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Models for collapse in trees and c -animals

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Abstract. We consider the phenomenon of collapse in a lattice model of a branched polymer in a dilute solution. We model the polymer as a lattice animal with a fixed cyclomatic index (c), and consider two alternative but equivalent interpretations in which the collapse is driven either by the contact interaction between non-bonded nearest neighbours, or by the decreasing quality of the solvent. We prove that the reduced limiting free energy is independent of c . For the contact model, this implies that, if a collapse transition exists at $\beta = \beta_0$ (where e^β is the fugacity) for trees ($c = 0$), then a collapse transition occurs at β_0 for all values of c . The critical point of the solvent model is $-\beta_0/2$, independent of c and, moreover, the critical exponent α is the same for both models, independent of c . We use these results to improve our numerical estimates of the temperature dependence of the limiting free energy and confirm our earlier estimate of the value of the cross-over exponent ϕ .

1. Introduction

Randomly branched polymers in dilute solution in a good solvent have been modelled both as lattice animals and as lattice trees (Lubensky and Isaacson 1979, Parisi and Sourlas 1981, Gaunt *et al* 1982, Janse van Rensburg and Madras 1992). If the temperature is lowered or, equivalently, if the solvent quality is decreased, branched polymers are thought to undergo a collapse transition from a *coil* to a *ball*. This transition comes about through a competition between the monomer–monomer interactions and the monomer–solvent interactions. Attractive monomer–monomer and repulsive monomer–solvent interactions will both favour collapse but these interactions can work in the same or in opposite directions.

Several lattice models have been constructed which show evidence of a transition of this type (Derrida and Herrmann 1983, Dickman and Schieve 1984, 1986, Dhar 1987, Lam 1987, 1988, Chang and Shapir 1988, Gaunt and Flesia 1990, 1991, Gaunt 1991, Flesia 1992). These models fall into two classes, in which the collapse is driven either by a fugacity which is associated with the cyclomatic index, or by a fugacity associated with non-bonded nearest-neighbour contacts. The effect of monomer–solvent interactions has not been explicitly included.

In order to investigate the relationship between trees and animals, Whittington *et al* (1983) introduced the idea of a c -animal, i.e. a lattice animal with fixed cyclomatic index (c). If $a_{n,c}$ is the number of weakly embeddable c -animals with n vertices,

they proved that

$$0 < \lim_{n \rightarrow \infty} n^{-1} \log a_{n,c} = \log \lambda_c < \infty \quad (1.1)$$

and that

$$\lambda_c = \lambda_0 \quad \forall c. \quad (1.2)$$

Assuming the functional form

$$a_{n,c} \sim n^{-\theta_c} \lambda_c^n \quad (1.3)$$

they conjectured that

$$\theta_c = \theta_0 - c \quad (1.4)$$

and subsequently this result was proved rigorously by Soteris and Whittington (1988).

In this paper, we study a contact model of collapsing c -animals and prove that the temperature dependence of the reduced limiting free energy is independent of c .

In addition, we introduce a new model in which the collapse is driven explicitly by solvent quality, i.e. by a repulsive interaction between each vertex of the animal and nearest-neighbour unoccupied sites of the lattice. We refer to this as the *solvent perimeter model*. For c -animals, we point out that the thermodynamics of the solvent perimeter model and the contact model are the same. This equivalence will not exist in more general models of branched polymers and the details of the competition between monomer–monomer and monomer–solvent effects in these models will be the subject of a separate publication.

We make use of this equivalence, and of the c -independence of the two models, to make improved numerical estimates of the temperature dependence of the reduced limiting free energy. We argue that the value of the cross-over exponent ϕ is the same for the two models and is independent of c .

2. Rigorous results

We consider c -animals weakly embedded in the d -dimensional simple hypercubic lattice. If the c -animal has n vertices and e edges then, by Euler's relation,

$$c = e - n + 1. \quad (2.1)$$

We call a pair of vertices in the c -animal which are a unit distance apart but not incident on a common edge, a *contact*. Similarly, we call an edge of the lattice, incident on exactly one vertex of the c -animal, a *solvent contact*, and we refer to the set of solvent contacts of a c -animal as the *solvent perimeter* of the c -animal. In figure 1 we show a c -animal on the square lattice with $n = 10$, $e = 11$, $c = 2$, k (the number of contacts) = 2, s (the solvent perimeter) = 14. By counting edges in two ways,

$$2dn = 2e + 2k + s \quad (2.2)$$

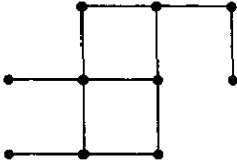


Figure 1. A 2-animal weakly embedded in the square lattice.

which together with (2.1) gives

$$s = 2[(d - 1)n + 1 - c - k]. \tag{2.3}$$

We write $a_{n,c}(k)$ for the number of c -animals with n vertices and k contacts, and $Z_{n,c}(\beta)$ for the corresponding partition function

$$Z_{n,c}(\beta) = \sum_k a_{n,c}(k)e^{\beta k}. \tag{2.4}$$

We note that $c = 0$ corresponds to trees and that Madras *et al* (1990) proved that the limit

$$\lim_{n \rightarrow \infty} n^{-1} \log Z_{n,0}(\beta) \equiv \mathcal{F}_0(\beta) \tag{2.5}$$

exists and is a monotone non-decreasing, continuous, convex function of β .

We now seek inequalities between $Z_{n,c}(\beta)$ and $Z_{n,c+1}(\beta)$ by extending constructions given in Whittington *et al* (1983). By adding a square at the top vertex of a c -animal, we obtain a $(c + 1)$ -animal with k unchanged, which yields the inequality

$$a_{n+3,c+1}(k) \geq a_{n,c}(k). \tag{2.6}$$

By deleting an appropriate edge in a $(c + 1)$ -animal with k contacts, we obtain a c -animal with $(k + 1)$ contacts and this construction leads to the inequality

$$a_{n,c+1}(k) \leq 2dn a_{n,c}(k + 1). \tag{2.7}$$

Taking logarithms in (2.6) and (2.7) and dividing by n , then letting $n \rightarrow \infty$ and using an inductive argument on c , immediately gives the existence of the limit

$$\mathcal{F}_c(\beta) \equiv \lim_{n \rightarrow \infty} n^{-1} \log Z_{n,c}(\beta) \tag{2.8}$$

with

$$\mathcal{F}_c(\beta) = \mathcal{F}_0(\beta) \quad \forall c. \tag{2.9}$$

We now investigate the relationship between the contact model and the solvent perimeter model for c -animals. Let $q_{n,c}(s)$ be the number of weakly embeddable c -animals with n vertices and s solvent contacts and define the partition function

$$Q_{n,c}(\beta) = \sum_s q_{n,c}(s)e^{\beta s}. \tag{2.10}$$

From (2.3),

$$Q_{n,c}(\beta) = e^{2\beta[(d-1)n+1-c]} \sum_k a_{n,c}(k) e^{-2\beta k} e^{2\beta[(d-1)n+1-c]} Z_{n,c}(-2\beta). \tag{2.11}$$

Taking logarithms, dividing by n and letting $n \rightarrow \infty$, gives

$$F_c(\beta) \equiv \lim_{n \rightarrow \infty} n^{-1} \log Q_{n,c}(\beta) = 2\beta(d-1) + \mathcal{F}_c(-2\beta). \tag{2.12}$$

We note that this not only gives an exact relationship between the reduced limiting free energies of the two models, but (2.11) gives a similar relationship between the partition functions for all n .

We have shown that the limiting thermodynamics is independent of c in each model, and that the limiting thermodynamics of one model determines that of the other. In particular, if a collapse transition exists the critical value of β for the contact model (β_0 , say) is independent of c and the critical point for the solvent perimeter model is then $-\frac{1}{2}\beta_0$, independent of c . Moreover, critical exponents such as α are the same for these two models, and independent of c .

3. Numerical results

In the last section, we showed that the β -dependence of the limiting free energy for c -animals is independent of c , and that there is a relationship between the contact and solvent perimeter models. We now explore how this knowledge can be used to improve our numerical estimates of the thermodynamics.

Recently, Gaunt and Flesia (1991) have estimated the β -dependence of the limiting free energy of the contact model for trees using new exact enumeration data for $n \leq 19$ on the square lattice and $n \leq 17$ on the simple cubic lattice. From these data, we can also calculate $Z_{n,c}(\beta)$ for values of $c = 1, 2, \dots$. In view of (1.3) and (1.4), we might expect better convergence of ratio estimates for larger values of c when $\beta = 0$ and, presumably, for all values of $\beta < \beta_0$. As an example, we show in figure 2 ratio estimates and linear extrapolants of $e^{\mathcal{F}_0}$ for the square lattice using the results for $c = 0, 1$ for two values of β . As expected the convergence is faster for larger c but, unfortunately, is accompanied by an increase in curvature, perhaps due to the effectively shorter series. Nevertheless, these additional estimators are very useful in forming our final estimates.

In a similar way, we can use the data for larger values of c to provide improved estimates of the cross-over exponent ϕ . From (2.9) we know that if the critical exponent α exists, then it must be independent of c . Assuming that α and ϕ are related by the ‘hyperscaling’ relation $2 - \alpha = 1/\phi$ (see e.g. Derrida and Herrmann 1983), we expect ϕ also to be independent of c . Defining the intensive heat capacity $C_{n,c}$ as

$$C_{n,c}(\beta) = n^{-1} \frac{d^2}{d\beta^2} \log Z_{n,c}(\beta) \tag{3.1}$$

we expect sharp peaks in $C_{n,c}(\beta)$ increasing smoothly in height as n increases. According to finite size scaling theory, the height $h_{n,c}$ scales as

$$h_{n,c} \sim n^{\alpha\phi}. \tag{3.2}$$

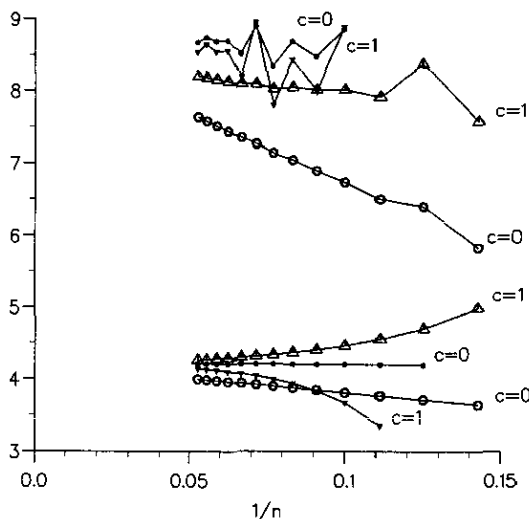


Figure 2. Ratio estimates (open symbols) and linear extrapolants (full symbols) of $e^{\mathcal{F}_0}$ for the square lattice for $c = 0, 1$ and $\beta = -1$ (lower curves) and $\beta = +1$ (upper curves).

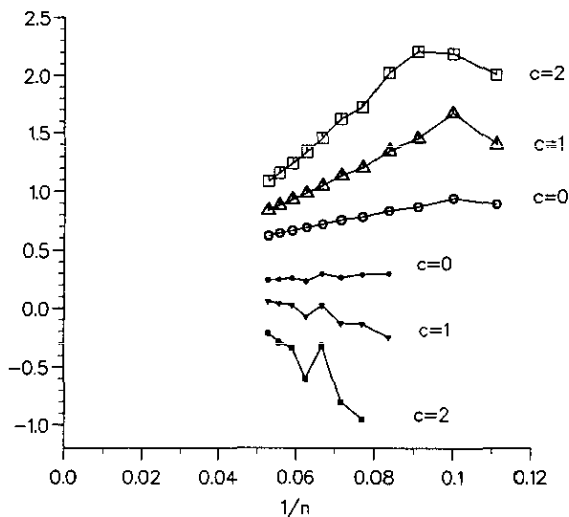


Figure 3. Ratio estimates (open symbols) and alternate linear extrapolants (full symbols) of $\alpha\phi$ for the square lattice for $c = 0, 1, 2$.

A suitable ratio estimator of $\alpha\phi$ is

$$(\alpha\phi)_{n,c} = \frac{\log(h_{n,c}/h_{n-1,c})}{\log(n/n-1)} \tag{3.3}$$

and we present values of $(\alpha\phi)_{n,c}$ and their alternate linear extrapolants for the square lattice plotted against $1/n$ for $c = 0, 1, 2$ in figure 3. The curves appear to have a common limit, implying that ϕ is independent of c . We estimate the value of

the common limit as

$$\alpha\phi = 0.20 \pm 0.06 \quad (3.4)$$

which, together with hyperscaling, gives

$$\phi = 0.60 \pm 0.03 \quad (d = 2). \quad (3.5)$$

The β -dependence of the free energy \mathcal{F}_0 for the contact model for trees on the square and simple cubic lattices has been estimated by Gaunt and Flesia (1991) for $\beta \leq 1.5$ and $\beta \leq 1.0$, respectively. We can make indirect estimates of the same quantity by estimating $F_0(\beta)$ (using data for various values of c) and making use of the identity (2.12). We find that this indirect route allows us to make reliable estimates of $\mathcal{F}_0(\beta)$ for considerably larger values of β . We give these estimates in table 1 for the square lattice, and compare with the direct estimates of Gaunt and Flesia (1991). Madras *et al* (1990) have shown that for the square lattice

$$\log \Lambda_0 \leq \mathcal{F}_0(\beta) \leq \log \lambda_0 \quad \beta < 0 \quad (3.6)$$

and

$$\max\{\log \lambda_0, 4C/\pi + \beta\} \leq \mathcal{F}_0(\beta) \leq \log \lambda_0 + \beta \quad \beta \geq 0 \quad (3.7)$$

where C is Catalan's constant, and Λ_0 ($\simeq 3.796$) and λ_0 ($\simeq 5.140$) are the growth constants for strongly and weakly embedded trees, respectively. The values of these bounds are also given in table 1 for comparison.

Table 1. Estimates of the limiting free energy of the contact model for trees on the square lattice. * indicates that no direct estimate was possible.

β	$\mathcal{F}_0(\beta)$			
	Direct estimate	Indirect estimate	Lower bound	Upper bound
-4.0	1.339 \pm 0.002	1.339 \pm 0.001	1.334	1.637
-3.0	1.348 \pm 0.002	1.347 \pm 0.001	1.334	1.637
-2.0	1.371 \pm 0.001	1.371 \pm 0.001	1.334	1.637
-1.0	1.439 \pm 0.001	1.439 \pm 0.001	1.334	1.637
0	1.637 \pm 0.002	1.637 \pm 0.002	1.637	1.637
1.0	2.16 \pm 0.04	2.20 \pm 0.04	2.166	2.637
1.5	2.50 \pm 0.20	2.55 \pm 0.15	2.666	3.137
2.0	*	3.0 \pm 0.20	3.166	3.637
2.5	*	3.45 \pm 0.25	3.666	4.137
3.0	*	3.9 \pm 0.30	4.166	4.637

4. Discussion

We have introduced a model of collapsing branched polymers which focuses directly on the solvent quality. For the case of c -animals, we have shown that the thermodynamics of this model and the thermodynamics of the contact model, are essentially

equivalent, and that the limiting free energy is independent of c . These results provide a variety of routes for estimating the limiting free energy, and the cross-over exponent ϕ , of the contact model for trees. The existence of these additional estimators is very helpful in making our final estimates. Another especially useful feature is that we are able to extend the range of values of β for which we can make reliable estimates of the limiting free energy.

It is important to realize that the above mapping does not exist for unrestricted lattice animals. More general models, in which there is a competition between contact interactions and solvent effects, will be discussed in a future publication.

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