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The collapse transition for lattice trees

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Abstract. We consider a lattice tree model for the collapse of dilute branched polymers in the good solvent regime in which the collapse is driven by a near-neighbour contact fugacity. We describe some rigorous results, including bounds, for the temperature dependence of the reduced limiting free energy and compare these results with numerical estimates derived from exact enumeration data. From the specific heat, we estimate the collapse temperature T_c and the cross-over exponent ϕ_0 in two and three dimensions. We find $\phi_0 = 0.60 \pm 0.03$ ($d=2$) and $\phi_0 = 0.82 \pm 0.03$ ($d=3$). Finally, we speculate on a possible roughening transition which may occur at a temperature $T_r < T_c$.

1. Introduction

Recently there has been considerable interest in the collapse of branched polymers. Randomly branched polymers in dilute solution in a good solvent have been modelled by lattice animals (i.e. by connected subgraphs of a lattice). As the solvent quality decreases, or alternatively the temperature decreases, the branched polymers become more compact and a tricritical collapse transition is expected to occur. For linear polymers, the existence of an analogous transition is well documented (see, for example, the references cited by Derrida and Herrmann 1983). The existence of a collapse transition in a directed animal model has been proved by Dhar (1987). A directed model for linear polymers has been studied by Binder *et al* (1990) who determined the location of the collapse transition exactly.

Two basic types of lattice animal model have been proposed to study the collapse of branched polymers. In one of these, the collapse is driven by some kind of near-neighbour fugacity and in the other by a cycle fugacity. However, several variants of these underlying models are possible. For example, the animals may be either weakly embedded or strongly embedded in the lattice (i.e. subgraphs or section graphs, respectively), and their size may be classified either by their site content or their bond content. A more extensive discussion of the various models has been given by Gaunt and Flesia (1990) and by Madras *et al* (1990). So far all workers (Derrida and Herrmann 1983, Dickman and Schieve 1984, Lam 1987, 1988, Chang and Shapir 1988, Madras *et al* 1988, 1990, Gaunt and Flesia 1990) have studied one or more versions of the cycle model. In addition, Gaunt and Flesia (1990) and Madras *et al* (1990) have studied the reduced limiting free energy of a near-neighbour *contact* model. (Two vertices form a contact if they are non-bonded near-neighbours.)

Yet another model is associated with *lattice trees*. Work by Lubensky and Isaacson (1979) first suggested that cycles are relatively unimportant in determining the universality class of branched polymers. This conclusion has been verified numerically (see

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e.g. Seitz and Klein 1981, Duarte and Ruskin 1981, Gaunt *et al* 1982) and has led to lattice trees being considered as a useful model of branched polymers in dilute solution in the good solvent regime. However, lattice trees may also be used as a model of a collapsing branched polymer. They have the advantage of simplicity in that instead of the plethora of models associated with lattice animals, there is just one lattice tree model. Clearly, all the cycle models are irrelevant for trees and amongst the near-neighbour fugacity models, only the contact model is non-trivial. Furthermore, the trees must be weakly embedded in the underlying lattice since for strongly embedded trees the number of contacts is zero by definition. Lastly, since the number of sites (n) and the number of bonds (b) in a tree are trivially related by $b = n - 1$, it is immaterial whether the size of the tree is classified by its site or bond content. Thus, the one and only tree model is described by a near-neighbour contact fugacity, with the lattice trees weakly embedded in the lattice and their size classified by their site content, say. We refer to this model as the t-model.

The partition function of the t-model is defined by

$$Z_n(\beta) = \sum_{\lambda} t_n(\lambda)\, e^{\beta\lambda} \tag{1.1}$$

where $t_n(\lambda)$ is the number of weakly embedded trees with n sites and λ near-neighbour contacts, and e^{β} is the contact fugacity. We note that $\beta > 0$ corresponds to attractive interactions and $\beta < 0$ to repulsive interactions. We define the reduced free energy by

$$F_n(\beta) = n^{-1} \log Z_n(\beta) \tag{1.2}$$

and the reduced limiting free energy by

$$\mathscr{F}(\beta) = \lim_{n\to\infty} F_n(\beta). \tag{1.3}$$

For a d-dimensional hypercubic lattice, Madras *et al* (1990) have proved a number of rigorous results relating to $\mathscr{F}(\beta)$, which we now summarize.

First, the limit in (1.3) exists for $-\infty \leqslant \beta < \infty$, and $\mathscr{F}(\beta)$ is monotone, non-decreasing, convex and continuous for $-\infty < \beta < \infty$. If Λ_0 and λ_0 are the growth constants for strongly and weakly embedded trees, respectively, then

$$\mathscr{F}(-\infty) = \log \Lambda_0 \tag{1.4}$$

and

$$\mathscr{F}(0) = \log \lambda_0 \tag{1.5}$$

although there is *no* proof that

$$\lim_{\beta\to-\infty} \mathscr{F}(\beta) = \log \Lambda_0. \tag{1.6}$$

For $\beta > 0$, $\mathscr{F}(\beta)$ is bounded below and above as follows

$$\max\{\mathscr{F}(0), (d-1)\beta\} \leqslant \mathscr{F}(\beta) \leqslant \mathscr{F}(0) + (d-1)\beta. \tag{1.7}$$

Dividing (1.7) by β and letting $\beta \to \infty$ gives

$$\lim_{\beta\to\infty} \mathscr{F}(\beta)/\beta = d - 1 \tag{1.8}$$

and, moreover, there is an asymptotic line

$$L(\beta) = (d-1)\beta + S \tag{1.9}$$

such that $\lim_{\beta\to\infty}\{\mathscr{F}(\beta)-L(\beta)\}=0$. Physically, S is interpreted as the reduced limiting entropy of the compact phase. It turns out that there are exponentially many maximally compact trees which implies that S is strictly positive. In fact, it can be proved that

$$\pi^{-d}\int_0^{\pi}\dots\int_0^{\pi}\log\left(2d-2\sum_{i=1}^{d}\cos\alpha_i\right)\mathrm{d}\alpha_1\dots\mathrm{d}\alpha_d\leqslant S\leqslant d\log d-(d-1)\log(d-1). \tag{1.10}$$

So, in particular, for the square lattice

$$(4\mathscr{C}/\pi=)1.166\ldots\leqslant S\leqslant 1.386\ldots \tag{1.11}$$

where $\mathscr{C}$ is Catalan's constant, and for the simple cubic lattice

$$1.673\ldots\leqslant S\leqslant 1.909\ldots. \tag{1.12}$$

In section 2, we compare the above rigorous results with numerical estimates of $\mathscr{F}(\beta)$ for the square and simple cubic lattices. As expected, $\mathscr{F}(\beta)$ is rather smooth and we have been unable to detect any sign of the singularity which is expected to occur for some value of $\beta=\beta_c>0$ corresponding to the collapse transition. In order to locate the transition point, β_c, we study the specific heat in section 3. Numerical estimates of the cross-over exponent, ϕ_0, are given in both two and three dimensions. We conclude, in section 4, with a summary and discussion of our results.

Our numerical estimates are based on a knowledge of $Z_n(\beta)$ for all $n\leqslant N$. They are given in appendix 1 up to $N=19$ on the square and diamond lattices, $N=17$ on the simple cubic lattice and $N=15$ on the body-centred cubic lattice. They were obtained from exact enumeration data derived by Martin (1990) using combinatorial techniques invented by Sykes (1986a, b, c, d). These data have already been given by Madras *et al* (1990) for the square and simple cubic lattices. The data for the other two lattices will appear in a future publication. In appendix 2, we give some data for bond and site trees.

2. Free energy

In this section, we report numerical estimates for the β-dependence of the reduced limiting free energy of the square and simple cubic lattices, and compare these estimates with the rigorous results described in section 1.

We begin by using the data given in appendix 1 to calculate the reduced free energy $F_n(\beta)$, defined in (1.2), for values of β in the interval $-4\leqslant\beta\leqslant 6$. The results for the simple cubic lattice are plotted in figure 1. The corresponding plot for the square lattice is very similar.

The reduced limiting free energy $\mathscr{F}(\beta)$ is the $n\to\infty$ limit of these curves and must lie somewhere between the rigorous lower and upper bounds given in the last section. These bounds are shown in figure 1 for the simple cubic lattice and have been plotted using the numerical estimates (Gaunt *et al* 1982)

$$\log\Lambda_0=2.061\pm0.007\qquad \log\lambda_0=2.351\pm0.007. \tag{2.1}$$

We note for use later that the corresponding estimates for the square lattice are (Gaunt *et al* 1982)

$$\log\Lambda_0=1.334\pm0.002\qquad \log\lambda_0=1.637\pm0.002. \tag{2.2}$$

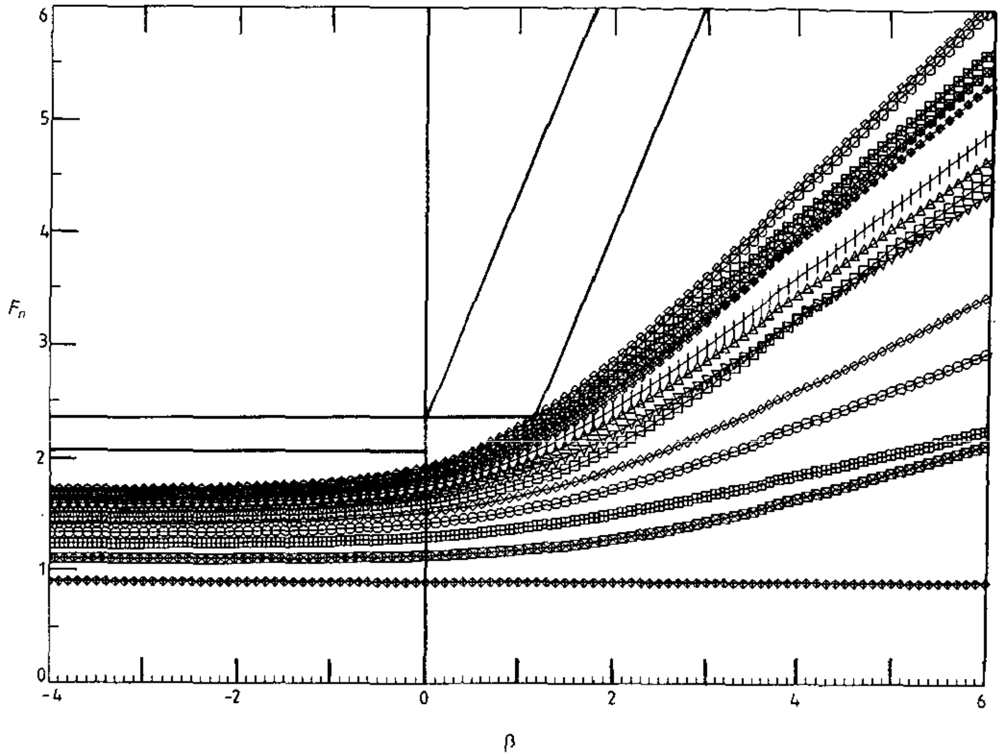

Figure 1. The reduced free energy, $F_n(\beta)$, of the simple cubic lattice or $n=3$–17. Upper and lower bounds to $\mathcal{F}(\beta)$ are included.

It is seen from figure 1 that for values of $n \leqslant 17$ on the simple cubic lattice, the $F_n(\beta)$ curves lie entirely outside the region delineated by the bounds and hence considerable extrapolation is required in order to estimate $\mathcal{F}(\beta)$, especially for large β (i.e. low temperatures).

The extrapolation methods which we have found most useful are the ratio and Padé approximant techniques (Gaunt and Guttmann 1974). The application of these techniques to problems of this kind has been described in detail elsewhere (Gaunt and Flesia 1990, Madras *et al* 1990). Estimates of $\mathcal{F}(\beta)$ from these two methods agree well with each other but the ratio estimates are usually more precise. For $\beta \leqslant 0$ and for small positive values of β, the results are very satisfactory. However, both methods rapidly become less useful for larger values of β and for $\beta \gtrsim 1.5$ (square) and $\beta \gtrsim 1$ (simple cubic) they fail to provide estimates of any reliability.

Our best estimates for the square and simple cubic lattices are tabulated in table 1 and plotted in figures 2 and 3, respectively. Upper and lower bounds to $\mathcal{F}(\beta)$ and to the asymptotic line $L(\beta)$ are given as continuous and dashed curves, respectively.

For $\beta \leqslant 0$, our results suggest very strongly that equation (1.6), for which there is no proof, is in fact correct, i.e. $\mathcal{F}(\beta)$ is asymptotic to $\log \Lambda_0$ as $\beta \to -\infty$. For $\beta > 0$, our results are consistent with a rather rapid approach to the asymptote $L(\beta)$. We have tried to estimate the limiting entropy S of the compact phase from the behaviour of $\{\mathcal{F}(\beta) - (d-1)\beta\}$ for increasing values of $\beta > 0$. This quantity is given in table 1 and suggests a value of S for the square and simple cubic lattices close or equal to the lower bounds in (1.11) and (1.12), respectively.

Table 1. Estimates of the limiting free energy $\mathcal{F}(\beta)$ and $\mathcal{F}(\beta)-(d-1)\beta$ for the square and simple cubic lattices.

	Square		Simple cubic	
β	$\mathcal{F}(\beta)$	$\mathcal{F}(\beta)-\beta$	$\mathcal{F}(\beta)$	$\mathcal{F}(\beta)-2\beta$
−4.0	1.339 ± 0.002		2.0647 ± 0.0005	
−3.5	1.342 ± 0.002		2.0677 ± 0.0007	
−3.0	1.348 ± 0.002		2.0728 ± 0.0008	
−2.5	1.356 ± 0.002		2.0811 ± 0.0008	
−2.0	1.371 ± 0.001		2.0948 ± 0.0009	
−1.5	1.396 ± 0.001		2.118 ± 0.001	
−1.0	1.439 ± 0.001		2.157 ± 0.001	
−0.5	1.513 ± 0.001		2.225 ± 0.001	
0	1.637 ± 0.002	1.637 ± 0.002	2.351 ± 0.007	2.351 ± 0.007
0.1	1.669 ± 0.002	1.569 ± 0.002	2.395 ± 0.002	2.195 ± 0.002
0.2	1.707 ± 0.002	1.507 ± 0.002	2.445 ± 0.004	2.045 ± 0.004
0.3	1.749 ± 0.002	1.449 ± 0.002	2.509 ± 0.007	1.909 ± 0.007
0.4	1.797 ± 0.003	1.397 ± 0.003	2.59 ± 0.01	1.79 ± 0.01
0.5	1.850 ± 0.005	1.350 ± 0.005	2.68 ± 0.02	1.68 ± 0.02
0.6	1.906 ± 0.006	1.306 ± 0.006	2.79 ± 0.04	1.59 ± 0.04
0.7	1.969 ± 0.007	1.269 ± 0.007	2.90 ± 0.08	1.50 ± 0.08
0.8	2.032 ± 0.009	1.232 ± 0.009	3.16 ± 0.15	1.56 ± 0.15
0.9	2.10 ± 0.02	1.20 ± 0.02	3.30 ± 0.20	1.50 ± 0.20
1.0	2.16 ± 0.04	1.16 ± 0.04	3.50 ± 0.25	1.50 ± 0.25
1.1	2.23 ± 0.04	1.13 ± 0.04		
1.2	2.29 ± 0.07	1.09 ± 0.07		
1.3	2.36 ± 0.10	1.06 ± 0.10		
1.4	2.44 ± 0.15	1.04 ± 0.15		
1.5	2.50 ± 0.20	1.0 ± 0.20		

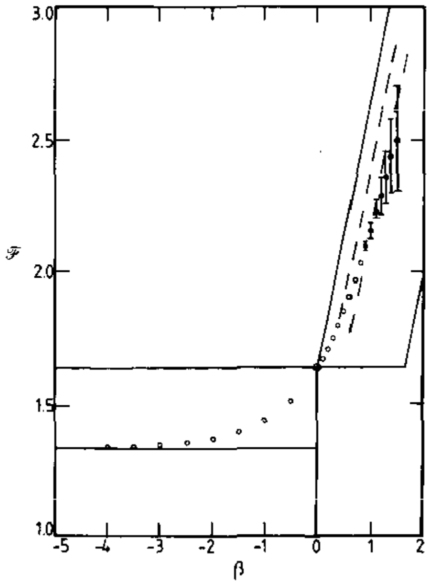

Figure 2. Numerical estimates of the reduced limiting free energy $\mathcal{F}(\beta)$ on the square lattice. Upper and lower bounds to $\mathcal{F}(\beta)$ and the asymptotic line $L(\beta)$, are included.

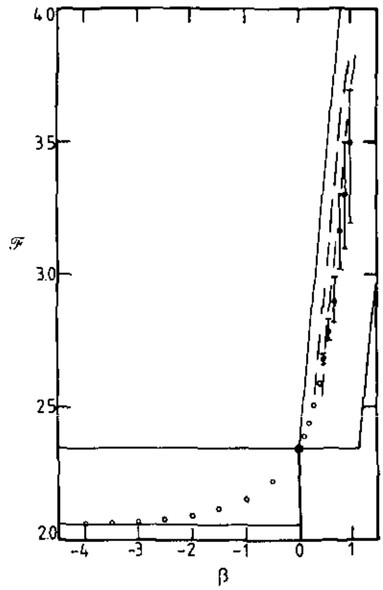

Figure 3. As figure 2 but on the simple cubic lattice.

Finally, we note that the plots of $\mathscr{F}(\beta)$ in figures 2 and 3 are very smooth and give no hint of the collapse transition which is expected to occur for some value of $\beta = \beta_c > 0$. Of course, we expect that for $\beta < 0$, corresponding to repulsive interactions, $\mathscr{F}(\beta)$ will be analytic.

3. Specific heat

Rather than attempt numerical differentiation of $\mathscr{F}(\beta)$ in order to obtain the specific heat, we follow the approach taken by other workers (for example, Chang and Shapir 1988) and differentiate the reduced free energy $F_n(\beta)$ *before* taking the $n \to \infty$ limit. Accordingly, we define the specific heat either through

$$\mathscr{C}'_n = \mathrm{d}^2 F_n / \mathrm{d}\beta^2 = (\langle \lambda^2 \rangle - \langle \lambda \rangle^2)/n \tag{3.1}$$

or through

$$\mathscr{C}_n = \beta^2 \, \mathrm{d}^2 F_n / \mathrm{d}\beta^2. \tag{3.2}$$

The relative merits of these different definitions have been discussed previously by Gaunt and Flesia (1990).

In figure 4, we plot $\mathscr{C}'_n$ against β for the square lattice for values of $n \leq 19$. All the curves are dominated by a single sharp peak which increases smoothly in height as n increases. Presumably this peak corresponds to the collapse transition. According to finite size scaling theory, the height h'_n of this peak should scale as $n^{\alpha_0 \phi_0}$, where ϕ_0 is the cross-over exponent and α_0 is the specific heat exponent. Assuming the hyper-scaling relation (Derrida and Herrmann 1983) $2 - \alpha_0 = 1/\phi_0$, gives the height scaling as

$$h'_n \sim n^{2\phi_0 - 1} \qquad n \to \infty. \tag{3.3}$$

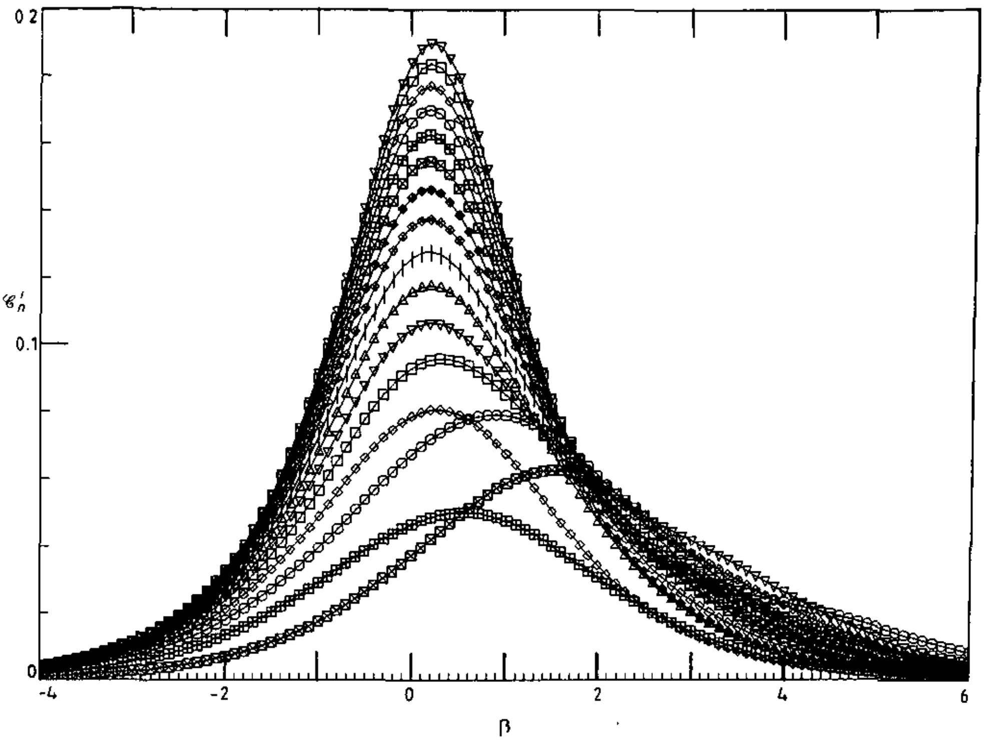

Figure 4. The specific heat, $\mathscr{C}'_n(\beta)$, of the square lattice for $n = 4$–19.

To estimate ϕ_0, we have calculated

$$\phi_{0,n} = \frac{1}{2}\left[\frac{\log(h'_n/h'_{n-1})}{\log(n/n-1)} + 1\right] \tag{3.4}$$

which should approach ϕ_0 as $n \to \infty$. In figure 5, we have plotted $\phi_{0,n}$ against $1/n$, together with the extrapolants (Gaunt and Guttmann 1974) calculated from alternate pairs of points. We estimate for the two-dimensional square lattice

$$\phi_0 = 0.60 \pm 0.03 \qquad d = 2. \tag{3.5}$$

In three dimensions, a similar analysis yields figure 6 and

$$\phi_0 = 0.82 \pm 0.03 \qquad d = 3. \tag{3.6}$$

The estimate in (3.6) is for the body-centred cubic lattice, although it is also consistent with less well-converged results for the simple cubic and diamond lattices. The plots of $\mathscr{C}'_n$ against β for the body-centred cubic lattice are given in figure 7. For $n = 15$ the curve has two distinct peaks and this is the first time that such behaviour has been reported for the function $\mathscr{C}'_n(\beta)$. We note that it does not occur for any other lattice, at least for the values of n that are currently available. Clearly, the height of the larger peak in figure 7 corresponds to the collapse and has been used in (3.4) to calculate $\phi_{0,15}$ for the body-centred cubic lattice. It is possible that the smaller peak corresponds to a roughening transition (Dickman and Schieve 1984), which takes place at a lower temperature, T_r, than the collapse transition at T_c. Anomalous low temperature

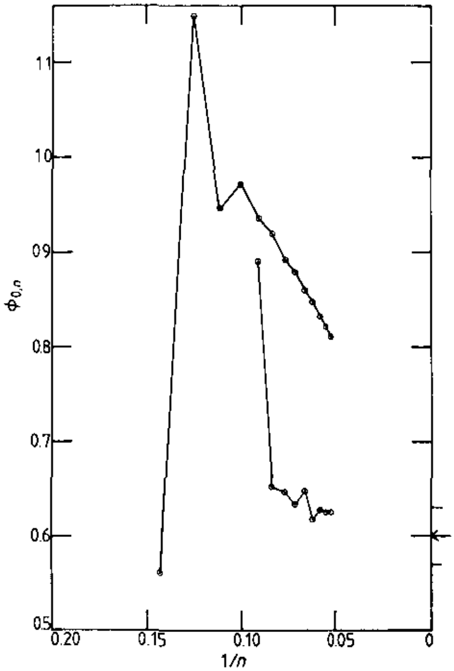

Figure 5. $\phi_{0,n}$ and their alternate extrapolants plotted against $1/n$ for the square lattice. Our best estimate of ϕ_0 is indicated on the right-hand axis.

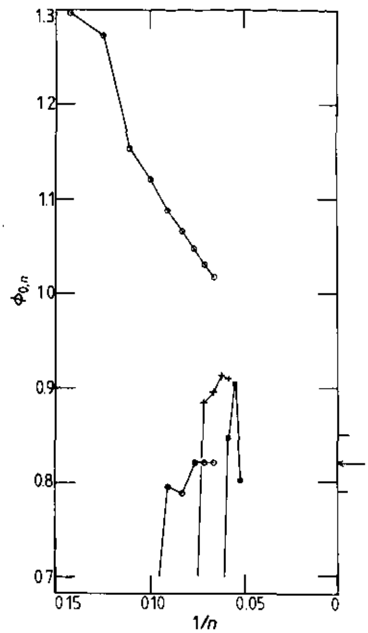

Figure 6. As figure 5 but for the body-centred cubic lattice (○), together with $\phi_{0,n}$ for the simple cubic (+) and diamond (■) lattices.

behaviour may be highlighted by calculating the specific heat $\mathscr{C}_n$ using the alternative definition in (3.2); the β^2-factor has the effect of diminishing the collapse relative to the roughening. Although evidence of roughening is found for all lattices in both two and three dimensions, the results for $\mathscr{C}_n$ are not easy to interpret and we refrain from presenting them here.

According to finite size scaling theory, the value of β at which $\mathscr{C}'_n$ has its principal maximum, namely $\beta_{\max}(n)$, should approach β_c as n increases like

$$\beta_{\max}(n)=\beta_c+An^{-\phi_0}+\ldots \qquad n\to\infty \tag{3.7}$$

where A is a constant amplitude. In figure 8, we plot $\beta_{\max}(n)$ against $1/n^{\phi_0}$ for several lattices in two and three dimensions using the central value of ϕ_0 in (3.5) and (3.6), respectively. In all cases, after some initial irregularities, the curves become quite smooth. For the square lattice, the curve passes through a minimum as n increases and we have tried to represent such behaviour by including in (3.7) an additional term as in

$$\beta_{\max}(n)=\beta_c+An^{-\phi_0}-Bn^{-1}+\ldots \qquad n\to\infty. \tag{3.8}$$

In fact, the presence of such an analytic term is expected for all lattices on general theoretical grounds. Assuming the values of ϕ_0 given in (3.5) and (3.6), we have solved (3.8) using successive triplets of $\beta_{\max}(n)$-values. This procedure gives sequences of estimates, $\beta_c(n)$, which we have tried to extrapolate linearly against $1/n$. For the diamond lattice, the data are too poorly converged for us to extract any estimate of

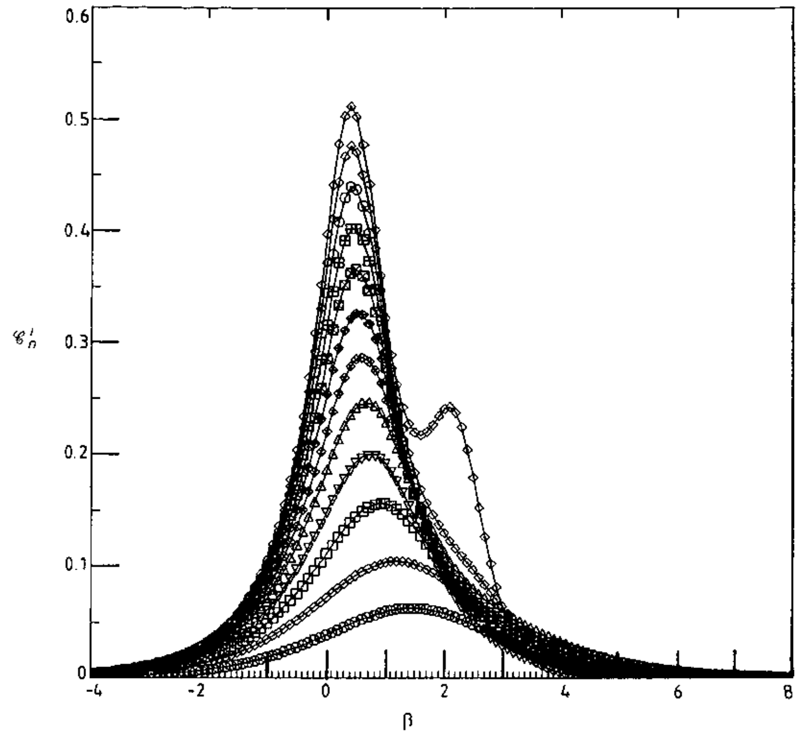

Figure 7. The specific heat, $\mathscr{C}'_n(\beta)$, of the body-centred cubic lattice for $n = 4$–15.

β_c. For the other lattices, we obtain the rather crude estimates

$$\begin{aligned} \beta_c = 1/T_c &= 0.5 \pm 0.1 && \text{(square)} \\ &= 0.35 \pm 0.3 && \text{(simple cubic)} \\ &= 0.33 \pm 0.1 && \text{(body-centred cubic).} \end{aligned} \tag{3.9}$$

The central estimates in (3.9) suggest that, before it collapses, a two-dimensional system has to be cooled to a lower temperature than one in three dimensions. This conclusion was also reached for the C-model, i.e. a cycle model of lattice animals, strongly embedded in the lattice with site counting (Derrida and Herrmann 1983, Lam 1987, 1988). The coordination numbers of the embedding lattice are also important. In three dimensions, it is expected that a system on the body-centred cubic lattice will collapse earlier than the same system on the simple cubic lattice (as the results in (3.9) show). This is because near-neighbours are more abundant in the former case.

4. Summary and discussion

In this paper we have investigated numerically, for the first time, the collapse that occurs in a lattice tree model of branched polymers. In section 1, we summarized some rigorous results (Madras *et al* 1990), including upper and lower bounds, for the

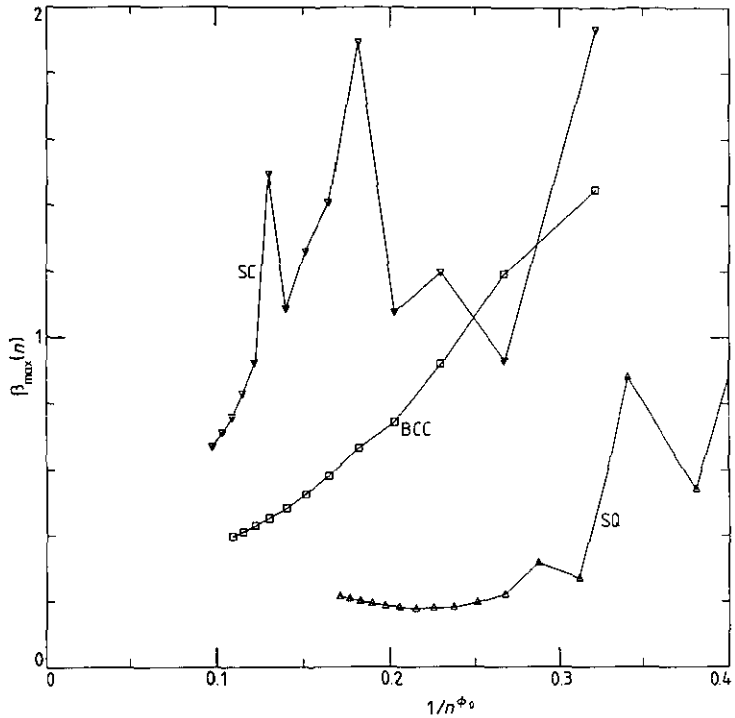

Figure 8. $\beta_{max}(n)$ plotted against $1/n^{0.60}$ for the square lattice and against $1/n^{0.82}$ for the simple cubic and body-centred cubic lattices.

temperature dependence of the reduced limiting free energy $\mathcal{F}(\beta)$. In addition, we reported in the appendices some new exact enumeration results for lattice trees, derived from data obtained by J L Martin and M F Sykes (see Madras *et al* 1990 and to be published). In section 2, these data were used to obtain numerical estimates of $\mathcal{F}(\beta)$ which compare very well for $\beta \leq 0$ and satisfactorily for small $\beta > 0$ with the rigorous bounds. Although there is no proof, it appears very likely that $\mathcal{F}(\beta)$ is asymptotic to $\log \Lambda_0$ as $\beta \to -\infty$. In addition, our numerical results support the conjecture that, for the square and simple cubic lattices, the reduced limiting entropy of the compact phase is equal to (or at least very close to) the rigorous lower bound in (1.10).

From the specific heat, we have obtained in section 3 estimates of the collapse transition T_c and the cross-over exponent ϕ_0 in two and three dimensions. Our best estimates for ϕ_0 are around 0.60 in two dimensions and 0.82 in three dimensions. Given ϕ_0, the specific heat exponent α_0 is given by the hyper-scaling relation (see Derrida and Herrmann 1983, Chang and Shapir 1988) $\alpha_0 = 2-(1/\phi_0)$.

These values of the exponent ϕ_0 are not in agreement with the Flory exponents (Daoud *et al* 1983) of $\phi_F = \frac{5}{6} = 0.833\ldots$ ($d=2$) and $\phi_F = \frac{11}{16} = 0.6875$ ($d=3$). This is not particularly surprising since the upper tricritical dimension for this problem is $d_t = 6$. It is perhaps more surprising that the Flory theory does not even predict the increase of ϕ_0 when going from $d=2$ to $d=3$.

The above values of ϕ_0 for lattice trees (t-model) may be compared with numerical estimates of ϕ for the C-model. In two dimensions, the best estimate is $\phi = 0.657 \pm 0.025$ obtained by Derrida and Herrmann (1983) using transfer matrices on finite strips together with finite size scaling. In three dimensions, Lam (1988) has used Monte

Carlo data to estimate $\phi \simeq 0.814$, while exact enumeration data give $\phi \approx 1$ (Chang and Shapir 1988). These results indicate that the t-model and C-model may be in different universality classes, although the evidence is not conclusive.

The two peaks in $\mathscr{C}'_{15}(\beta)$ for the body-centred cubic lattice and the anomalous low temperature behaviour of $\mathscr{C}_n(T)$ for both two- and three-dimensional lattices have been interpreted in terms of a possible roughening transition. The possibility of a roughening transition was first suggested by Dickman and Schieve (1984) for the C-model of collapse in lattice animals. Evidence which *may* indicate roughening in the C-model has been obtained for two- and three-dimensional lattices using both Monte Carlo techniques (Dickman and Schieve 1984, Lam 1987) and exact enumeration data (Gaunt and Flesia 1990). Anomalous low temperature behaviour, *possibly* related to roughening, has been observed therefore in both a lattice animal cycle (C-) model and the lattice tree contact (t-) model in both two and three dimensions.

Acknowledgments

We have benefited from discussions with all our colleagues in the King's College Statistical Physics Group. Particular thanks are due to J L Martin and M F Sykes who together derived the exact enumeration data from which the data in the appendix were derived. We are grateful to G S Joyce for evaluating the integral in (1.10) when $d = 3$. We also acknowledge stimulating discussions with S G Whittington. This research was financially supported, in part, by the SERC (grant number GR/G 05834).

Appendix 1. Partition functions $Z_n(\beta)$ with $x = e^{\beta}$

Square

$Z_1 = 1 \qquad Z_2 = 2 \qquad Z_3 = 6$

$Z_4 = 18 + 4x \qquad Z_5 = 55 + 32x \qquad Z_6 = 174 + 160x + 30x^2$

$Z_7 = 570 + 672x + 332x^2 \qquad Z_8 = 1908 + 2712x + 2030x^2 + 336x^3$

$Z_9 = 6473 + 10\,880x + 9972x^2 + 4064x^3 + 192x^4$

$Z_{10} = 22\,202 + 43\,220x + 46\,004x^2 + 27\,392x^3 + 6062x^4$

$Z_{11} = 76\,886 + 169\,784x + 207\,444x^2 + 148\,728x^3 + 63\,852x^4 + 5696x^5$

$Z_{12} = 268\,352 + 662\,424x + 912\,378x^2 + 755\,936x^3 + 435\,330x^4 + 111\,112x^5 + 4830x^6$

$$Z_{13} = 942\,651 + 2\,573\,976x + 3\,923\,948x^2 + 3\,718\,712x^3 + 2\,497\,462x^4 + 1\,047\,168x^5 + 173\,400x^6$$

$$Z_{14} = 3\,329\,608 + 9\,967\,932x + 16\,621\,216x^2 + 17\,685\,192x^3 + 13\,472\,960x^4 + 7\,173\,256x^5 + 2\,280\,164x^6 + 196\,608x^7$$

$$Z_{15} = 11\,817\,582 + 38\,489\,344x + 69\,641\,568x^2 + 81\,730\,120x^3 + 69\,928\,992x^4 + 43\,064\,560x^5 + 19\,087\,660x^6 + 4\,218\,176x^7 + 180\,674x^8$$

$$Z_{16}=42\,120\,340+148\,278\,528x+289\,148\,184x^2+370\,021\,256x^3+349\,897\,084x^4$$
$$+243\,682\,636x^5+129\,300\,260x^6+45\,287\,440x^7+6\,961\,342x^8+100\,352x^9$$

$$Z_{17}=150\,682\,450+570\,197\,440x+1\,191\,271\,268x^2+1\,649\,049\,272x^3+1\,699\,165\,082x^4$$
$$+1\,320\,197\,000x^5+795\,256\,592x^6+355\,393\,128x^7+99\,763\,798x^8$$
$$+9\,630\,560x^9$$

$$Z_{18}=540\,832\,274+2\,189\,348\,656x+4\,876\,431\,544x^2+7\,252\,368\,728x^3$$
$$+8\,068\,090\,292x^4+6\,885\,986\,552x^5+4\,626\,204\,916x^6+2\,408\,178\,984x^7$$
$$+922\,980\,400x^8+197\,901\,280x^9+11\,189\,428x^{10}$$

$$Z_{19}=1\,946\,892\,842+8\,395\,558\,272x+19\,853\,269\,060x^2+31\,536\,512\,904x^3$$
$$+37\,628\,498\,868x^4+34\,838\,434\,432x^5+25\,760\,261\,240x^6$$
$$+15\,095\,548\,080x^7+6\,936\,931\,892x^8+2\,230\,866\,664x^9+359\,409\,332x^{10}$$
$$+9\,934\,752x^{11}.$$

Diamond

$Z_1=1$ $\quad Z_2=2$ $\quad Z_3=6$ $\quad Z_4=22$ $\quad Z_5=91$

$Z_6=396+12x$ $\quad Z_7=1782+144x$ $\quad Z_8=8186+1248x$

$Z_9=38\,199+9120x+192x^2$ $\quad Z_{10}=180\,544+60\,504x+3318x^2+128x^3$

$$Z_{11}=862\,642+377\,520x+37\,836x^2+2048x^3$$

$$Z_{12}=4\,161\,378+2\,259\,888x+348\,966x^2+26\,664x^3$$

$$Z_{13}=20\,245\,844+13\,148\,256x+2\,820\,900x^2+294\,464x^3+8064x^4$$

$$Z_{14}=99\,248\,728+74\,993\,100x+20\,851\,026x^2+2\,896\,056x^3+162\,816x^4+5292x^5$$

$$Z_{15}=489\,826\,224+421\,826\,784x+144\,575\,364x^2+25\,871\,376x^3+2\,260\,878x^4$$
$$+105\,840x^5$$

$$Z_{16}=2\,431\,989\,718+2\,349\,583\,788x+956\,672\,442x^2+213\,316\,024x^3+25\,643\,988x^4$$
$$+1\,770\,072x^5$$

$$Z_{17}=12\,139\,384\,729+12\,996\,154\,944x+6\,114\,841\,356x^2+1\,646\,561\,296x^3$$
$$+255\,815\,532x^4+23\,851\,032x^5+577\,584x^6$$

$$Z_{18}=60\,883\,076\,058+71\,522\,393\,940x+38\,082\,029\,826x^2+12\,049\,148\,736x^3$$
$$+2\,318\,999\,586x^4+280\,161\,948x^5+13\,708\,980x^6+320\,760x^7$$

$$Z_{19}=306\,652\,125\,954+392\,142\,612\,648x+232\,532\,813\,844x^2+84\,481\,367\,760x^3$$
$$+19\,506\,872\,034x^4+2\,939\,600\,352x^5+227\,075\,520x^6+7\,698\,240x^7.$$

Simple cubic

$Z_1=1$ $\quad Z_2=3$ $\quad Z_3=15$ $\quad Z_4=83+12x$

$Z_5 = 486 + 192x \qquad Z_6 = 2967 + 1992x + 270x^2$

$Z_7 = 18\,748 + 17\,616x + 5700x^2 + 400x^3$

$Z_8 = 121\,725 + 145\,872x + 73\,902x^2 + 16\,104x^3 + 384x^5$

$Z_9 = 807\,381 + 1\,173\,216x + 785\,448x^2 + 299\,472x^3 + 29\,280x^4 + 9216x^5$

$$Z_{10} = 5\,447\,203 + 9\,296\,964x + 7\,608\,912x^2 + 3\,986\,592x^3 + 970\,845x^4 + 167\,760x^5 + 33\,024x^6$$

$$Z_{11} = 37\,264\,974 + 73\,034\,952x + 70\,171\,248x^2 + 45\,126\,408x^3 + 17\,533\,428x^4 + 4\,004\,592x^5 + 919\,680x^6 + 104\,880x^7$$

$$Z_{12} = 257\,896\,500 + 570\,616\,752x + 627\,603\,288x^2 + 469\,676\,808x^3 + 240\,021\,897x^4 + 80\,393\,760x^5 + 19\,664\,922x^6 + 4\,958\,880x^7 + 94\,500x^9$$

$$Z_{13} = 1\,802\,312\,605 + 4\,442\,485\,104x + 5\,494\,079\,484x^2 + 4\,654\,566\,416x^3 + 2\,850\,265\,746x^4 + 1\,261\,429\,248x^5 + 393\,237\,032x^6 + 117\,012\,768x^7 + 13\,714\,224x^8 + 3\,024\,000x^9$$

$$Z_{14} = 12\,701\,190\,885 + 34\,507\,622\,736x + 47\,335\,340\,712x^2 + 44\,629\,965\,192x^3 + 31\,267\,320\,963x^4 + 16\,759\,746\,024x^5 + 6\,685\,661\,748x^6 + 2\,258\,748\,744x^7 + 529\,155\,132x^8 + 87\,143\,832x^9 + 12\,835\,236x^{10}$$

$$Z_{15} = 90\,157\,130\,289 + 267\,647\,434\,752x + 402\,881\,113\,224x^2 + 417\,554\,922\,912x^3 + 326\,433\,287\,382x^4 + 201\,109\,725\,768x^5 + 97\,191\,844\,656x^6 + 38\,621\,502\,576x^7 + 12\,136\,805\,082x^8 + 2\,793\,699\,792x^9 + 490\,539\,864x^{10} + 59\,724\,096x^{11}$$

$$Z_{16} = 644\,022\,007\,040 + 2\,073\,965\,899\,752x + 3\,396\,362\,370\,270x^2 + 3\,832\,392\,373\,520x^3 + 3\,291\,565\,921\,095x^4 + 2\,263\,013\,083\,236x^5 + 1\,262\,410\,265\,762x^6 + 585\,705\,055\,176x^7 + 222\,946\,129\,560x^8 + 67\,977\,369\,624x^9 + 15\,138\,726\,168x^{10} + 3\,075\,171\,048x^{11} + 131\,441\,760x^{12} + 37\,544\,640x^{13}$$

$$Z_{17} = 4\,626\,159\,163\,233 + 16\,061\,510\,248\,344x + 28\,413\,305\,010\,864x^2 + 34\,637\,466\,582\,840x^3 + 32\,323\,821\,031\,008x^4 + 24\,369\,368\,927\,352x^5 + 15\,197\,610\,620\,388x^6 + 8\,021\,550\,231\,096x^7 + 3\,559\,862\,088\,072x^8 + 1\,320\,293\,720\,400x^9 + 383\,349\,428\,328x^{10} + 93\,494\,805\,744x^{11} + 14\,202\,593\,592x^{12} + 1\,465\,427\,712x^{13} + 178\,124\,544x^{14}.$$

Body-centred cubic

$Z_1 = 1 \qquad Z_2 = 4 \qquad Z_3 = 28 \qquad Z_4 = 204 + 48x$

$Z_5 = 1562 + 864x + 144x^2 \qquad Z_6 = 12\,544 + 10\,824x + 4032x^2 + 960x^3$

$Z_7 = 104\,756 + 120\,048x + 71\,136x^2 + 26\,608x^3 + 7344x^4$

$$Z_8 = 900\,168 + 1\,279\,344x + 1\,001\,412x^2 + 524\,752x^3 + 220\,776x^4 + 57\,024x^5 + 2816x^6$$

$$Z_9 = 7\,901\,843 + 13\,415\,424x + 12\,729\,888x^2 + 8\,478\,544x^3 + 4\,572\,576x^4 + 1\,873\,584x^5 + 552\,088x^6 + 44\,160x^7$$

$$Z_{10} = 70\,545\,284 + 139\,356\,264x + 154\,046\,760x^2 + 121\,832\,944x^3 + 78\,940\,680x^4 + 41\,397\,648x^5 + 18\,049\,700x^6 + 5\,309\,952x^7 + 798\,288x^8$$

$$Z_{11} = 638\,589\,820 + 1\,438\,759\,872x + 1\,810\,272\,744x^2 + 1\,637\,483\,904x^3 + 1\,220\,529\,240x^4 + 758\,618\,640x^5 + 407\,983\,040x^6 + 176\,859\,312x^7 + 58\,034\,952x^8 + 11\,236\,304x^9 + 378\,000x^{10}$$

$$Z_{12} = 5\,847\,741\,388 + 14\,797\,602\,912x + 20\,839\,131\,300x^2 + 21\,115\,886\,128x^3 + 17\,597\,289\,060x^4 + 12\,444\,614\,544x^5 + 7\,723\,757\,976x^6 + 4\,128\,654\,192x^7 + 1\,853\,249\,760x^8 + 655\,744\,368x^9 + 150\,059\,244x^{10} + 14\,405\,520x^{11}$$

$$Z_{13} = 54\,073\,952\,472 + 151\,836\,363\,792x + 236\,264\,310\,264x^2 + 264\,433\,527\,616x^3 + 242\,265\,305\,232x^4 + 189\,919\,078\,224x^5 + 131\,635\,620\,752x^6 + 80\,760\,938\,880x^7 + 43\,631\,955\,612x^8 + 20\,184\,138\,528x^9 + 7\,592\,349\,408x^{10} + 2\,024\,575\,056x^{11} + 307\,128\,840x^{12} + 12\,147\,840x^{13}$$

$$Z_{14} = 504\,210\,769\,416 + 1\,555\,713\,958\,704x + 2\,648\,010\,933\,408x^2 + 3\,238\,334\,740\,208x^3 + 3\,226\,458\,327\,804x^4 + 2\,757\,673\,722\,048x^5 + 2\,091\,825\,408\,512x^6 + 1\,422\,907\,772\,304x^7 + 871\,605\,859\,524x^8 + 475\,787\,185\,832x^9 + 226\,671\,366\,192x^{10} + 90\,147\,469\,728x^{11} + 27\,117\,230\,596x^{12} + 5\,630\,305\,200x^{13} + 403\,790\,640x^{14} + 39\,655\,424x^{15}$$

$$Z_{15} = 4\,735\,591\,774\,476 + 15\,925\,717\,164\,240x + 29\,414\,288\,060\,664x^2 + 38\,968\,278\,158\,176x^3 + 41\,882\,015\,193\,744x^4 + 38\,610\,300\,779\,664x^5 + 31\,625\,742\,605\,544x^6 + 23\,384\,443\,224\,576x^7 + 15\,743\,620\,564\,572x^8 + 9\,646\,044\,839\,008x^9 + 5\,329\,876\,746\,336x^{10} + 2\,611\,080\,091\,392x^{11} + 1\,088\,802\,260\,900x^{12} + 367\,415\,527\,152x^{13} + 89\,064\,438\,480x^{14} + 12\,584\,378\,528x^{15} + 1\,047\,822\,336x^{16} + 28\,311\,552x^{18}.$$

Appendix 2. Bond and site trees

Using the data in appendix 1, we can derive the number of trees with n sites, weakly and strongly embedded in the lattice, i.e. bond and site trees, respectively. From the definition of $Z_n(\beta)$ in (1.1), we see that the coefficient independent of x is the number of strongly embedded trees, and that the number of weakly embedded trees is obtained by putting $x = 1$ and summing. This procedure supplements the previously known data as follows:

Square. The bond trees given by Whittington *et al* (1983) for $n \leq 15$ are supplemented by

$$1\,624\,797\,422 \quad (n = 16) \qquad 7\,840\,606\,590 \quad (n = 17)$$

$$37\,979\,513\,054 \quad (n = 18) \qquad 184\,592\,118\,338 \quad (n = 19)$$

while the site trees given by Duarte and Ruskin (1981), Gaunt *et al* (1982) and Whittington *et al* (1983) for $n \leq 17$ extend as

$$540\,832\,274 \quad (n = 18) \qquad 1\,946\,892\,842 \quad (n = 19).$$

Diamond. Site trees have been given by Duarte and Ruskin (1981) for $n \leq 12$ and continue as

$$20\,245\,844 \quad (n = 13) \qquad 99\,248\,728 \quad (n = 14)$$

$$489\,826\,224 \quad (n = 15) \qquad 2\,431\,989\,718 \quad (n = 16)$$

$$12\,139\,384\,729 \quad (n = 17) \qquad 60\,883\,076\,058 \quad (n = 18)$$

$$306\,652\,125\,954 \quad (n = 19).$$

Bond trees for $n \leq 19$ are given in table 2.

Simple cubic. Bond and site trees given by both Gaunt *et al* (1982) and Whittington *et al* (1983) for $n \leq 11$ are extended by

$$2\,270\,927\,307 \quad (n = 12) \qquad 21\,032\,126\,627 \quad (n = 13)$$

$$196\,774\,731\,204 \quad (n = 14) \qquad 1\,857\,077\,730\,393 \quad (n = 15)$$

$$17\,658\,743\,358\,651 \quad (n = 16) \qquad 169\,023\,638\,003\,517 \quad (n = 17)$$

Table 2. Bond trees for the diamond and body-centred cubic lattices.

n	t_n (diamond)	t_n (body-centred cubic)
1	1	1
2	2	4
3	6	28
4	22	252
5	91	2 570
6	408	28 360
7	1 926	329 892
8	9 434	3 986 292
9	47 511	49 568 107
10	244 494	630 277 520
11	1 280 046	8 158 745 828
12	6 796 896	107 168 136 392
13	36 517 528	1 424 941 392 516
14	198 157 018	19 142 538 495 540
15	1 084 466 466	259 435 941 941 340
16	5 978 976 032	
17	33 177 186 473	
18	185 149 839 834	
19	1 038 490 166 352	

for bond trees, and for site trees by

257 896 500	$(n=12)$	1 802 312 605	$(n=13)$
12 701 190 885	$(n=14)$	90 157 130 289	$(n=15)$
644 022 007 040	$(n=16)$	4 626 159 163 233	$(n=17)$.

Body-centred cubic. Site trees have been given by Duarte and Ruskin (1981) for $n \leqslant 9$ and continue as

70 545 284	$(n=10)$	638 589 820	$(n=11)$
5 847 741 388	$(n=12)$	54 073 952 472	$(n=13)$
504 210 769 416	$(n=14)$	4 735 591 774 476	$(n=15)$.

Bond trees for $n \leqslant 15$ are given in table 2.

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