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J. Phys. A: Math. Gen. 27 (1994) 5813–5830. Printed in the UK

Non-universality in the collapse of two-dimensional branched polymers

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Received 12 November 1993, in final form 3 June 1994

Abstract. In this paper we study the complete phase diagram of a model of interacting branched polymers. The model we consider is a lattice animal one, where the collapse transition can be driven both by a contact fugacity between two occupied nearest neighbours and by a fugacity related to each occupied edge. Using a Potts model formulation of the problem we conjecture the existence of two different universality classes for the θ transitions (with thermal exponents, ν and ϕ, equal to $(\frac{1}{2}, \frac{2}{3})$ and $(\frac{8}{13}, \frac{8}{13})$), separated by a higher-order percolation point. We also present convincing numerical evidence for these exponent values using a transfer-matrix approach. We discuss the possibility of a collapse–collapse transition and we predict the behaviour of our model when an adsorbing surface is included.

1. Introduction

Linear polymers consist of monomers with a functionality of two. The study of such polymers has witnessed great progress following the work of de Gennes [1, 2]. This is especially true in two dimensions, where many critical properties were determined using Coulomb gas [3] or conformal invariance [4] methods. An area in which much progress was made recently is that of the collapse of a linear polymer when the quality that the solution decreases and the polymer passes through the so-called θ-transition (or θ-point) [5, 6].

In contrast, much less is known about branched polymers (BP) which are made of monomers of higher functionality. In lattice statistical mechanics, these BP are described by lattice animals. Lattice animals in d dimensions can be related to the Yang–Lee edge singularity in $d-2$ dimensions [7]. Unfortunately, this technique does not allow a complete determination of critical exponents in $d = 2$. There also exists evidence that lattice animals may not be conformally invariant [8]. Still, quite accurate estimates of critical exponents for $d = 2$ lattice animals can be found in the literature [9].

In the present paper we will study the collapse transitions that branched polymers in two dimensions may undergo in dilute solution in a poor solvent when the temperature is lowered. To be more specific, consider a lattice animal consisting of s occupied vertices and b occupied edges, on, for example, a square lattice. We call a *contact* a pair of nearest-neighbour occupied vertices which are not connected through an occupied edge (figure 1). We denote the number of such contacts by I. The model for the collapse of branched polymers which we will study in this paper is defined by giving a weight $x^s y^b \tau^I$ to such an animal. Here x, y and τ are fugacities for vertices, edges and contacts, respectively.

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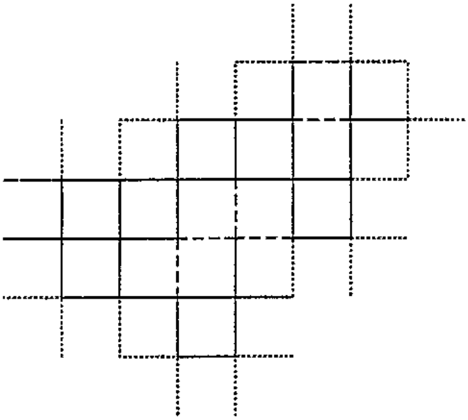

Figure 1. An example of a lattice animal in a square lattice made of $s = 25$ sites, $b = 31$ bonds, $l = 6$ contacts, $t = 32$ perimeter edges, $m = 26$ solvent contacts and $c = 7$ cycles.

We are interested in the following quantities. First we define a partition function Z_s as

$$Z_s = \sum_{b,l} C_{s,b,l} y^b \tau^l \tag{1.1}$$

where $C_{s,b,l}$ is the number of distinct lattice animals (modulo translation) with s occupied vertices, b occupied edges and l contacts, We expect that for large s and fixed y and τ, Z_s grows exponentially so that the dimensionless free energy per monomer is given by

$$f = -\lim_{s\to\infty} \frac{1}{s} \log Z_s = -\log \mu \tag{1.2}$$

where μ is a non-universal quantity which depends on the details of the lattice. As a consequence, the grand-canonical partition function Z

$$Z = \sum_s x^s Z_s \tag{1.3}$$

will have a critical point at $x = x_c = 1/\mu$ and then we can rewrite (1.2) as

$$f = \log x_c(y, \tau) \tag{1.4}$$

where we have now explicitly denoted the dependence of x_c on y and τ. Another quantity of interest is a linear measure $\langle R \rangle_s$ (e.g. we can take the radius of gyration) of an animal of s occupied vertices (by $\langle \cdot \rangle_s$ we denote the average over all animals with s vertices). As usual, the asymptotic behaviour of this quantity defines the exponent ν as

$$\langle R \rangle_s \sim s^\nu \qquad s \to \infty. \tag{1.5}$$

For $\tau = 0$, contacts are forbidden (strong embeddings) and the lattice animals are referred to as *site* animals. For this case our model coincides with the so-called *cycle* model for BP collapse (this name stems from the fact that the number of cycles, c, in the animal is given by $c = b - s + 1$, so that the weight of an animal in this case can also be rewritten as $z^s y^c$, with $z = xy$). Recently, it was argued by one of us (CV) that the collapse (or θ-) transition in the *cycle* model of BP is in the universality class of the tri-critical zero-state Potts model [10]. For y (respectively x) $= 1$, we recover the so-called *contact* models for the θ-transition of *edge* animals (weak embeddings) counted by vertices (resp. edges). It can be argued that these models are more physical as collapse models, and indeed they are natural extension of such models for linear polymers (where one always has $s = b + 1$).

It has been argued that the θ-points of contact and cycle models may be in different universality classes [11].

In the present paper we will study the phase diagram of the branched polymers for general τ using both analytic reasonings and transfer-matrix calculations. Indeed, we will find strong evidence for the existence of two distinct universality classes separated by a higher-order multicritical point which is described by percolation exponents. We will also discuss the nature of the collapsed phase.

It is interesting to remark that for after a simple transformation our model reduces to a model recently introduced by Flesia *et al* [12] and studied by those authors in the canonical ensemble (our model, in fact, is studied in a grand-canonical ensemble). The phase diagram which we obtain will look at first sight similar to the one proposed by these authors, but is in fact different in several quantitative aspects.

This paper is organized as follows. In section 2 we show how our branched polymers can be obtained as graphs in the high-temperature expansion of an appropriate Potts model. This relation was already derived by Coniglio some years ago [13]. We will supplement his work with some new insights which can be obtained from more recent studies of Potts models. In section 3 we will present the result of transfer-matrix calculations which will give evidence for the existence of two distinct universality classes for the collapse of branched polymers which in section 2 were conjectured to be the tri-critical zero-state Potts model and the Ising model universality classes. In section 4 we discuss the collapsed phase. Finally, in section 5, we present some concluding remarks, including the expected behaviour of the interacting branched polymers near a surface.

2. The Potts model and branched polymers

The description of branched polymers using the Potts model has been introduced by several authors in the past [14–17]. We now briefly recall their main results.

In the q-state Potts model [18, 19], one has at each site i of a lattice a 'spin' variable which can be in any of q different states or 'colours': $\sigma_i = 1, \ldots, q$. To describe branched polymers, we introduce the following reduced Hamiltoninan $\mathcal{H}_p$:

$$\mathcal{H}_p = J \sum_{\langle i,j\rangle} \delta_{\sigma_i \sigma_j} + L \sum_{\langle i,j\rangle} \delta_{\sigma_i 1} \delta_{\sigma_j 1} + H \sum_i \delta_{\sigma_i 1} . \tag{2.1}$$

Using standard high-temperature expansion techniques [19], a 'partition function' Z for lattice animals can be obtained in the limit $q \to 1$. One then finds in the thermodynamic limit

$$Z = \sum_{\{\mathcal{G}_1\}} (pv)^b \exp(-Hs)(1-p)^t \tag{2.2}$$

where the set $\mathcal{G}_1$ contains all (unrooted) lattice animals with b occupied edges, s occupied vertices and t perimeter edges (a perimeter edge is an empty edge between an occupied vertex and a nearest-neighbour vertex, which can be occupied or empty); see figure 1. In equation (2.2), $p = 1 - \exp(-J - L)$ and $v = (\exp J - 1)/(\exp(J + L) - 1)$. When $v = 1$ (or $L = 0$), f is equal to the usual generating function of bond percolation. It is well known that, on the square lattice, bond percolation is critical for $p = p_c = \frac{1}{2}$ and $H = 0$ [20]. The plane $L = 0$, and in particular the line $L = H = 0$, will play a major role in our further discussions and will be referred to as the percolation plane and the percolation line, respectively.

For any animal we have the relation

$$4s = 2b + t + l \tag{2.3}$$

(square lattice!!) which allows us to rewrite (2.2) as

$$Z = \sum_{\{\mathcal{G}_1\}} x^s y^b \tau^l \tag{2.4}$$

with

$$x = \exp(-H - 4(J + L)) \tag{2.5a}$$

$$y = \left[\exp(J) - 1\right] \exp(J + L) \tag{2.5b}$$

and

$$\tau = \exp(J + L)\,. \tag{2.5c}$$

Thus Z indeed coincides with the 'partition function' for the interacting animal problem introduced in the previous section, while the equations (2.5) express the fugacities of our BP model in terms of the Potts–Hamiltonian parameters.

Next we turn briefly to the two-point correlation function which will also occur in the transfer-matrix calculations (section 3). The two-point correlation function Γ_{kl} for the Potts model (2.1) is defined as

$$\Gamma_{kl} = \langle \delta_{\sigma_k 1} \delta_{\sigma_l 1} \rangle - \langle \delta_{\sigma_k 1} \rangle \langle \delta_{\sigma_l 1} \rangle\,. \tag{2.6}$$

Again using high-temperature expansion techniques, it can be shown that

$$g_{kl} \equiv \left.\frac{\partial \Gamma_{kl}}{\partial q}\right|_{q=1} = \sum_{\{\mathcal{G}_2\}} x^s y^b \tau^l \tag{2.7}$$

where the set $\mathcal{G}_2$ contains all lattice animals that pass through both the sites k and l.

It is our aim in this paper to study the phase diagram of the interacting BP as can be derived from (2.4) and (2.7). In sections 2.1 and 2.2 we first give some results which can be obtained from the relations derived so far and which can be considered to be exact.

2.1. *The role of the percolation plane*

The percolation plane is given in terms of the fugacities x, y and τ by

$$y = \tau^2 - \tau\,. \tag{2.8a}$$

The percolation line is given by the additional equation

$$x = \tau^{-4}\,. \tag{2.8b}$$

Along this line the percolation threshold $p = p_c = \frac{1}{2}, H = 0$ is located at $\tau = 2$, and thus $y = 2, x = \frac{1}{16}$. Within the percolation plane this point is fully repulsive in a renormalization-group sense. The relevant scaling dimensions are well known by now [3] and are $y_t = \frac{3}{4}, y_H = \frac{91}{48}$.

More important however is the fact that, in the space of parameters of the Hamiltonian (2.1), the percolation fixed point is *fully* repulsive [21]. The third relevant scaling dimension can be related to a magnetic exponent of the Potts model which is given by $\frac{19}{48}$. The role played by this fully repulsive percolation fixed point will be further discussed below (section 2.4).

There is another limit for which the model (2.1) is solvable. Indeed, in the limit $H \to -\infty$, the probability that the Potts spin has 'colour' 1 becomes 0, and thus the model reduces to a $(q-1)$-state Potts model . For the case of interest here $(q \to 1)$, we thus find that for

$$H \to -\infty \qquad \text{or} \qquad x\tau^4 \to \infty \tag{2.9}$$

the branched polymers are described by a zero-state Potts model. It is known that this model describes spanning trees [19]. For values of the parameters x, y, τ which satisfy (2.9) our branched polymers will thus behave like trees which span the whole lattice. We will investigate below when this is the case.

2.2. *Results for the contact model of edge lattice animals*

The information we have obtained so far can be applied to the contact model of edge animals (counted by vertices, i.e. $y = 1$). For small τ we expect that the critical exponents of the animal are equal to those that were determined for non-interacting animals [5]. If we increase τ the animals will collapse at a critical value of τ which we denote as $\tau_{\theta,I}$. Using the results of section 2.1 we can obtain a lower bound for $\tau_{\theta,I}$ and some information on the behaviour of the fully collapsed animals ($\tau \to \infty$). First, the plane $y = 1$ intersect the percolation line for

$$\tau = \tau_p = \frac{1+\sqrt{5}}{2} \qquad x = x_p = \left(\frac{1+\sqrt{5}}{2}\right)^{-4}. \tag{2.10}$$

At this point, the percolation probability p equals $(-1+\sqrt{5})/(1+\sqrt{5})$, less than the value at the percolation threshold $p_c = \frac{1}{2}$.

Subcritical percolation clusters behave like branched polymers, and from this we obtain a (non-rigorous) lower bound on the value $\tau_{\theta,I}$, i.e.

$$\tau_{\theta,I} > \frac{1+\sqrt{5}}{2}\,. \tag{2.11}$$

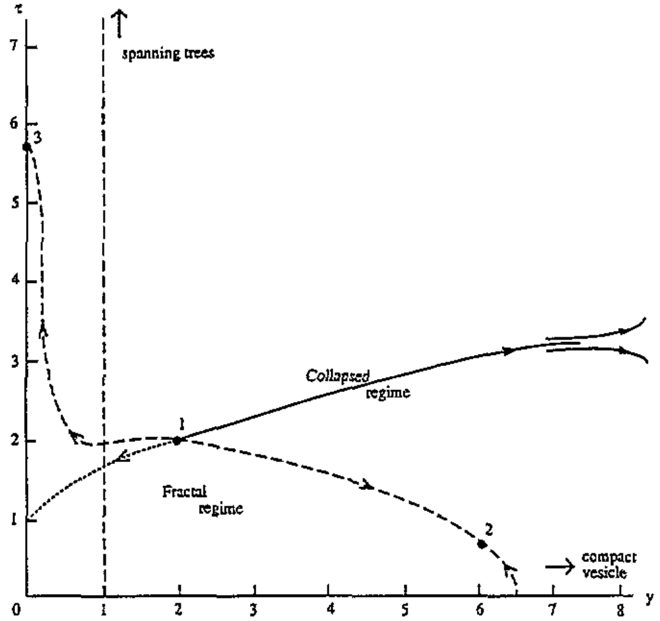

Figure 2. Projection of the phase diagram in the (y, τ) plane. The arrows indicate renormalization-group flows. We have indicated three critical points: (1) percolation point, (2) tricritical zero-state Potts point, and (3) Ising critical point. The full curve is the location of supercritical percolation, while the dotted curve indicates subcritical percolation. The broken curve is the line of theta transitions. The line at $y = 1$ is the the line along which our model coincides with the contact model of site animals. In the plane $\tau = 0$ our model coincides with the cycle model.

This inequality will indeed be satisfied by our transfer-matrix results.

Secondly, it can be shown that the condition (2.9) is satisfied for our model at $y = 1, \tau \to \infty$. We thus arrive at the important conclusion that in the contact model, edge animals collapse into spanning tree configurations. The proof is a simple consequence of results obtained in [22]. In that reference it was shown that for $y = 1$ and for $\tau \to \infty$

$$\lim_{\tau\to\infty} \frac{f}{\log\tau} = -1 \, . \tag{2.12}$$

Then, using (1.2) it follows that for the contact model of edge animals, $x_c(y = 1, \tau) \sim \tau^{-1}$ when $\tau \to \infty$. In that limit, condition (2.9) is therefore fulfilled and we conclude that the critical, collapsed edge animals in the contact model become like spanning trees for $\tau \to \infty$. On the basis of renormalization-group (RG) ideas we may expect this to be true everywhere in the collapsed phase when the animal is investigated at large enough scales.

In figure 2, which contains the phase diagram of the lattice animals as will be derived in this paper, we show the knowledge we have obtained so far on the phase diagram of the interacting lattice animals. We feel that at least this part can be considered as exact (through non-rigorous) information. As we have discussed above, the percolation point is fully repulsive in the (x, y, τ)-parameter space, and thus two critical lines must come out of the percolation plane at the percolation threshold. We don't know the exact location of these lines, neither have we, so far, any exact information on the nature of the transition along these lines. Yet, as discussed below, we can obtain some conjectural information on these lines, which will then be verified in the next section, using transfer-matrix calculations.

2.3. *The cycle model*

As noted in the introduction, for $\tau = 0$ we recover the cycle model of lattice animal collapse. The collapse of branched polymers in this model was studied using the transfer-matrix technique [23]. The transition was located at $x = x_{\theta,c} = 0.0230 \pm 0.004$, $y = y_{\theta,c} = 6.48 \pm 0.12$. The exponents at this θ-point were determined numerically to be $\nu_{\theta,c} = 0.5095 \pm 0.003$, $\phi_{\theta,c} = 0.657 \pm 0.025$.

In a recent letter [10] some new results were obtained for this model. First, it was shown, using a mapping onto the vesicle model of Fisher *et al* [24, 25] that for $y > y_{\theta,c}$, the equation of the critical line is $x = y^{-2}$. Secondly, for the special case of branched polymers without holes (which are also called discs [26]) the exact exponents at the θ-point were determined as

$$\nu_{\theta,c} = \tfrac{1}{2} \qquad \phi_{\theta,c} = \tfrac{2}{3}\,. \tag{2.13}$$

It is not completely clear whether this result still holds for animals with holes. In fact, it has been shown recently [26] that the nature of the collapsed phase differs depending on whether one includes holes or not. On the other hand, one can give non-rigorous arguments [10] which show that the θ-point in the cycle model of BP (with holes) is described by the tri-critical zero-state Potts model universality class, for which the critical exponents are just again those given by (2.13). So it seems that, at least for $\tau = 0$, the presence/absence of holes is irrelevant, i.e. does not have any effect on the exponents at the collapse transition. In this respect, it is also interesting to remark that exact renormalization-group calculations performed on a Sierpinski gasket [27, 28] show this to be the case on a fractal lattice.

We will repeat the arguments of [10] below, as they can be extended to the collapse transition in our more general model (2.4) for all τ.

2.4. *Relation with the Potts lattice gas*

For general q, the Potts model (2.1) can be transformed [19] into a Potts lattice gas by considering the state $\sigma_i = 1$ as the state $t_i = 1$ of a Potts lattice gas. When $t_i = 0$, the Potts model can be in any of the remaining $(q-1)$ Potts states which we will denote by $\mu_i = 1, \ldots, q-1$. The Hamiltonian $\mathcal{H}_p$ now becomes

$$\mathcal{H}_p = J \sum_{\langle i,j \rangle} t_i t_j (\delta_{\mu_i \mu_j} - 1) + M \sum_{\langle i,j \rangle} t_i t_j + \Delta \sum_i t_i \tag{2.14}$$

with $\Delta = -H - 4(J + L)$ (working again on the square lattice) and $M = L + 2J$. For some purposes it is convenient to rewrite the lattice-gas part of (2.15) into an Ising language ($t_i = (s_i + 1)/2$) as

$$\mathcal{H}_p = \tfrac{1}{4} J \sum_{\langle i,j \rangle} (1 + s_i)(1 + s_j)(\delta_{\mu_i \mu_j} - 1) + K \sum_{\langle i,j \rangle} s_i s_j + h \sum_i s_i \tag{2.15}$$

now with $K = M/4$, $h = M + \Delta/2$.

The model (2.14) has been studied a lot in the past, and is known to contain several fixed points: q-state Potts (for $H = 0$, $L = 0$ or $\Delta = -4J$, $M = 2J$ or $K = J/2$, $h = 0$), Ising fixed point ($J = 0, h = 0$), a tri-critical $(q-1)$-state Potts point (at unknown parameter values), ...

Another long-known fact [29] is that for $q = 2$, the model (2.14) describes the properties of Ising clusters, i.e. of connected sets of nearest-neighbour sites for which the Ising variable

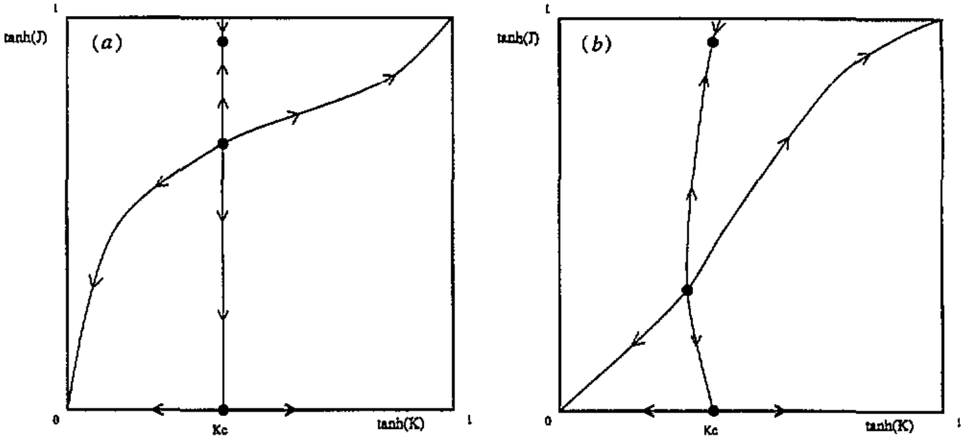

Figure 3. Qualitative representation of the phase diagram of the q-state Potts lattice-gas model in the plane $h = 0$ for (a) $q = 2$ and for (b) $q = 1$.

is in the same state (Ising correlated percolation). Recently, using conformal invariance and renormalization-group arguments, the precise connection between Ising clusters and the fixed points of (2.14) for $q = 2$ was clarified [30]. We will use the results obtained there, and an assumption that the renormalization-group flow will not change qualitatively when we pass from $q = 2$ (Ising clusters) to $q = 1$ (lattice animals).

In figure 3(a) we have therefore drawn the phase diagram of the model (2.15) in the plane $h = 0$, for $q = 2$ as obtained in [30]. When $J = 0$ we recover of course the zero-field Ising model. For $J > 0$ the graphs which appear in the high-temperature expansion of (2.15) are so-called bond diluted Ising clusters. These are the clusters of a correlated site-bond percolation problem and they are obtained as follows: first we group sets of nearest-neighbour sites for which the Ising variable is in the same state, and then the bonds between these sites are randomly occupied with a probability $p_B = 1 - \exp(-J)$. When $J \to \infty$, all bonds are occupied and the graphs are called *clusters*. Under the RG, these clusters are attracted to a fixed point at an unknown value of $J > 2K_c$. In [30] it was shown that this is the tri-critical one-state Potts fixed point which is present in the phase diagram of (2.15) for $q = 2$. As shown by Coniglio and Klein [31] a special role is played by the line $K = J/2$ where the percolative properties of the bond diluted clusters can be related in a unique way to the thermodynamic properties of the Ising model. The graphs are also called *droplets* along this line and are nowadays often used in the Swendsen–Wang Monte Carlo algorithm [32]. Along this droplet line at $K = K_c$ one finds for general q, the q-state Potts fixed point of (2.15). For $q = 2$, this is again an Ising fixed point. In the plane $h = 0$, there are thus three non-trivial fixed points which are, for $q = 2$, situated on the line $K = K_c$: *Ising, Ising droplet and Ising cluster (or tri-critical one-state Potts) fixed* point. We will refer to this line as the critical line.

What remains of this phase diagram when $q \to 1$? Along the line $h = 0, K = J/2$, the model (2.15) corresponds to the q = 1-state Potts model [31]. This line is in fact the percolation line of section 2.1. From the vesicle analogy studied in [10] we finally know that the θ-point in the cycle model (situated at $\tau = 0$ or $J \to \infty$) also lies in the plane $h = 0$. All this information and the expected continuity of RG flows as a function of q leads us to the conjecture that the θ-point in the cycle model is attracted to a fixed point at some finite value of $J > K_c$, and, more interestingly, that this fixed point is the tri-critical zero-state Potts fixed point of (2.15), with thermal exponents $\nu = \frac{1}{2}$ and $\phi = \frac{2}{3}$. It is not clear to us whether the Ising fixed point is still present in the model when $q \to 1$. It is, however, present for larger q values, and can also be recovered for $q \to 1$ by a proper extension of the parameter space of the model (2.1). We therefore would like to conjecture that there is still an Ising fixed (or critical) point in the small J-region of the phase diagram. The resulting phase diagram is drawn in figure 3(*b*). The critical line is no longer straight, and there is no *a priori* reason why the line should be in the plane $h = 0$ (though we repeat that the percolation fixed point, and the point at $J = \infty$ are certainly in this plane).

Having thus determined a phase diagram for the model (2.15), we can, using some simple algebra, determine the corresponding phase diagram in the (x, y, τ)-parameter space. The result is shown in figure 2. The critical line now becomes a line of θ-transitions coming out of the percolation fixed point. We then expect that from $0 \leqslant \tau < 2$, the collapse is in the universality class of the tri-critical zero-state Potts model. Along this line, which includes the cycle model at $\tau = 0$, we are led to predict

$$\nu_{\theta,\mathrm{c}} = \tfrac{1}{2} \qquad \phi_{\theta,\mathrm{c}} = \tfrac{2}{3} . \tag{2.16}$$

When $\tau > 2$, the nature of the transition changes. Points along this line, including the θ-point of contacts models at $y = 1$, are attracted to the Ising critical point and we therefore expect

$$\nu_{\theta,I} = \tfrac{8}{15} \qquad \phi_{\theta,\mathrm{c}} = \tfrac{8}{15} . \tag{2.17}$$

We thus find that indeed cycle and contact models are in different universality classes. The exact location of the line of θ-transitions is not known. A possibility is that it lies within the plane $h = 0$, which in (x, y, τ) parameters can be written as

$$x(y + \tau)^2 = 1 . \tag{2.18}$$

As a final remark, we admit that the results presented in this subsection are of very conjectural nature and that they depend on several uncontrolled assumptions. In the next section we will use transfer-matrix calculations to study the location of the critical line and to get independent estimates of the critical exponents along that line. They will to a large extent confirm the conjectures (2.16) and (2.17).

3. Transfer-matrix calculations

Transfer-matrix calculations for interacting branched polymers were pioneered by Derrida and Hermann [23] who investigated the cycle model ($\tau = 0$) for strips with width $\mathcal{L}$ up to 7. We have extended their work to the more general model defined in (2.4) and (2.7).

In transfer-matrix calculations one determines the correlation function g_{OR} between two columns a distance R apart. For $R \to \infty$ this correlation function can be related to the largest eigenvalue λ_0 of the transfer matrix and is given as

$$g_{OR} \sim \lambda_0^R . \tag{3.1}$$

From (3.1) it follows that the correlation length ξ is given by

$$\xi = -(\log(\lambda_0))^{-1} . \tag{3.2}$$

For $\lambda_0 \to 1^-$, $\xi \to \infty$. Thus, for a given y and τ fixed we can determine the critical value $x_c(\tau, y)$ by the requirement

$$\lambda_0(x_c, y, \tau) = 1 . \qquad (3.3)$$

This method allows us to determine the location of the critical plane.

The maximum width $\mathcal{L}$ that can be studied is determined by memory requirements. In our calculations, due to the rather 'complicated' form of the interactions (we have to discriminate configurations according to the number of occupied vertices, edges and number of contacts) the matrices grow very large rapidly (table 1), and our calculations were limited to widths $\mathcal{L} \leqslant 7$.

Table 1. Sizes of the transfer matrix as a function of the strip width $\mathcal{L}$.

$\mathcal{L}$	Matrix size
2	4
3	10
4	34
5	97
6	338
7	1102
8	3937

Table 2. Values of the critical fugacity x_c, as a function of the strip width, for two points located along the percolation line, i.e. ($y = 1$, $\tau = (1+\sqrt{5})/2$) and ($y = 6$, $\tau = 3$). For each size, x_c has been evaluated using the condition $\lambda_0(x_c, y, \tau) = 1$, where λ_0 is the largest eigenvalue of the transfer matrix (see section 3). Both sequences are nicely converging to the exact values (2.10*b*) $16/(1+\sqrt{5})^4$ and $\frac{1}{81}$.

$\mathcal{L}$	$y = 1,\ \tau = (1+\sqrt{5})/2$	$y = 6,\ \tau = 3$
2	0.201 657 812 5	0.013 197 079 8
3	0.175 290 991 2	0.012 574 691 6
4	0.166 263 687 6	0.012 428 972 4
5	0.162 089 696 2	0.012 384 187 6
6	0.159 839 636 9	0.012 368 247 6
7	0.158 507 415 6	0.012 362 069 6
Exact	0.145 898 034	0.012 345 678 9

To get an idea of the accuracy that can be expected, we determined x_c for some points along the exactly known percolation line (table 2). As a first example, for $y = 1$ the percolation line is intersected at the values of τ and x given by (2.10). In table 2 we give our estimates of x_c keeping y and τ fixed at 1 and τ_p, respectively. These values were determined using (3.3). There is a very nice convergence to the exact value of x_c. We give similar results for the intersection of the percolation line with the plane $y = 6$, which occurs at $\tau = 3$, $x_c = \frac{1}{81}$.

Besides determining the critical plane $x_c(y, \tau)$ we are also interested in the location of the tri-critical θ-lines and the values of exponents along those lines. To determine these we used finite-size scaling (FSS) methods. (We did not use any methods from conformal invariance (CI) as there are indications that this symmetry does not hold for non-interacting branched polymers [8]. The question of the validity of CI for interacting BP is outside the scope of this paper.)

We focused our attention on the density $\rho_{\mathcal{L}}(x, y, \tau)$ of occupied vertices. This is defined as

$$\rho_{\mathcal{L}}(x, y, \tau) \equiv \frac{1}{\mathcal{L}} \lim_{R\to\infty} \frac{1}{R}\left[x\frac{\partial}{\partial x}\log g_{OR}\right] \tag{3.4}$$

which from (2.7) can be written as

$$\rho_{\mathcal{L}}(x, y, \tau) = \frac{1}{\mathcal{L}} \lim_{R\to\infty} \frac{1}{R} \frac{\sum_{\mathcal{G}_R} s x^s y^b \tau^I}{\sum_{\mathcal{G}_R} x^s y^b \tau^I} . \tag{3.5}$$

The set $\mathcal{G}_R$ contains all BP going through sites in column O and column R. Using (3.1) this density can be rewritten as

$$\rho_{\mathcal{L}}(x, y, \tau) = \frac{1}{\mathcal{L}} \frac{\partial \log \lambda_0}{\partial \log x} . \tag{3.6}$$

In our calculations we fix y and then study $\hat{\rho}_{\mathcal{L}}(\tau) \equiv \rho_{\mathcal{L}}(x_c(\tau, y), y, \tau)$ as a function of τ.

Starting from the usual scaling relations we can derive the scaling of $\hat{\rho}_{\mathcal{L}}(\tau)$ near the tri-critical point $\tau_\theta(y)$. The result is

$$\hat{\rho}_{\mathcal{L}}(\tau) \sim \mathcal{L}^{1/\nu_\theta - 2} F\big((\tau - \tau_\theta(y))\mathcal{L}^{\phi_\theta/\nu_\theta}\big) \tag{3.7}$$

where F is a scaling function. (We have used this quantity because, as in the case of the θ-point of linear polymers [33], $\hat{\rho}_{\mathcal{L}}$ seems to be less influenced by numerical effects then the correlation length ξ, which is more commonly used in FSS studies with the transfer matrix).

From $\hat{\rho}_{\mathcal{L}}$, we calculate

$$r_{\mathcal{L}}(\tau) \equiv \left[\frac{\log\big(\hat{\rho}_{(\mathcal{L}+1}(\tau))/\hat{\rho}_{\mathcal{L}}(\tau)\big)}{\log((\mathcal{L}+1)/\mathcal{L})} + 2\right]^{-1} . \tag{3.8}$$

Graphs of $r_{\mathcal{L}}$ versus τ for different $\mathcal{L}$ should then intersect. The value of τ and $r_{\mathcal{L}}$ at the intersection give finite-size estimates of τ_θ and ν_θ, respectively.

In figure 4 we have presented such graphs for $y = 1$, while in table 3 we present our numerical values for their intersections as a function of $\mathcal{L}$. An extrapolation of these data then gives the final estimates (at $y = 1$)

$$\tau_{\theta,I} = 1.95 \pm 0.1 \qquad \nu_{\theta,I} = 0.535 \pm 0.015 \tag{3.9}$$

for the θ point of the contact model. These values are clearly in agreement with the predictions in section 2. Our value of $\tau_{\theta,I}$ satisfies the bound (2.11) while our value for $\nu_{\theta,I}$ is in full agreement with the Ising-value $\nu = \frac{8}{15}$.

To get also an estimate of $\phi_{\theta,I}$ we calculated the quantity

$$t_{\mathcal{L}}(\tau) \equiv -\frac{1}{\hat{\rho}_{\mathcal{L}}(\tau)} \frac{\mathrm{d}\hat{\rho}_{\mathcal{L}}}{\mathrm{d}\tau} \tag{3.10}$$

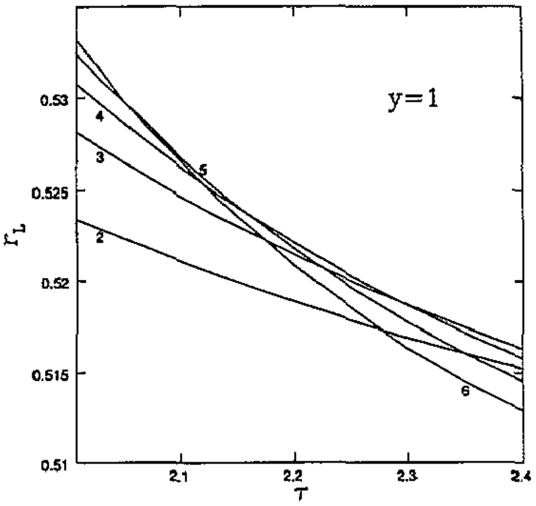

Figure 4. Plot of the values $r_{\mathcal{L}}$ (3.8) versus τ for $y = 1$. For large $\mathcal{L}$ the curves should intersect at ($\tau_{\theta,I}$, $\nu_{\theta,I}$). The intersections points are reported in table 3.

Table 3. Estimates of the critical exponents ($\nu_{\theta,I}$ and $\phi_{\theta,I}$) for different strip widths at $y = 1$. The values are obtained looking at the crossing points of the lines in figure 4. The asymptotic results (equations (3.9) and (3.12)) have been obtained looking at these intersection points in the range $y < 2$.

$\mathcal{L}$	ν_θ	ϕ_θ
3	0.511 14	0.842
4	0.518 30	0.676
5	0.524 94	0.609
6	0.529 73	0.56

which scales as

$$t_{\mathcal{L}} \sim \mathcal{L}^{\phi_\theta/\nu_\theta} \tag{3.11}$$

at $\tau = \tau_\theta(y)$. Numerical estimates of the crossover exponent obtained in this way are less accurate because they involve a second derivative (calculated numerically) of the eigenvalue λ_0. Values for ϕ_θ, at $y = 1$, are also given in table 3 and they lead to the final result

$$\phi_{\theta,I} = 0.55 \pm 0.015\,. \tag{3.12}$$

This value is again consistent with the prediction $\phi_{\theta,I} = \frac{8}{15}$.

We have also performed similar calculations at $y = 0.2, 0.4, 0.6, 0.8, 1.5$; the estimates for $\nu_{\theta,I}$ and $\phi_{\theta,I}$ we obtained are within the numerical errors, equal to those given by (3.9) and (3.12).

As a first conclusion then, our numerical results are in full agreement with the conjecture that for $y < 2$ the theta point of branched polymers is described by Ising exponents.

We have made completely similar calculations for $y > 2$, where we have determined $\tau_c(y)$ for a few y values. In figure 5 we present graphs of $r_{\mathcal{L}}$ versus τ for $y = 6$. As can be seen in table 4 the estimates for $\nu_{\theta,c}$ go through a maximum, and no reliable extrapolation

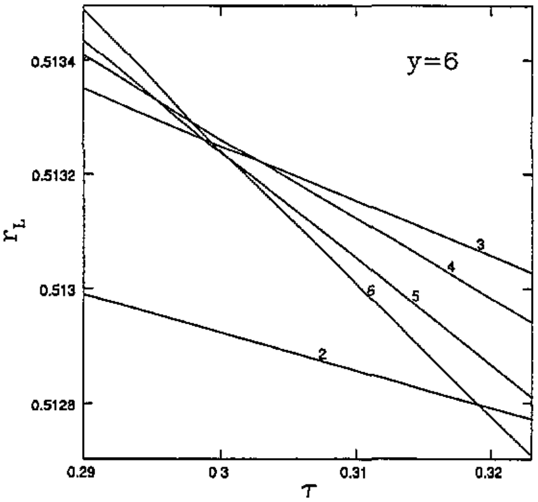

Figure 5. Plot of the values $r_{\mathcal{L}}$ (3.8) versus τ for $y = 6$. For large $\mathcal{L}$ the curves should intersect at $(\tau_{\theta,c}, \nu_{\theta,c})$. The intersections points are reported in table 4.

Table 4. Estimates of the critical exponents ($\nu_{\theta,c}$ and $\phi_{\theta,c}$) for different strip widths at $y = 6$. The values are obtained looking at the crossing points of the lines in figure 4. The asymptotic results (equation (3.13)) have been obtained looking at these intersection points in the range $y > 2$.

$\mathcal{L}$	ν_θ	ϕ_θ
3	0.51225	0.592
4	0.51326	0.624
5	0.51333	0.661
6	0.51329	0.662

can be obtained. For $y \sim 6.2$, finite-size estimates of $\nu_{\theta,c}$ are nearly independent of $\mathcal{L}$ indicating that here we are close to the tri-critical fixed point. At this point our results for the thermal exponents are

$$\nu_{\theta,c} = 0.51 \pm 0.01 \qquad \phi_{\theta,c} = 0.65 \pm 0.1 \,. \tag{3.13}$$

These values are, within their accuracy, equal to those obtained by Derrida and Hermann [23] for the cycle model ($\tau = 0$).

The values (3.13) are also clearly different from the values for $y < 2$ as given in (3.10) and (3.12). This is the most evident for ϕ_θ. On the basis of this, we conclude that indeed there are two different universality classes for θ-collapses of BP, one including the contact model, the other including the cycle model.

Secondly, we remark that our value for $\phi_{\theta,c}$ is in agreement with the prediction in (2.17). The same cannot be said about $\nu_{\theta,c}$, but we have to take into account that the error bar on $\nu_{\theta,c}$ is much smaller. We can argue that, due to the maximum in our finite-size estimates for this exponent, we have to go to considerably larger $\mathcal{L}$-values to find the true asymptotic behaviour. We can also remark that, in a similar study [33] of the θ-point of linear polymers, the exponent $\nu_\theta = 0.55 \pm 0.01$ was obtained, seemingly excluding the now generally accepted exact value $\nu_\theta = \frac{4}{7}$ [5].

We think it is fair to say that the present calculations do not allow us to confirm nor to disprove the prediction (2.16) for $\nu_{\theta,c}$. The question of whether the θ-point of BP (with holes) in the regime $y > 2$ (or $\tau < 2$) is in the universality class of the tri-critical zero-state Potts model thus remains open.

Finally we have investigated whether the lines of θ-points lie in the plane given by (2.18). We find that, within the numerical accuracy, this is true for $y > 2$, but not for the line of Ising transitions.

4. The collapsed phase

We finally turn to a study of the collapsed phase and the possibility of a collapse–collapse transition. A proper discussion of the collapsed phase requires the introduction of the concept of solvent contact [12]. A *solvent contact* is a perimeter edge that is not a contact, so that the number of such solvent contacts m in a given animal is

$$m = t - I \,. \tag{4.1}$$

In section 2, we showed that for $y = 1$, $\tau \to \infty$, the critical properties of BP become those of spanning trees, for which by definition $m = c = 0$, and as a consequence for large s, $I = b = s$. Furthermore, we can expect on the basis of RG ideas that the latter is true for all $\tau > \tau_{\theta,I}$ when we look at large enough length scales. We are therefore led to predict that

$$\langle I \rangle_s \sim s \qquad \text{for} \quad y = 1,\ \tau > \tau_{\theta,I} \,. \tag{4.2}$$

On the other hand, for the collapsed phase in the cycle model, some exact results were recently determined by Flesia *et al* [26]. They showed that

$$\langle m \rangle_s \sim s \qquad \text{for} \quad \tau = 0,\ y > y_{\theta,c} \,. \tag{4.3}$$

The cycle model includes only animals without contacts ($\tau = 0$) so that trivially we have $\langle I \rangle_s = 0$.

One can now ask whether there exists a transition between these two physically distinct collapsed phases or whether quantities like, for example, $\langle m \rangle_s$ change analytically when we pass from the cycle to the contact model. Numerical evidence for such a collapse–collapse transition was provided in [12].

Using the Potts description of the interacting lattice animals we can get information on the asymptotic form (for $y \to \infty$, $\tau \to \infty$, but keeping $w = \tau/y$ fixed) of a possible collapse–collapse transition line.

Using (2.3) and (4.1) we can rewrite (2.4) as

$$Z = \sum_{\{\mathcal{G}_1\}} (xy^2)^s (y^{-m/2}) (w)^I \,. \tag{4.4}$$

When $y \to \infty$, equation (4.4) will contain only graphs which have $m = 0$, i.e. which span the lattice (and consequently $s = N$). For that case, from (2.3), $I = 2s - b$, and we finally have

$$Z \sim \sum_{\{\mathcal{G}_s\}} w^{-b} \tag{4.5}$$

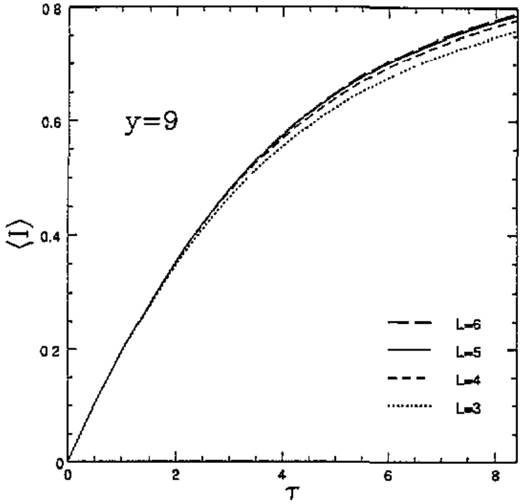

Figure 6. Average number of contacts $\langle I\rangle$ versus τ for $y = 9$ at criticality (4.5) in a finite strip for $\mathcal{L} = 3, 4, 5$.

where the sum is over graphs which span the lattice. It is well known [19] that (4.5) is the high-temperature expansion for the q-state Potts model when $q \to 0$ with

$$w = 1/(\exp(J) - 1)\,. \tag{4.6}$$

Thus, in the large-y, large-τ region our lattice animals are described by the zero-state Potts model. This model is known [19] to have only a transition at $J_c = 0$, or for $w \to \infty$. In fact, at this point the graphs contributing to (4.5) become the spanning trees which we already encountered in section 2.2.

In conclusion then, for $y \to \infty$ and $\tau \to \infty$, the only transition in the model can be for $w \to \infty$, or, stated otherwise, any possible collapse–collapse transition line should asymptotically become parallel to the τ-axis.

We have looked for evidence of this transition again using the transfer matrix. Unfortunately, the technique of locating the transition using a plot of $r(\tau)$ versus τ cannot be applied in this case, because everywhere in the collapsed phase we have $\nu = \frac{1}{2}$, so a crossing of curves for different $\mathcal{L}$ values is not to be expected, and indeed turns out not to occur.

An alternative method is to look at averages and fluctuations in the number of contacts. We have therefore looked at the average number of contacts $\langle I\rangle$ which is defined as

$$\langle I\rangle = \lim_{s\to\infty} \frac{\langle I\rangle_s}{s} = \lim_{s\to\infty} \frac{\sum_{b,I} C_{s,b,I}\, I y^b \tau^I}{s \sum_{b,I} C_{s,b,I}\, y^b \tau^I}\,. \tag{4.7}$$

Using the definitions (1.1) and (1.2), we can write $\langle I\rangle$ as

$$\langle I\rangle = \frac{\partial \log Z_s}{\partial \log \tau} = -\frac{\partial \log x_c(\tau, y)}{\partial \log \tau}\,. \tag{4.8}$$

In figure 6 we show numerical results for $\langle I\rangle$ as a function of τ at $y = 9$ for different values of $\mathcal{L}$. These results give evidence that the collapse–collapse transition (if it exists) is continuous and not first order.

To localize the transition one can look at the fluctuations ΔI in the number of contacts:

$$\Delta I = \lim_{s\to\infty} \frac{(\langle I^2\rangle_s - \langle I\rangle_s^2)}{s} = -\frac{\partial^2}{\partial(\log\tau)^2}\log x_c(\tau, y)\,. \tag{4.9}$$

We have made extensive explorations in the phase diagram looking for a peak in ΔI growing with L, but we did not find any evidence for such behaviour. We believe this to be strong numerical evidence against the existence of the collapse–collapse transition.

5. Remarks and conclusions

In this paper we have given numerical and analytical results for the critical behaviour of a model for interacting BP. We have determined the critical surface and the location of lines and points of higher-order transitions (figure 2) .

For small y and τ values the behaviour of large lattice animals ($s \to \infty$) is essentially that of non-interacting animals; we thus expect, e.g., that $\nu = 0.64\ldots$ [9] for animals in this regime.

When one increases y or τ, the animal collapses. For $y < 2$, the collapse is in the Ising universality class with the exponents given by (2.16). The animal collapses into a tree-like structure.

When $2 < y \leqslant 6.48\ldots$, the collapse is in a different universality class with exponents which are possibly those of the tri-critical zero-state Potts model, and are given in (2.18). Further work remains to be done to confirm the predicted exponent values along that line. The animal collapses into a compact configuration with no contacts, but (see (4.3)) a number of solvent contacts proportional to s. The two collapse lines are separated by a higher-order critical point which is of percolation type. At this point, we expect, using the well known percolation exponent, that $\nu = \frac{48}{91}$ and $\phi = \frac{3}{4}/\frac{91}{48} = \frac{36}{91}$.

Finally, we have given numerical evidence for the presence of only one collapsed phase.

The results presented here can be extended in several directions. In section 1, we discussed the exponential growth of the quantity Z_s for large s. Magnetic-like exponents occur in the corrections to this leading behaviour. More precisely, we expect Z_s to behave as

$$Z_s(y, \tau) \sim x_c(\tau, y)^{-s} s^{-\Theta}\,. \tag{5.1}$$

For non-interacting BP, Θ is known to be exactly 1, while on the basis of the vesicle analogy $\Theta = 2$ was predicted along the cycle-model collapse branch [10]. So far we have no result for Θ along the Ising line. It is furthermore known that, for example, along the percolation line for $p > p_c$, or in general in a collapsed phase, that (5.3) does not always give the correct form of Z_s [34].

We also did not discuss any surface exponents. In fact these are not even known completely for the non-interacting branched polymers [35, 36]. Still, we can make some predictions for these exponents along the two lines of θ-collapses.

An especially interesting exponent is the surface crossover exponent, which is associated with the adsorption of the BP onto the surface when the attraction with the boundary reaches a critical value (the 'special' surface transition [37]).

Along the cycle-model collapse line, again using the vesicle analogy, the adsorption of the tri-critical BP can be related to the adsorption of a self-avoiding walk, a problem for which exact results exist. This leads us to predict that in this case the surface crossover exponent, which we denote as ϕ_s, equals $\frac{1}{3}$.

Adsorption onto a surface (which is one-dimensional in $d = 2$) is not possible in general, because it would imply the existence of a phase transition in $d = 1$. Only for models like $\mathcal{O}(n)$-models with $n < 1$ is such a transition is possible. Therefore, we are led to predict that along the 'Ising'-line of θ-transition there is no adsorption possible. If we denote by ω_c the 'critical value' of some fugacity for monomer–surface interactions then we expect ω_c to diverge when τ goes to $\tau_{\theta,I}$ from below (if we consider, e.g., the case $y = 1$).

We are currently investigating these adsorption processes, because a confirmation of the above predictions could give considerable further evidence for the correctness of the universality classes which we proposed here.

The model we have studied can be related to the 'solvent' model of Flesia *et al* [12]. The authors of that reference study a model in the canonical ensemble (i.e. for fixed s) with a free energy $Z_{F,s}$ which is defined as

$$Z_{F,s} = \sum u^m w^I \tag{5.2}$$

where the sum runs over the set of all distinct BP with s (fixed!) occupied edges, m solvent contacts and I contacts. Comparing with (4.4) we immediately see that this is just our model in the canonical ensemble with $u = y^{-1/2}$. Using these relations our phase diagram can be compared with that of [12]. In that work, the location of the tri-critical lines is determined, together with the associated crossover exponents, using the exact enumeration data of [22]. While both phase diagrams agree to some extent, in the present work we have added substantial quantitative information. The relation with the Potts model as discussed in section 2 also allowed us to give conjectures on the exact values of the critical exponents along the tri-critical lines. Furthermore, we find no evidence of a collapse–collapse transition. We suspect that the transition found in [12] is an effect of the use of finite animals in a region where spanning graphs dominate.

Finally, we can think of extending our model to $d = 3$. Several of the arguments in section 2 seem to also go through in that case. The role of the percolation line and plane should be similar, and we can also expect an Ising-like branch. Whether the other branch of collapse transitions is still tri-critical zero-state Potts is not so clear (in any case the exponents of that model in $d = 3$ are not known) but the vesicle analogy has been extended to this dimension, so that numerical estimates for the exponents along the branch now exist [38]. Of course a numerical investigation of our model in $d = 3$ would be much more difficult, but could be envisaged using techniques that were recently established for the simulation of $d = 3$-vesicles [38].

Acknowledgments

We would like to thank S G Whittington for a critical reading of and several useful comments on an earlier version of this paper. We also would like to thank A L Stella for a critical reading of the manuscript, and C Micheletti for help in computer work. Finally, one of us (CV) would like to thank the IUAP-Belgium for financial support.

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