

## Vesicles, the Tricritical-0-State Potts Model, and the Collapse of Branched Polymers

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We relate a cycle model for the collapse of branched polymers without holes (in  $d=2$ ) to the problem of self-avoiding rings with an area fugacity, studied in the context of vesicles. This relation together with arguments which show that the collapse transition of branched polymers (with holes) is described by the tricritical-zero-state Potts model allows a determination of all critical exponents at this collapse point;  $\nu = \frac{1}{2}$ ,  $\phi = \frac{2}{3}$ ,  $\tau = 2$ , in agreement with numerical results. We also comment on the universality of this result.

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Linear polymers consist of monomers with a functionality which is 2. The study of critical properties of such polymers has seen great progress following the work of de Gennes [1]. This is especially true in two dimensions where the principle of conformal invariance [2] or the Coulomb gas method [3] have allowed an exact determination of many critical properties [4]. An area in which recently much progress has been made is that of the collapse of a linear polymer under the influence of attractive interactions between the monomers. The critical exponents at the two-dimensional collapse transition (also called theta point) are now known exactly [5,6].

In contrast, much less is known about branched polymers (BP's) which are made of monomers with a functionality which is greater than 2. In statistical mechanics, these BP are described by lattice animals. Exact results for lattice animals are few [7]. There even exists evidence that lattice animals are not conformally invariant [2]. Besides being models for BP, lattice animals occur in many physically important situations such as in the study of vesicles [8,9], equilibrium DLA [10], or (in dimensions greater than two) in the study of membranes and surfaces [11]. In the present paper we will study the collapse of branched polymers. Several models have been introduced to describe this collapse. These models are commonly divided into cycle and contact models [12]. There are recent claims that these two models may not be in the same universality class [13]. In this paper, we will show that the collapse transition in the cycle models is described by a zero-state tricritical Potts model [14], leading to a full and exact determination of all critical exponents. At the end of this Letter, we will briefly comment on the universality question.

A (site) lattice animal consists of a connected set of nearest-neighbor sites on a lattice. Here we will work in  $d=2$ , and, to fix attention, consider the square lattice. If we think of a site as representing a monomer of a BP in a dilute solution we may give a weight  $\lambda_s^s$  to such an animal, where  $s$  is the number of sites in the animal and  $\lambda_s$  is the fugacity for one monomer. In the cycle model of BP collapse we next introduce an attraction between the monomers by giving each pair of nearest-neighbor sites in

the animal a weight  $\lambda_b$ . The grand canonical partition function for the animal problem is then defined by

$$Z(\lambda_s, \lambda_b) = \sum_{s,b} C(s,b) \lambda_s^s \lambda_b^b, \quad (1)$$

where  $C(s,b)$  is the number of lattice animals with  $s$  sites and  $b$  nearest-neighbor pairs (Fig. 1). At fixed  $\lambda_b$  the partition sum (1) will diverge at a critical value  $\lambda_s^c(\lambda_b)$  of the site fugacity. When  $\lambda_b=1$  we have the noninteracting site animals but upon increasing  $\lambda_b$  the branched polymer will collapse at a critical value  $\lambda_b^*$  [we denote  $\lambda_s^c(\lambda_b^*)$  by  $\lambda_s^*$ ]. This collapse has been studied numerically by Monte Carlo methods [15] and by transfer matrix techniques [16].

We first consider a subset of lattice animals, namely, those without internal holes. In the following we will show that the statistics of these lattice animals can be mapped onto that of self-avoiding rings with an area fugacity, which have been studied in the context of vesicles [8,9] and are well understood by now. The proof is simple. We draw, on the dual lattice, a self-avoiding ring (SAR) around the lattice animal (Fig. 1). It is now easy to see that the area  $A$  inside the ring equals the number

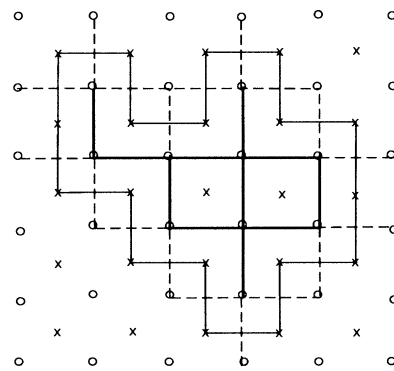


FIG. 1. A lattice animal of  $s=10$  sites,  $b=11$  bonds (thick full lines), and  $t=18$  perimeter bonds (dashed lines) on the square lattice (dots). Also shown is a self-avoiding ring (thin full line) on the dual lattice (crosses).

of sites in the animals, while the number of steps  $N$  of the ring is equal to the number of perimeter bonds ( $t$ ) of the animal. This latter number can be immediately related to  $s$  and  $b$  by (square lattice)  $4s = 2b + t$ . Combining these results we get the following equivalences between animals and rings:

$$s = A, \quad b = (4A - N)/2. \tag{2}$$

We thus arrive at the conclusion that the statistics (1) of the animals with weight  $\lambda_s^s \lambda_b^b$  is equal to the statistics of SAR's with weight  $K^N p^A$  where the step fugacity  $K$  and the area fugacity  $p$  are given by

$$K = \lambda_b^{-1/2}, \quad p = \lambda_s \lambda_b^2. \tag{3}$$

The latter problem is that studied in the context of vesicles, and its phase diagram is shown in Fig. 2 [8,9].

Evidently, at  $p = 1$ , the vesicle problem reduces to that of the noninteracting SAR which has a critical fugacity  $K^*$  (which equals  $0.3790523\dots$  on the square lattice [17]) and a fractal dimension  $D$  which is  $\frac{4}{3}$  [4]. More recently, it has been shown that the dimension of the interior of the ring,  $D_I$ , equals 2 [18,19]. When  $p$  is decreased below 1, the vesicles behave like branched polymers while for  $p > 1$  they are inflated and have  $D_I = 2$  [8,9]. (For  $p > 1$ , the critical step fugacity is zero.)

Returning now to the lattice animals without holes (Fig. 2) we see that in the absence of interactions ( $\lambda_b = 1$ ), upon increasing  $\lambda_s$  to its critical value we move along the line  $K = 1$  until we meet the branched polymer line. Thus we recover the known fact that these noninteracting lattice animals are the same as deflated vesicles. Now, increasing  $\lambda_s$  at fixed  $\lambda_b > 1$  we move along lines of constant  $K$  and have branched polymer behavior until at  $\lambda_b^* = K_*^2$  we hit the SAR fixed point. Here our BP's

which are the interiors of the rings collapse and have a fractal dimension  $\bar{D} = D_I = 2$  ( $v = D_I^{-1} = \frac{1}{2}$ ). For  $\lambda_b > \lambda_b^*$  we reach the inflated vesicle phase where the branched polymers are compact. In fact when, upon increasing  $\lambda_s$  (for  $\lambda_b > \lambda_b^*$ ) we cross the line  $p = 1$ , the size of the lattice animal will make a discontinuous jump from a finite to an infinite value [9], implying that here we have a true first-order transition, and also implying that the theta point has all the characteristics of a tricritical point.

In this picture, it is clear that the crossover exponent  $\phi$  at the BP theta point is determined by the SAR thermal exponent leading to  $\phi = \frac{4}{3}/2 = \frac{2}{3}$ . A final exponent ( $\tau$ ) in which we are interested is of "magnetic" type and appears in the expression for the number  $\tilde{C}_s(\lambda_b)$  of BP of  $s$  sites which is defined as

$$\tilde{C}_s(\lambda_b) \equiv \sum_b C(s, b) \lambda_b^b. \tag{4a}$$

This quantity, for large  $s$ , goes as

$$\tilde{C}_s(\lambda_b) \sim [\lambda_s^c(\lambda_b)]^{-s} s^{-\tau}, \tag{4b}$$

which defines the exponent  $\tau$ .

For  $\lambda_b < \lambda_b^*$ , we expect  $\tau = 1$ , the appropriate value for noninteracting BP [7]. The value of  $\tau$  can, through the relations (2) and (3), be determined from a knowledge of the number of self-avoiding rings of area  $A$ . This number has been determined for  $K = 1$  from an exact enumeration of self-avoiding rings [20] and its value is indeed consistent with the BP value  $\tau = 1$ . Using the exact enumeration data of Enting and Guttmann [20], we can also get a numerical estimation of  $\tau$  at the theta point. The value we obtain is  $\tau = 2.0 \pm 0.1$ .

To conclude our study of lattice animals without holes we make some remarks. First, at the theta point,  $\lambda_s^*$  and  $\lambda_b^*$  obey the equation  $\lambda_s^* \lambda_b^{*2} = 1$ . For  $\lambda_b > \lambda_b^*$ , the critical curve is given by  $\lambda_s^c = \lambda_b^{-2}$ . Second, we remark that at their  $\theta$  point, these BP already have a compact interior but a surface which is still fractal (with  $D = \frac{4}{3}$ ).

We now return to the more realistic lattice animals *with* holes. All the above equivalences still hold true if we draw SAR's around both exterior and interior boundaries of the animal. Thus the cycle model of interacting animals can again be mapped into vesicles with  $p$  and  $K$  still given by [3]. Now, however, the vesicles will contain holes (such objects are also called punctured discs [21]). The arguments given in Ref. [9] on the phase diagram of the vesicle problem can immediately be extended to this case [22]. The critical line has the same qualitative behavior as in Fig. 2 [e.g.,  $K_c(p) = 0$  for  $p > 1, \dots$ ]. Furthermore, if we denote by  $N$  the length of the total perimeter (i.e., of external boundary plus boundaries of the holes), then one can show that the average area  $\langle A \rangle$  scales like  $N$  in the deflated regime, and like  $N^2$  in the inflated regime [22]. Thus, for  $p < 1$  the punctured discs are still highly ramified objects. Clearly when  $p \rightarrow 0$  the vesicles with holes behave like noninteracting BP.

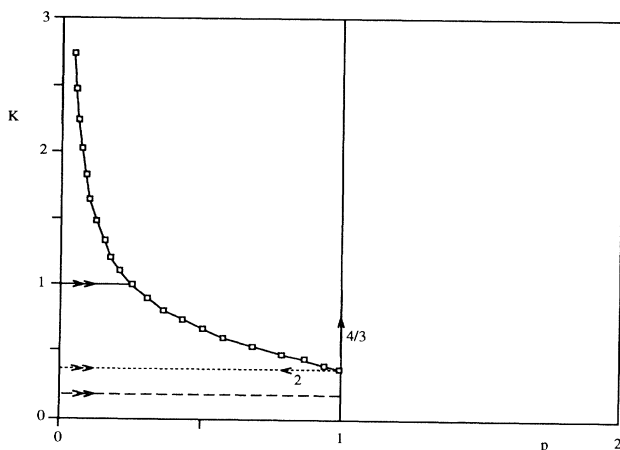


FIG. 2. The phase diagram of the vesicle problem. The open squares are the numerical results of Ref. [9]. At the SAR point ( $p = 1$ ) we have indicated the relevant eigenvalues. Also shown are horizontal lines of increasing  $\lambda_s$  (fixed  $\lambda_b$ ) for  $\lambda_b = 1$  (full line),  $\lambda_b = \lambda_b^*$  (dotted line), and  $\lambda_b > \lambda_b^*$  (dashed line).

Furthermore, arguments of fields theoretic type [23] indicate that holes are irrelevant for noninteracting BP's. Taking all these results together, there is thus strong evidence that BP's still collapse at  $p = \lambda_s^* \lambda_b^{*2} = 1$ , also in the presence of holes.

This prediction is indeed in agreement with the numerical data of Ref. [16]. Using the values  $\lambda_s^* = 0.0230 \pm 0.004$  and  $\lambda_b^* = 6.48 \pm 0.12$  from that reference we find  $\lambda_s^* \lambda_b^{*2} = 0.97 \pm 0.05$ , consistent with the above prediction.

Are the exponent values ( $\nu = \frac{1}{2}$ ,  $\phi = \frac{2}{3}$ ) the same for the BP's with holes? Or, in other words, are holes also irrelevant at the theta point? The numerical estimates of Ref. [14] are  $\phi = 0.657 \pm 0.025$  and  $\nu = 0.5095 \pm 0.003$ . In interpreting these data we must realize that the calculations of Ref. [16] used strips of width up to 7 only, and that the estimates of exponents crucially depend on the precise location of the  $\theta$  point. It is therefore our feeling that the error bars on  $\nu$  are underestimated. (In this respect it is interesting to note, e.g., that a similar calculation for the theta point of linear polymers gave  $\nu = 0.55 \pm 0.01$  [24], seemingly excluding the exact value  $\nu = \frac{4}{7}$  [5].) The estimate of  $\phi$  is, however, definitely consistent with our prediction.

Additional evidence comes from a mapping of the interacting animal problem (with holes) onto a Potts lattice gas. This mapping has been introduced by other authors [23,25,26] but we will further exploit its consequences using similarities between the present problem and that of the Ising clusters, which was recently solved [27]. These arguments, though nonrigorous, will give evidence that the  $\theta$  point of BP's is described by a tricritical-zero-state Potts model whose exponents [3]  $\nu = \frac{1}{2}$ ,  $\phi = \frac{2}{3}$  are precisely those obtained above. We start by considering the Potts lattice gas [14] in which Potts variables  $\sigma_i = 1, \dots, (q-1)$  are coupled to lattice gas variables  $t_i = 0, 1$ . The reduced Hamiltonian is

$$H = J \sum_{\langle i,j \rangle} t_i t_j (\delta_{\sigma_i \sigma_j} - 1) + \Delta \sum_i t_i + M \sum_{\langle i,j \rangle} t_i t_j. \quad (5)$$

If we call  $Z_p$  the partition function of the Potts model (5), then it is known [23,25,26] that the function  $G = (d \ln Z_p / dq)$  ( $q=1$ ) is the generating function for the interacting lattice animals using the following parameter

values [24] (again take the square lattice):

$$\Delta = \ln \lambda_s, \quad M = \ln \lambda_b, \quad J \rightarrow \infty. \quad (6)$$

The phase diagram of (5) has been studied extensively [14,28]. It is known to contain several fixed points such as an Ising fixed point (for  $J=0$ ), a critical- $q$ -state Potts fixed point, and critical- and tricritical- $(q-1)$ -state Potts points. Another long-known fact [29] is that for  $q=2, J \rightarrow \infty$  the model (5) describes the properties of Ising clusters, i.e., of connected sets of nearest-neighbor sites for which the Ising variable 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 (5) for  $q=2$  was clarified [27]. 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) to relate the collapse transition in the cycle model of lattice animals to the zero-state tricritical Potts model.

In Fig. 3(a) we have therefore drawn part of the phase diagram of (3) for the case  $q=2$  as determined in Ref. [27]. We will consider clusters of down spins and for convenience work with Ising parameters ( $K_{IS} = M/4, h = \Delta/2 + M$ ) instead of lattice gas parameters. There are, in the plane  $J = \infty$ , three critical regimes. For  $K_{IS} < K_{IS}^*$  (the Ising critical temperature) the clusters behave as those of uncorrelated percolation (full line). For  $K_{IS} > K_{IS}^*, h = 0$ , there is a line of first-order (dashed line) percolative transitions. Precisely at the Ising critical point there is a tricritical point separating both regimes. This tricritical point is, under renormalization, attracted to the tricritical-one-state Potts fixed point located at  $K_{IS} = K_{IS}^*, h = 0$  and an unknown but finite value of  $J$  [27].

We now return to the lattice animals. As discussed above, these are again described by (5) for  $J \rightarrow \infty$ , but now  $q=1$ . Converting (6) to Ising variables we get

$$K_{IS} = [\ln \lambda_b] / 4, \quad h = \ln \lambda_b + \frac{1}{2} \ln \lambda_s. \quad (7)$$

In Fig. 3(b) we have drawn the expected phase diagram of the animals as a function of  $K_{IS}$  and  $h$ . First for  $\lambda_b = 1$ , we get the critical point of the noninteracting lat-

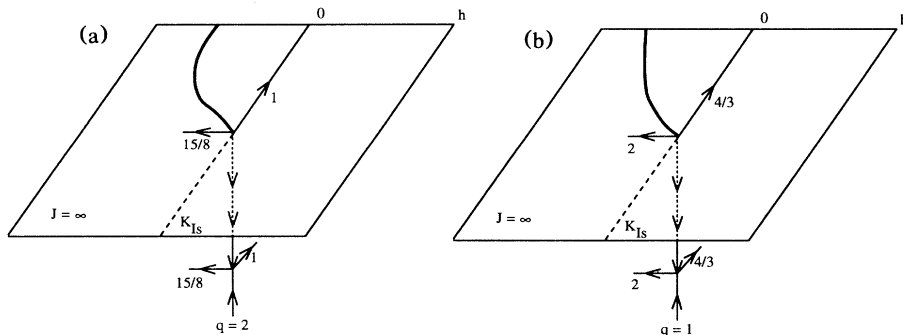


FIG. 3. (a) Part of the phase diagram of the Hamiltonian (5) for  $q=2$ . Shown is the plane  $J = \infty$  and the tricritical fixed point which attracts the critical Ising clusters (see text). (b) The phase diagram of the lattice animal collapse (see text).

tice animals at  $h = [\ln \lambda_s^c(1)]/2 < 0$  [because  $\lambda_s^c(1) < 1$ ]. Putting on  $\lambda_b$  means increasing  $K_{IS}$ . At the critical value  $\lambda_b^*$  the BP's collapse. For  $\lambda_b > \lambda_b^*$  we have a first-order transition. Now notice that the form of the critical line  $\lambda_s^c = \lambda_b^{-2}$  which we found from the vesicle analogy for  $\lambda_b \geq \lambda_b^*$  implies that the  $\theta$  point and the line of first-order transitions are located along the line  $h=0$ . We now notice the complete similarity of the plane  $J=\infty$  for the cases  $q=2$  and  $q=1$ . [In fact, for the punctured disks there is a symmetry  $p \leftrightarrow 1/p$  which interchanges the inside and outside of the disk (or vesicle). In the case  $q=2$ , this corresponds to  $h \leftrightarrow -h$  symmetry in the Ising model which interchanges clusters of down spins and clusters of up spins. Thus, in both Figs. 3(a) and 3(b) there is a second line which is not drawn of second-order transitions. Both lines meet at the  $\theta$  point.] We will therefore assume that also the renormalization group flow does not change qualitatively when we go from  $q=2$  to  $q=1$ , and thus that the collapse point of BP's is attracted to the tricritical-zero-state Potts model.

The exponents of the tricritical Potts model were calculated by Nienhuis [3] and they lead, for  $q=0$  to  $\nu = \frac{1}{2}$  and  $\phi = \frac{2}{3}$ , in agreement with what we found in the vesicle picture.

The leading magnetic exponent  $y_H$  of the model equals 2. This exponent describes the behavior of the correlation function for the model (5) which for  $q \rightarrow 1$  can be expressed in terms of the number of branched polymers  $\tilde{C}_s(\lambda_b)$ . This allows one to relate the exponents  $\tau$  and  $y_H$  with the result [30]

$$\tau = 2/y_H + 1. \quad (8)$$

In this way we are led to predict  $\tau=2$ . This is indeed in agreement with the numerical result discussed earlier.

It thus seems that indeed the  $\theta$  point of the cycle model of branched polymers is described by the exponents of the zero-state tricritical Potts model. As noted in the introduction, another model for the collapse of BP is the contact model. We now briefly comment on the universality question. The contact model can also be described by the Hamiltonian (5), but now in the plane  $\Delta=0$  [26]. Again using similarities with the case  $q=2$ , it seems that the  $\theta$  point of contact models cannot be in the domain of attraction of the tricritical-zero-state Potts model. The model (5) also contains a percolation fixed point which is fully repulsive. One is thus led to a picture in which two distinct  $\theta$  points, one for contact, the other for cycle models, are separated by the higher-order percolation fixed point. Details of these reasonings will be published elsewhere.

In conclusion then, we have determined the critical exponents of cycle models of branched polymers at their collapse transition. In addition to BP's without holes we could also determine the location of the collapse point in terms of the critical fugacity of SAR's. This is known exactly on the hexagonal lattice [4] so that for that lattice

the location of the  $\theta$  point is at  $\lambda_b^* = K_*^{-2} = 2 + \sqrt{2}$ ,  $\lambda_s^* = (\lambda_b^*)^{-2} = (2 + \sqrt{2})^{-2}$ .

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  - [30] To obtain this result, we have used a hyperscaling relation which may not hold for noninteracting BP, but which is certainly valid for the tricritical Potts model.