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## LETTER TO THE EDITOR

# Collapse transitions in animals and vesicles

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**Abstract.** We discuss the relationship between the solvent model of collapse in strongly and weakly embeddable lattice animals, and a model recently introduced by Vanderzande and by Stella *et al.* We show that there are important qualitative differences in the behaviour predicted by these two models in the compact regime.

Collapse transitions in lattice animals (as a model of branched polymers in dilute solution) and in vesicles have been studied theoretically by a number of authors. For the animal problem, the transition from an expanded to a collapsed state can be driven by a cycle fugacity (Derrida and Herrmann 1983), by a contact fugacity (Madras *et al* 1990, Gaunt and Flesia 1991, Flesia and Gaunt 1992) or by a solvent fugacity (Flesia 1993). In this letter we shall be particularly interested in the latter case. The transition in vesicles is controlled by a pressure difference between the inside and the outside of the vesicle (Fisher *et al* 1991). When the internal pressure exceeds the external pressure the vesicle is an expanded object, but it collapses as soon as the external pressure exceeds the internal pressure. A connection between the transitions in animals and in vesicles has been investigated recently by Vanderzande (1993) and by Stella *et al* (1992), and the primary purpose of this letter is to explore this connection further.

The nature of the phase transition for vesicles in hypercubic lattices is rather well understood (Fisher *et al* 1991, Banavar *et al* 1991). We focus on the square ( $Z^2$ ) and simple cubic ( $Z^3$ ) lattices though many of our results are more generally applicable. A vesicle is a disc in  $Z^2$ , i.e. a self-avoiding polygon and its interior, or a ball in  $Z^3$ , i.e. a plaquette surface homeomorphic to a sphere, and its interior. We write  $m$  for the number of edges in the polygon, or for the number of plaquettes in the surface,  $n$  for the enclosed area or volume, and  $v_m(n)$  for the number of vesicles per lattice site. We can define the generating function  $A_n(x)$  by the equation

$$A_n(x) = \sum_m v_m(n) x^m \quad (1)$$

and it follows from the arguments of Fisher *et al* (1991) that

$$\mathcal{A}(x) = \lim_{n \rightarrow \infty} n^{-1} \log A_n(x) \quad (2)$$

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is monotone non-decreasing, continuous, log-convex and almost everywhere differentiable. Moreover, there exists an  $x_0 < 1$  such that  $\mathcal{A}(x)$  is zero for  $x < x_0$  and positive for  $x > x_0$ . It follows from numerical estimates of the connective constant for self-avoiding walks on the square lattice that in two dimensions  $x_0 \approx 0.379$ . The value of the limit

$$\lim_{n \rightarrow \infty} \langle m \rangle / n$$

is determined by the logarithmic derivative of  $\mathcal{A}(x)$ , since the order of the derivative and limit can be interchanged everywhere that the derivative of  $\mathcal{A}(x)$  exists. This implies that  $\langle m \rangle = o(n)$  for all  $x < x_0$ , and  $\langle m \rangle \sim n$  for almost all  $x > x_0$ .

Vanderzande (1993) and Stella *et al* (1992) have noticed that a model involving a proper subset of strongly embeddable animals can be mapped into the vesicle problem. The subset of animals considered by Vanderzande and by Stella *et al* is the set of animals which are dual to a vesicle. That is, each vertex in the animal is replaced by its dual cell and the union of these cells must be homeomorphic to a disc in  $Z^2$  or to a ball in  $Z^3$ . Loosely speaking, the animals have no internal 'holes' and, since the animals are a subset of the strongly embeddable animals, every pair of adjacent vertices are connected by an edge. For brevity, we call this model the *disc model*. The thermodynamics of this model in the ensemble in which the number of vertices of the animal is constant is precisely the thermodynamics of the vesicle problem with  $n$  constant. Hence the disc model has a phase transition. In order to describe this transition we now introduce some notation about lattice animals.

Consider a lattice animal, weakly embeddable in the lattice, with  $n$  vertices,  $e$  edges and with cyclomatic index  $c$ . We define a *contact* as a pair of nearest-neighbour occupied vertices not directly connected by an occupied edge. Similarly we define a *solvent contact* as an edge which joins a vertex of the animal to a neighbouring unoccupied vertex. If the number of contacts is  $k$  and the number of solvent contacts is  $s$ , then (using Euler's relation)

$$s = (2d - 2)n + 2 - 2c - 2k \quad (3)$$

where  $d$  is the dimension of the lattice.

In the disc model the number of vertices in the animal corresponds to the area of the disc or the volume of the ball and the number of solvent contacts ( $s$ ) of the animal corresponds to the perimeter ( $m$ ) of the disc or to the area ( $m$ ) of the plaquette sphere bounding the ball. This mapping, together with the results of Fisher *et al.* (1991), shows that in the compact regime  $\langle s \rangle = o(n)$ , while for almost all values of  $x$  in the expanded regime  $\langle s \rangle \sim n$ .

We next describe some known results for the *solvent models* for strongly embeddable animals. In this model for the collapse transition in animals, there is a fugacity associated with the number of solvent contacts. Let  $a_n(s, k)$  be the number of animals with  $n$  vertices,  $s$  solvent contacts and  $k$  contacts. Since for strongly embeddable animals  $k = 0$ , the partition function is

$$\hat{Q}_n(\beta) = \sum_s a_n(s, 0) e^{\beta s} \quad (4)$$

and the corresponding limiting free energy is

$$\hat{\mathcal{F}}(\beta) = \lim_{n \rightarrow \infty} n^{-1} \log \hat{Q}_n(\beta). \quad (5)$$

It is straightforward to show that the limit exists and that  $\hat{\mathcal{F}}(\beta)$  is convex, monotone non-decreasing, continuous and differentiable almost everywhere. This model can be mapped into the model studied (using transfer matrix methods) by Derrida and Herrmann (1983) and their work predicts a transition at  $\hat{\beta}_c \approx -0.935$ .

We now derive some additional results for the solvent model for strongly embeddable animals and compare these results with those for the disc model. Define the *site perimeter* as the number of vertices which are not in the animal but which are incident on at least one edge of the lattice which is a solvent contact of the animal. Let  $\hat{a}_n(s, m)$  be the number of strongly embeddable animals with  $n$  vertices, site perimeter  $m$  and with  $s$  solvent contacts. Hence  $a_n(s, 0) = \sum_m \hat{a}_n(s, m)$ . For the site percolation problem, define  $\hat{P}_n(p)$  to be the probability that the origin is in a cluster of  $n$  vertices at vertex occupation probability  $p$ . Then

$$\hat{P}_n(p) = \sum_{s, m} n \hat{a}_n(s, m) p^n (1-p)^m. \quad (6)$$

Take  $\beta < 0$ . Clearly  $2dm \geq s \geq m$ , so that  $e^{2dm\beta} \leq e^{s\beta} \leq e^{m\beta}$ . Hence

$$\begin{aligned} \hat{Q}_n(\beta) &= \sum_s a_n(s, 0) e^{s\beta} \\ &= \sum_{m, s} \hat{a}_n(s, m) e^{s\beta} \\ &\leq \sum_{m, s} \hat{a}_n(s, m) e^{m\beta} \\ &= \hat{P}_n(1 - e^\beta) / n(1 - e^\beta)^n \end{aligned} \quad (7)$$

and, similarly,

$$\begin{aligned} \hat{Q}_n(\beta) &= \sum_{m, s} \hat{a}_n(s, m) e^{s\beta} \\ &\geq \sum_{m, s} \hat{a}_n(s, m) e^{2dm\beta} \\ &= \hat{P}_n(1 - e^{2d\beta}) / n(1 - e^{2d\beta})^n. \end{aligned} \quad (8)$$

Taking logarithms, dividing by  $n$  and letting  $n$  go to infinity gives, for  $\beta < 0$

$$\hat{\mathcal{F}}(\beta) \leq -\log(1 - e^\beta) + \lim_{n \rightarrow \infty} n^{-1} \log \hat{P}_n(1 - e^\beta) \quad (9)$$

and

$$\hat{\mathcal{F}}(\beta) \geq -\log(1 - e^{2d\beta}) + \lim_{n \rightarrow \infty} n^{-1} \log \hat{P}_n(1 - e^{2d\beta}). \quad (10)$$

Since  $\hat{P}_n$  is a probability it is bounded above by 1 and hence equation (9) gives

$$\hat{\mathcal{F}}(\beta) \leq -\log(1 - e^\beta). \quad (11)$$

Let  $\hat{p}_c$  be the critical probability for site percolation. From Kesten (1982, Theorem 5.2, p. 98), given  $p > \hat{p}_c$  there exists numbers  $\pi$ ,  $\theta$  and  $C$  such that  $1 \geq \hat{P}_n(p) \geq \pi C \theta^{1/d} n^{(d-1)/d}$  and hence for  $p > \hat{p}_c$

$$\lim_{n \rightarrow \infty} n^{-1} \log \hat{P}_n(p) = 0. \quad (12)$$

Using this in equation (10) gives for  $\beta < (1/2d) \log(1 - \hat{p}_c)$

$$\hat{\mathcal{F}}(\beta) \geq -\log(1 - e^{2d\beta}) \quad (13)$$

and since  $\hat{\mathcal{F}}$  is a non-decreasing function we have for  $\beta > (1/2d) \log(1 - \hat{p}_c)$

$$\hat{\mathcal{F}}(\beta) \geq -\log \hat{p}_c. \quad (14)$$

Equations (13) and (11) imply that

$$\lim_{\beta \rightarrow -\infty} \hat{\mathcal{F}}(\beta) = 0 \quad (15)$$

while for all  $\beta > -\infty$

$$\hat{\mathcal{F}}(\beta) > 0. \quad (16)$$

From this, it follows immediately that  $\langle s \rangle \sim n$  for almost all  $\beta > -\infty$ , in contrast to the behaviour of the disc model. (In the grand canonical ensemble this implies that there is no vertical line in the phase diagram for this model, analogous to the one in figure 2 of Vanderzande (1993) for the disc model.) This is an important qualitative distinction between the thermodynamics of the two models. It occurs because most strongly embeddable animals are non-simply connected while the subset of animals considered by Vanderzande and by Stella *et al*, being dual to discs, cannot have 'holes'. It is the additional perimeter associated with the 'holes' in strongly embeddable animals which leads to the different  $n$ -dependence of  $\langle s \rangle$  in the compact regime.

For the solvent model for weakly embeddable animals we define the canonical partition function

$$Q_n(\beta) = \sum_{s,k} a_n(s, k) e^{\beta s}. \quad (17)$$

It is easy to show (by a concatenation argument) that the limiting reduced free energy

$$\mathcal{F}(\beta) = \lim_{n \rightarrow \infty} n^{-1} \log Q_n(\beta) \quad (18)$$

exists and is a convex function of  $\beta$ . Moreover,  $\mathcal{F}(\beta)$  is monotone non-decreasing and continuous. For the square lattice,  $\mathcal{F}(-\log \sqrt{2}) = \log 4$  and we have argued that  $\mathcal{F}(\beta)$  is singular at  $\beta = \beta_c = -\log \sqrt{2}$  (Flesia *et al* 1992). (A corresponding singularity is thought to exist for the simple cubic lattice.) In addition we can show that  $\mathcal{F}(\beta) \geq 4C/\pi$ , where  $\mathcal{C}$  is Catalan's constant, so that the free energy is bounded away from zero, but we have not rigorously ruled out the possibility that  $\mathcal{F}(\beta)$  is a constant for  $\beta \leq -\log \sqrt{2}$ . However, we have estimated the value of  $\mathcal{F}(\beta)$ , by a ratio analysis of exact enumeration data, and find  $\mathcal{F}(-0.5) = 1.29 \pm 0.04$  and  $\mathcal{F}(-0.7) = 1.19 \pm 0.06$ . These results strongly suggest that  $\mathcal{F}(\beta) < \log 4$  when  $\beta < -\log \sqrt{2}$ , and hence that the qualitative behaviour for this model is also different from that of the disc model.

In summary, we have discussed the relationship of the disc model to the solvent models for strongly and weakly embeddable animals. We have shown that the strongly

embeddable case is qualitatively different from the disc model in the compact regime and we have argued that this is probably also the case for weakly embeddable animals. The disc model is of interest in its own right but its behaviour may not be indicative of the behaviour of other models of the collapse transition in branched polymers.

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