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Critical behavior of two-dimensional vesicles in the deflated regime

Jayanth R. Banavar and Amos Maritan*
Department of Physics and Materials Research Laboratory, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802

Attilio Stella
Dipartimento di Fisica, Universita di Bologna, I-40126 Bologna, Italy and Centro Interuniversitario Struttura della Materia, Universita di Padova, Padova 35131, Italy
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The critical behavior of two-dimensional vesicles in the deflated regime is studied analytically using a mapping onto a gauge model, scaling arguments, and exact inequalities. In agreement with the results of earlier studies the critical behavior is governed by a branched-polymer fixed point. The shape of the critical line in the gauge model is deduced in the weak and in the infinitely deflated regime.

Recently there has been considerable interest in understanding the behavior of vesicles[1] as a prototype of more general systems such as interfaces, membranes, and random surfaces.[2] Real vesicles, e.g., red blood cells, exhibit a variety of well-defined but fluctuating shapes.[3] Using an arsenal of techniques (including Monte Carlo simulation, series expansions, and scaling analysis), Leibler, Fisher, and co-workers[1] have carried out detailed studies of two-dimensional (2D) vesicles with a fixed number of monomers forming a closed, planar, self-avoiding walk. Even in two dimensions the behavior is very rich, characterized by continuously variable fractal shapes, several universality classes, including self-avoiding walk (SAW) and branched polymers (BP), and novel dynamical phenomena such as flicker. An internal pressure increment Δp acts on the vesicle controlling the internal area of the vesicle. When $\Delta p > 0$, the vesicle becomes circular. Our focus is on the deflated regime ($\Delta p < 0$), where numerical simulations have suggested that the vesicles collapse to form a branched polymer. Very few, if any, analytic results are available in this regime.

We work in the grand canonical ensemble on a square lattice with lattice spacing a. (We expect that our results are independent of the lattice structure.) The generating function is given by

$$G(K,W) = \sum_{S:\, O \in \partial S} K^{|\partial S|} W^{|S|}, \qquad (1)$$

where the sum is over the set of 2D vesicles (self-avoiding rings) with the constraint that the origin be one of the boundary sites. Each vesicle S has an area $|S|$ (the number of elementary plaquettes enclosed) and a self-avoiding perimeter $|\partial S|$ in units of a (the number of monomers). K and W are fugacities associated with the perimeter length and the enclosed area, respectively. In the notation of Leibler, Fisher, and co-workers, $W = e^{\bar{p}}$ ($\bar{p} = \Delta p a^2 / k_B T$). Our results are best explained in the context of Fig. 1. $W = 1$ corresponds to the well-understood case of a pure SAW. We focus on $W < 1$ corresponding to the deflated regime [when $W > 1$, $G(K,W)$ is divergent for $K > 0$]. We find that (a) the pure SAW fixed point is unstable when $W < 1$. The two eigenvalues (critical exponents) are $\frac{4}{3}$ and 2; (b) the shape of the critical line close to $W = 1$ is given by $K_c(W) - K_c(W=1) \sim (1 - W)^{2/3}$. Further, for $W = 1$, we recover the Duplantier[4] result that the average area is proportional to the square of the radius of gyration of the perimeter; (c) based on a scaling analysis, we find that for $W < 1$ the average area is proportional to the average perimeter; (d) in the $W \to 0$ limit, the critical line $K_c(W) \sim W^{-1/2}$; (e) in this limit, the average area is equal to one-half the average perimeter; and (f) in the notation of Ref. 1, the values of the exponents are $\nu = \nu_A = \frac{3}{4}$, $\phi = 2$, $\nu_A^- = \frac{1}{2}$, and $\tau = \frac{1}{3}$. All these agree with the results of computer simulations and the physical arguments presented in Ref. 1.

Results (a), (d), and (e) are exact, while (b) and (c) are based on highly plausible and standard scaling assumptions. Result (a) is derived by constructing an Ising gauge model interacting with $O(n)$ fields whose free energy (in the $n \to 0$ limit) is related to $G(K,W)$ in Eq. (1)

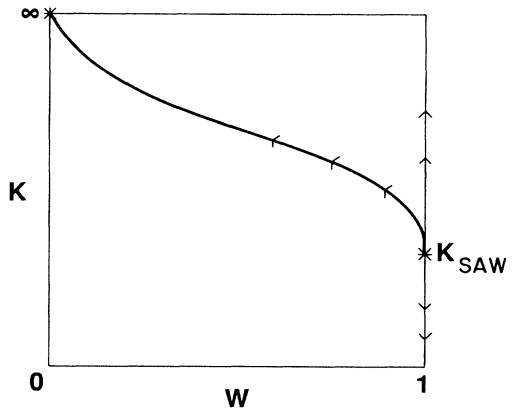

FIG. 1. Schematic phase diagram in the (K,W) plane. The asterisk indicates fixed points, the arrows show the renormalization-group flows, and the critical line separates regions where the generating function $G(K,W)$ is finite and infinite.

and carrying out a renormalization-group analysis on it. Results (d) and (e) are derived using rigorous inequalities. Result (a) shows that for $W \lesssim 1$, the critical behavior is different from that of the pure SAW. Results (c) and (e) suggest that the critical behavior for all $W < 1$ is the same and is governed by the $W \to 0$ fixed point. We find that in this limiting case, the configurations are rings with no internal points. On the dual lattice this corresponds to branched polymers with no loops, with the exclusion of those configurations which violate the self-avoidance of the vesicle perimeter and the internal point constraint in the direct lattice. These exclusions operate in the small length scale limit and most likely lead to the fixed point at $W=0$ being a standard BP fixed point. In the simplest scenario, therefore, the critical behavior for all $W < 1$ is governed by a BP fixed point.

We now proceed to a brief description of how our results were obtained. Consider a reduced Hamiltonian

$$H = K \sum_{\langle i,j \rangle} \sigma_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + u \sum_{[i,j,k,l]} \sigma_{ij}\sigma_{jk}\sigma_{kl}\sigma_{li} , \tag{2}$$

where $\langle i,j \rangle$ denotes nearest-neighbor sites, $[i,j,k,l]$ refers to a plaquette with vertices i, j, k, and l, $\sigma_{ij} = \pm 1$, and $\mathbf{S}_i$ is an n-component vector having a modulus $\sqrt{n}$. The Hamiltonian equation (2) is invariant under local gauge transformations $\mathbf{S}_i \to \epsilon_i \mathbf{S}_i$, $\sigma_{ij} = \epsilon_i \sigma_{ij} \epsilon_j$ with $\epsilon_i = \pm 1$. Following de Gennes,[5] we are interested in the $n \to 0$ limit. As $u \to \infty$, the second term in Eq. (2) is maximized by the choice $\sigma_{ij} = 1$, modulo a gauge transformation. In this limit we recover the pure SAW. The partition function of Eq. (2) can be obtained by first tracing over the $\mathbf{S}_i$'s and then over the σ_{ij}'s. The former is analogous to the earlier work of de Gennes and leads to closed loops denoted by Γ, except that we have an additional contribution $\prod_{\langle i,j \rangle \in \Gamma} \times \sigma_{ij}$. The trace over σ_{ij} is carried out, following Kadanoff,[6] and leads to the following result:

$$Z(K,W) = (2\cosh u)^V \times \left[1 + nVK^2 + n \sum_S K^{|\partial S|} W^{|S|} + O(n^2) \right] , \tag{3}$$

where $W = \tanh u$, V is the total number of lattice sites, and the $\sum_S$ denotes a sum over all vesicles without any restriction as to the location of the origin. The first term on the right-hand side is the partition function of the pure gauge model, whereas the nVK^2 term arises due to trivial loops formed by a bond of the lattice being traversed twice. We note that for any translationally invariant $f(S)$, $\sum_S f(S) = V \sum_{S:\, O \in \partial S} f(S)/|\partial S|$. It follows that

$$\lim_{n \to 0} K \frac{\partial}{\partial K} \frac{\ln Z(K,W)}{nV} = 2K^2 + G(K,W) , \tag{4}$$

and the singularity structure for Eqs. (1) and (2) are the same. This equivalence allows us to glean information about Eq. (1) by carrying out a renormalization-group analysis of Eq. (2). We envisage carrying out a decimation of the gauge variables[6] and an unspecified renormalization-group scheme on the spin variables. The renormalization of u coming from the O(n)-invariant part of the Hamiltonian involves closed loops of $\mathbf{S}_i$ and is of order n and vanishes in the $n \to 0$ limit. The u renormalization arises entirely from the decimation of the gauge variables and for a rescaling factor, b is[6]

$$W' = W^{b^2} . \tag{5}$$

In the $W \leq 1$ regime, there are two fixed points of W, $W^* = 1$ and $W^* = 0$. The former case includes the pure SAW with a critical value K_c and critical exponents $1/\nu_{\mathrm{SAW}} = y_1 = \frac{4}{3}$ (following from the exact result of Nienhuis[7]) and $y_2 = 2$ [following from Eq. (5)]. The critical line $K_c(W)$ is defined as the value of K which separates finite and infinite values of G. The shape of $K_c(W)$ in the $W \to 1-$ limit is readily shown, using standard crossover scaling assumptions, to be (Fig. 1)

$$\Delta K_c = K_c(W) - K_c(W=1) \sim (1-W)^{y_1/y_2} . \tag{6}$$

In order to define averages in the grand canonical ensemble that coincides with the microcanonical averages, we work with $\tilde{G}(K,W)$, obtained by taking a sufficient number of derivatives of $G(K,W)$ with respect to K (or W) so that $\tilde{G} \sim \Delta K^{-\psi}$ [$\psi > 0$; $\Delta K = K_c(W) - K$]; if this is valid for $\Delta K \ll \Delta K_c$, then the average area and average perimeter are

$$\langle |S| \rangle \cong W \left| \frac{dK_c}{dW} \right| \Delta K^{-1} , \quad \langle |\partial S| \rangle \cong \Delta K^{-1} , \tag{7}$$

respectively. Since there are only two fixed points of W, $W^* = 0$ and $W^* = 1$, the critical line $K_c(W)$ is analytic in the $0 < W < 1$ regime. Thus, the average perimeter is proportional to the average area. This simple relationship has also been observed in computer simulations.

We now focus on the crossover scaling form of the average area near $W^* = 1$ (the pure SAW):

$$\langle |S| \rangle \sim \Delta K^{-2x} F(Z) , \tag{8}$$

where $Z = (1-W)\Delta K^{-y_2/y_1}$. As $W \to 1$, $Z \to 0$ and $F \to$ const so that the W dependence disappears as it must for the pure SAW. As $Z \to \infty$ [for a fixed $W \lesssim 1$, this happens when (K,W) is much closer to the critical line $(K_c(W),W)$ than to the SAW critical point $(K_c(1),1)$], $F(Z) \to Z^{(y_1 - y_2)/y_2}$ so that Eq. (7) is recovered.

Further, this fixes the exponent x to be equal to $1/y_1 = \mu_{\mathrm{SAW}}$. This result has been noted by Leibler, Fisher, and co-workers[1] and has been derived by Duplantier.[4]

From topological consideration, any self-avoiding ring on a square lattice satisfies the equality $|S| = -1 + |\partial S|/2 + N_i$, where N_i is the number of internal points (inside the vesicle, but not at the boundary). We derive two inequalities for $G(K,W)$ from this equation, as follows:

(i) Since $N_i \geq 0$, $|\partial S|/2 - 1 \leq |S|$. Substituting into Eq. (1), $G(K,W) \leq W^{-1} G(KW^{1/2},1)$. The right-hand side is the generating function of a pure SAW and diverges for $KW^{1/2} > K_{\mathrm{SAW}} \equiv K_c$ ($W=1$). This implies that $K_c(W) > K_{\mathrm{SAW}}/W^{1/2}$.

(ii) A lower bound for $G(K,W)$ may be obtained by restricting the statistical sum in Eq. (1) to ring configurations without any internal sites ($|S| = -1 + |\partial S|/2$).

Then

$$G(K,W) \geq \sum_{\substack{S \in \mathrm{BP} \\ O \in \partial S}} K^{2|S|+2} W^{|S|},$$

where BP refers to the above-mentioned ring configurations. Using standard methods,[8] one can show that the right-hand side diverges at a critical value of $K^2W \equiv K_{\mathrm{BP}}$. Thus, $K_c(W) < (K_{\mathrm{BP}}/W)^{1/2}$.

In the limit of $W \to 0$, $K_c(W) \sim 1/W^{1/2}$, and the critical behavior is dominated by the BP configurations. The $S \in \mathrm{BP}$ are sums over branched-polymer configurations on the dual lattice with some short-range restrictions related to the self-avoidance of the perimeter and the absence of internal sites. These differences are expected to be irrelevant in determining the critical behavior. The same analysis on a hexagonal and triangular lattices gives qualitatively similar results. $K_c(W) \sim W^{-1/4}$ for the hexagonal lattice, whereas $K_c(W) \sim W^{-1}$ for the triangular case in the $W \to 0$ limit. The proportionality constant between the area and the perimeter is $\frac{1}{2}$, $\frac{1}{4}$, and 1 for the square, hexagonal, and triangular lattices in the $W \to 0$ limit. The behavior of the critical line near $W = 1$ is identical for all the lattices.

Interesting effects have been observed in Monte Carlo simulations[1] in the deflated regime on adding an energy cost due to curvature and its effect on the branched-polymer behavior. A modification of Eq. (2) may be used as a Hamiltonian for this problem. However, the problem has proved to be intractable, thus far. The SAW fixed point is stable against curvature effects. A likely scenario is that the BP fixed point is also stable on adding a curvature energy. However, should the BP fixed point be unstable, entropic considerations suggest that the resulting configurations are at least as crumpled as the SAW. It is straightforward to generalize Eq. (1) to higher dimensions where the sum is now over self-avoiding rings and for each ring, we sum over all self-avoiding surfaces spanning the ring. Studies of the corresponding gauge model are underway.

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