

1.  $v = k+1$  ( $S = \{0,1,k\}$ ),  $2 \leq k \leq z-1$ :

$$\lambda = z-1 + \frac{k}{k-1} \left[ \binom{z-1}{k} (k-1) \right]^{1/k}, \quad (18)$$

$$s = \left[ \binom{z-1}{k} (k-1) \right]^{-1/k}. \quad (19)$$

Note that in this case, for fixed  $k$ ,

$$\lambda \sim (z-1) \left[ 1 + \frac{k}{(k-1)^{1-1/k}} \left( \frac{1}{k!} \right)^{1/k} \right] \quad (20)$$

as  $z$  goes to infinity. For  $k=2,3,4,5$ , the coefficient of  $z-1$  in Eq. (20) is  $1 + \sqrt{2} \approx 2.4142$ ,  $2.04004$ ,  $1.792805$ ,  $1.6331196$ , respectively.

2.  $v \leq z$  ( $S = \{0,1, \dots, z-1\}$ ):

$$\lambda = (z-1) \left( 1 + \frac{1}{z-2} \right)^{z-2} = \frac{(z-1)^{z-1}}{(z-2)^{z-2}}, \quad (21)$$

$$s = \frac{1}{z-2}. \quad (22)$$

The result in Eq. (21) agrees with the result of Fisher and Essam [28] and with the fact that in this case one can solve explicitly for  $P_n(v)$  to obtain

$$P_n(v) = \binom{(z-1)(n-1)}{n-1} \frac{1}{(z-2)(n-1)+1} \quad (23)$$

[see Penrose [29], Eq. (4) and note that  $P_n(v) = b_{n-2}(z-1)$ ].

TABLE VI. The growth constant  $\lambda(v)$  for trees on the Bethe lattice for  $v \leq z$ , 6, 5, 4, and 3.

$z$	$v \leq z$	$v \leq 6$	$v \leq 5$	$v \leq 4$	$v \leq 3$
12	28.531 167 06	28.526 187 70	28.479 122 19	28.117 664 01	25.832 396 97
8	17.651 384 60	17.650 462 25	17.634 097 02	17.460 761 28	16.165 151 39
6	12.207 031 25	12.207 031 25	12.203 112 42	12.121 540 58	11.324 555 32

3.  $v \leq 4$  ( $S = \{0, 1, 2, 3\}$ ):

$$\lambda = (z-1) \left( 1 + \frac{1-2/(z-1)}{A} + \frac{1}{2} \frac{1-1/(z-1)}{(1-2/(z-1))} A + \frac{1}{6} \frac{1-1/(z-1)}{1-2/(z-1)} A^2 \right), \tag{24}$$

where

$$A \equiv \frac{B}{[1-1/(z-1)]^{1/3}} + \frac{1}{4} \frac{[1-1/(z-1)]^{1/3}}{B} - \frac{1}{2} \tag{25}$$

and

$$B \equiv \left[ \frac{11}{8} - \frac{47}{8(z-1)} + \frac{6}{(z-1)^2} + \left( 1 - \frac{2}{z-1} \right) \sqrt[3]{\frac{15}{8} - \frac{69}{8(z-1)} + \frac{9}{(z-1)^2}} \right]^{1/3}. \tag{26}$$

In this case

$$\lambda \sim (z-1) \left( 1 + \frac{1}{b} + \frac{1}{2}b + \frac{1}{6}b^2 \right) \approx 2.660\ 324\ 085(z-1) \tag{27}$$

as  $z$  goes to infinity, where

$$b = \frac{1-2(11/8 + \sqrt[3]{15/8})^{1/3} + 4(11/8 + \sqrt[3]{15/8})^{2/3}}{4(11/8 + \sqrt[3]{15/8})^{1/3}} \approx 1.078\ 616\ 89. \tag{28}$$

Other cases can be solved numerically. Tables VI and VII show the results for  $\lambda$  for the cases corresponding to Tables I and II from Sec. II. Tables VIII and IX show the results for  $\lambda/\lambda(v)$  for the cases corresponding to Tables III and IV from Sec. II.

Equations (20) and (27) show that, for these two cases,  $\lambda(v)$  is asymptotically a linear function of  $z-1$ . This result can be generalized as follows. Equation (15) can be rewritten as

$$\sum_{j \in S - \{0\}} (j-1) \binom{z-1}{j} s^j = 1. \tag{29}$$

Let  $p = |S|$ . Assuming  $p \geq 3$  and  $\{0, 1\} \subset S$ , the number of nonzero terms on the left-hand side of Eq. (29) is  $p-2$ , therefore there exists  $m \in S - \{0, 1\}$  such that

$$(m-1) \binom{z-1}{m} s^m \geq \frac{1}{p-2}. \tag{30}$$

With one such  $m$  fixed, from Eq. (30) and the equation

$$\binom{z-1}{j} = \frac{(z-1)^j}{j!} \prod_{i=1}^{j-1} \left( 1 - \frac{i}{z-1} \right) \tag{31}$$

we obtain

$$s \geq \frac{(m!)^{1/m}}{(z-1)(p-2)^{1/m}(m-1)^{1/m} \{ \prod_{i=1}^{m-1} [1-i/(z-1)] \}^{1/m}} \equiv \frac{B_z}{z-1}. \tag{32}$$

Similarly each term on the left-hand side of Eq. (29) must be less than one. Hence

$$(m-1) \binom{z-1}{m} s^m < 1 \tag{33}$$

and so

$$s \leq \frac{(m!)^{1/m}}{(z-1)(m-1)^{1/m} \{ \prod_{i=1}^{m-1} [1-i/(z-1)] \}^{1/m}} \equiv \frac{A_z}{z-1}. \tag{34}$$

Using the bounds in Eqs. (32) and (34) in Eq. (14) we obtain

$$\sum_{j \in S} j \binom{z-1}{j} \left[ \frac{B_z}{(z-1)} \right]^{j-1} \leq \lambda(v) \leq \sum_{j \in S} j \binom{z-1}{j} \left[ \frac{A_z}{(z-1)} \right]^{j-1}. \tag{35}$$

Using equation (31), equation (35) becomes

$$(z-1) \sum_{j \in S} \frac{j B_z^{j-1}}{j!} \prod_{i=1}^{j-1} \left( 1 - \frac{i}{z-1} \right) \leq \lambda(v) \leq (z-1) \sum_{j \in S} \frac{j A_z^{j-1}}{j!} \prod_{i=1}^{j-1} \left( 1 - \frac{i}{z-1} \right). \tag{36}$$

Note that  $\lim_{z \rightarrow \infty} A_z = A$ , a constant, and  $\lim_{z \rightarrow \infty} B_z = B = A/(p-2)^{1/m}$ , a constant. Therefore, there exists constants  $c_1$  and  $c_2$ , which depend on  $S$ , such that

$$c_1 \leq \liminf_{z \rightarrow \infty} \frac{\lambda(v)}{z-1} \leq \limsup_{z \rightarrow \infty} \frac{\lambda(v)}{z-1} \leq c_2. \tag{37}$$

TABLE VII. The growth constant  $\lambda(v)$  for trees on the Bethe lattice for  $v=3, 4, 5, 6$ , and  $z$ .

$z$	$v=3$	$v=4$	$v=5$	$v=6$	$v=z$
12	25.832 396 97	21.365 634 85	18.479 068 92	16.626 656 55	12.356 131 41
8	16.165 151 39	13.181 927 95	11.268 114 50	10.032 256 04	8.5069 930 66
6	11.324 555 32	9.0716 264 26	7.6239 862 27	6.6493 848 89	6.6493 848 89

In the case  $S=\{0,1,k\}$ ,  $p=3$ ,  $m=k$ , and  $c_1=c_2$  so  $\lim_{z \rightarrow \infty} \lambda(v)/(z-1)=c_1$  and this is equivalent to the result in Eq. (20).

The above analysis was for planted trees. We now wish to relate these results to the corresponding results for rooted trees. Let  $R(x)=\sum_{n=0}^{\infty} R_n(v)x^n$  be the ordinary generating function for  $R_n(v)$ . Let  $S$  be the set of possible numbers of children for a vertex (other than the root) under the branch point restriction  $v$ . Note that  $0 \in S$ . We can derive a functional equation for the generating function  $R(x)$  by constructing a recurrence relation for the sequence of  $R_n$ 's in terms of the  $P_n$ 's as follows. Start with any  $n$ -vertex rooted subtree of  $\mathcal{T}_z$  for  $n \geq 2$ . First remove the root vertex  $v_0$  (and any edges incident on it). We are then left with  $j$  rooted trees where  $j$  is the number of children of  $v_0$  ( $1 \leq j \leq z$ ,  $j-1 \in S$ ) and the roots of the trees are the children of  $v_0$ . Now we can add a new bond and vertex (which will become the new root) to the root of each of these trees to obtain  $j$  planted subtrees of  $\mathcal{T}_z$ . Let  $m_i$  be the number of vertices in the  $i$ th planted subtree. Note that  $\sum_{i=1}^k m_i = n-1+j$ . This implies the following recurrence relation for  $R_n, n \geq 2$ :

$$R_n = \sum_{j-1 \in S, j > 0} \binom{z}{j} \times \sum_{\{m_i, i=1, \dots, j; \sum_{i=1}^j m_i = n-1+j\}} P_{m_1} P_{m_2} \dots P_{m_j}. \quad (38)$$

Multiplying both sides by  $x^n$ , summing from  $n=2, \dots, \infty$  and then using the fact that  $P_0=P_1=0$ ,  $P_2=1$  and  $R_0=0$ ,  $R_1=1$  leads to the following functional equation:

$$R(x) = x + x \sum_{j \in S} \binom{z}{j+1} \left[ \frac{P(x)}{x} \right]^{j+1}, \quad (39)$$

which can be rewritten as

$$R(x) = x + x \sum_{j \in S} \frac{z}{j+1} \binom{z-1}{j} \left[ \frac{P(x)}{x} \right]^{j+1}. \quad (40)$$

By the definition of  $R_n$  and  $P_n$  it is clear that  $P_n \leq R_{n-1}$ . From this and Eq. (40) we obtain

$$\frac{P(x)}{x} \leq R(x) \leq x + z \left[ \frac{P(x)}{x} \right]^2. \quad (41)$$

Since  $P(x)/x$  has the same radius of convergence as  $P(x)$ , the bounds in Eq. (41) imply that the radius of convergence for  $R(x)$  is equal to the radius of convergence for  $P(x)$ . Hence the growth constant  $\lambda$  is the same for both  $P_n$  and  $R_n$ . We also know (from Bender's Theorem 5) that

$$\frac{P(x)}{x} = A(x)(1-\lambda x)^{1/2} + B(x), \quad (42)$$

where  $A(x)$  and  $B(x)$  are analytic in a disk with radius greater than  $1/\lambda$ . Using Eqs. (42) and (39) yields

$$\begin{aligned} R(x) &= x + x \sum_{j \in S} \binom{z}{j+1} [A(x)(1-\lambda x)^{1/2} + B(x)]^{j+1} = x + x \sum_{j \in S} \binom{z}{j+1} \left[ \sum_{l=0}^{j+1} \binom{j+1}{l} A(x)^l (1-\lambda x)^{l/2} B(x)^{j+1-l} \right] \\ &= x + x \sum_{l=0}^{k+1} (1-\lambda x)^{l/2} A(x)^l \sum_{j \in S, j \geq l-1} \binom{z}{j+1} \binom{j+1}{l} B(x)^{j+1-l} \\ &= x + x \sum_{l=0}^{\lfloor \frac{k+1}{2} \rfloor} (1-\lambda x)^l A(x)^{2l} \sum_{j \in S, j \geq 2l-1} \binom{z}{j+1} \binom{j+1}{2l} B(x)^{j+1-2l} + (1-\lambda x)^{1/2} x \sum_{l=0}^k (1-\lambda x)^l A(x)^{2l+1} \\ &\quad \times \sum_{j \in S, j \geq 2l} \binom{z}{j+1} \binom{j+1}{2l+1} B(x)^{j-2l}. \end{aligned} \quad (43)$$

TABLE VIII. The ratio  $q(v)=\lambda/\lambda(v)$  for Bethe lattice trees.

$z$	$q(v \leq 5)$	$q(v \leq 4)$	$q(v \leq 3)$
12	1.001 653	1.014 529	1.104 280
8	1.000 928	1.010 864	1.091 884
6	1.000 321	1.007 053	1.077 926

Since the  $l=0, j=0$  term in the final sum is nonzero,  $R(x)=\hat{B}(x)+(1-\lambda x)^{1/2}\hat{A}(x)$ , where  $\hat{A}(x)$  and  $\hat{B}(x)$  are analytic in a disk with radius larger than  $1/\lambda$ . This implies by Darboux's theorem that  $R_n/\lambda^n=O(n^{-3/2})$  as claimed in Eq. (8).

#### IV. CONCLUSION

In this paper we have investigated the way in which the growth constants of animals and trees in various lattices depend on (a) the coordination number of the lattice and (b) valence restrictions imposed on the tree or animal. Our results describe the specifics of how the growth constant increases as the coordination number increases, increases as the maximum valence restriction is relaxed, and decreases as  $k$  increases for the special case of allowed branch vertex valence  $k$  only. Roughly speaking, the growth constants increase more or less linearly with coordination number, though we do not expect this increase to be strictly linear.

For the Bethe lattice with coordination number  $z$  we have proved that the growth constant is bounded above and below by linear functions of  $z$  for large  $z$ , which is presumably related to the quasilinear behavior observed for the regular lattices. We have used Eqs. (15) and (14) to calculate numerical values of  $\lambda(v)$  for integer values of  $z$  up to 100. It is not difficult to prove that  $\lambda(v \leq 2) < \lambda(v = z - 1) < \lambda(v = z - 2) < \dots < \lambda(v = 3)$  and the nonstrict inequalities  $\lambda(v = 3) = \lambda(v \leq 3) \leq \lambda(v \leq 4) \leq \dots \leq \lambda(v \leq z - 1)$ .

TABLE IX. The ratio  $q(v)=\lambda/\lambda(v)$  for Bethe lattice trees.

$z$	$q(v = 3)$	$q(v = 4)$	$q(v = 5)$	$q(v = 6)$
12	1.104 280	1.335 143	1.543 703	1.715 690
8	1.091 884	1.338 990	1.566 408	1.759 371
6	1.077 926	1.345 628	1.601 135	1.835 814

We observe, from the numerical data, that  $\lambda(v \leq 2) < \lambda(v = z - 1) < \lambda(v = z - 2) < \dots < \lambda(v = 3) = \lambda(v \leq 3) < \lambda(v \leq 4) < \dots < \lambda(v \leq z - 1)$ . In addition, for fixed  $v$ ,  $\lambda(v)$  is essentially indistinguishable from a linear function of  $z - 1$  even for small values of  $z$ .

A remarkable feature of our results is that the ratio  $\lambda/\lambda(v)$  is almost independent of the lattice considered. Indeed for the cases where  $v=3, 4$ , or  $5$  (Tables IV and IX), the variation is comparable with the error estimates for the series analysis and the Bethe lattice values of these ratios are very close to those found for the two- and three-dimensional lattices. Understanding why these ratios are almost lattice independent may provide insight into how valence restrictions affect the generation of new topologies as the molecular weight of a given branched polymer is increased.

We have proved that the results on the Bethe lattice are upper bounds for the corresponding results on regular lattices and we expect that, as the dimension of the regular lattices goes to infinity, the Bethe lattice upper bound will become sharper. In light of these results it would be interesting to obtain data for valence restricted trees in higher dimensions, and to construct a  $1/d$  expansion about the Bethe lattice results.

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