Phase Structure of Systems of Self-Avoiding Surfaces

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Models of self-avoiding random surfaces with chemical potentials for topological quantities in three and four dimensions are investigated by Monte Carlo methods. We explore the phase diagrams and find first- and second-order transition lines and triple points.

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In a recent paper[1] we investigated the thermodynamical behavior of self-avoiding random loops by Monte Carlo simulations. In this Letter we report on the self-avoiding random-surface problem. Random surfaces are a useful concept in different regions of physics. An analog of Symanzik's polymer description of quantum field theories[2] is the random-surface formulation of gauge theory (see Fröhlich[3] and references therein). The string quantization problem has been formulated as summation over random surfaces.[4] Moreover, there are possible applications[5] of random surfaces to the physics of microemulsions whose stability relies on a balance of entropy and energy of the interfaces (see de Gennes and Taupin[6] and references therein). For previous Monte Carlo simulations of random surfaces, see Ref. 7.

We consider systems of self-avoiding random surfaces in three and four dimensions on simple cubic lattices of size L with periodic boundary conditions. A configuration $c \in \mathcal{C}$ of closed self-avoiding surfaces comprises a collection of plaquettes in the lattice such that each link in c is contained in two plaquettes. Thus the surfaces may not intersect at a common link, but two (locally) distinct surfaces are allowed to touch at a vertex. The latter fact turns out to be crucial for the existence of a "droplet phase" as will be discussed below. We shall refer to such common points as "contact points."

The Euler characteristic of a configuration c of surfaces reads, in terms of the numbers of occupied sites, links, and plaquettes,

$$\chi(c) = n_{\text{sites}} - n_{\text{links}} + n_{\text{plaq}}, \tag{1}$$

where for closed self-avoiding surfaces $n_{\text{links}} = 2n_{\text{plaq}}$.

A configuration can be generated iteratively as follows. Starting from an old configuration we get a new one by a local change in a unit three-dimensional cube under the condition that the new one is allowed. A local change means the replacement of empty plaquettes by occupied ones and vice versa (i.e., Sterling and Greensite's "change-a-cube" operation[7]).

By a Monte Carlo simulation we generate samples of equilibrium ensembles of configurations c_i. In our heat-bath updating procedure we sequentially sweep all ($\frac{d}{3}$) L^d unit cubes and accept the new configuration with probability

$$w_{\text{new}}/(w_{\text{old}} + w_{\text{new}}), \tag{2}$$

where the w's are the Boltzmann factors

$$w = \exp(-\text{energy}/kT). \tag{3}$$

The thermal average of a variable A is then approximated by

$$\langle A \rangle \approx \frac{1}{N} \sum_{i=1}^{N} A(c_i). \tag{4}$$

In the following we discuss three variants of models of self-avoiding random surfaces. They are related by slight modifications of the corresponding partition functions. The first simple model that we consider is defined by

$$Z_1(\beta) = \sum_{c \in \mathcal{C}} \exp[-\beta s(c)], \tag{5}$$

where the energy of a configuration c is taken to be proportional to the total surface, $s(c)$ is the number of plaquettes, and $\beta = \epsilon/kT$ with ϵ the energy of one plaquette. Note that this model would be equivalent to the Z_2 lattice gauge model if the self-avoidance condition were not imposed.

In general a phase transition of a system shows up in a singularity of the free-energy density $-kT \ln Z\, L^{-d}$ in the thermodynamic limit $L \to \infty$. We investigate this in terms of several observables as a function of the inverse temperature β. The average energy should be discontinuous,

$$E_{\pm} = E(\beta_{\text{tr}} \pm \epsilon), \quad E_+ < E_-, \tag{6}$$

at a first-order transition point β_{tr} and vary like

$$\langle E \rangle \approx E_{\text{tr}} + \text{const} \times (\beta - \beta_{\text{tr}})^{1-\alpha} \tag{7}$$

at a second-order one. On finite lattices these behaviors are smeared out by finite-size effects. Therefore it is hard to decide whether an observed rapid decrease of $\langle E \rangle$ as a function of β signals a phase transition of first, second, or higher order, or no transition at all. That is why we employed some more refined methods (see, e.g., Creutz, Jacobs, and Rebbi[8]) to investigate phase transitions (thermal cycles; cold, hot, or mixed starts; different lattice sizes). Figure 1

shows the average energy $\langle s \rangle$ and Euler characteristic $\langle \chi \rangle$ obtained in a "β cycle" by a typical Monte Carlo simulation on a lattice in three dimensions. They show evidence of a second-order phase transition at $\beta_{tr} = 0.36$. This result is supported by many additional Monte Carlo runs for different lattice size. Intuitively the critical behavior of this self-avoiding surface gas can be understood in a manner analogous to the case of self-avoiding loops, which we investigate in Ref. 1. We observe that $\langle \chi \rangle$ is positive in the low-temperature phase $\beta > \beta_{tr}$; therefore, a typical configuration consists predominantly of relatively small, separated components. In the region of the transition temperature large surfaces appear and long-range fluctuations generate critical behavior—a second-order phase transition. In the high-temperature phase $\langle \chi \rangle$ is negative and a typical configuration consists of a single connected object with many handles similar to a sponge. Note that the average Euler characteristic vanishes at the critical temperature,

$$\langle \chi \rangle = 0 \quad \text{for } \beta = \beta_{tr}, \tag{8}$$

i.e., the mean curvature vanishes. This flatness might be related to scale invariance.

The corresponding measurements in four dimensions show markedly different results. We find hysteresis loops in the β cycles of both the energy and the Euler characteristic (cf. Fig. 2) indicating a first-order phase transition at $\beta_{tr} = 0.68$ with an energy jump $\Delta s\, L^{-d} = 0.45$. The occurrence of a first-order transition contrasts with the loop-gas case, where we observed a second-order phase transition both in two and three dimensions. This might be due to topological effects, the formation of handles in the "sponge phase." On the other hand, the observed different types of transitions are in agreement with those of Z_2 lattice gauge theories in three and four dimensions.[9]

Apparently the handles (more precisely $-\chi$, the negative of the Euler characteristic) drive the phase transition, as similarly the monopoles do for the U(1) lattice gauge model.[10] It is therefore suggestive to introduce a "chemical potential" for $-\chi$, and to consider a second model defined by the partition function

$$Z_{II}(\beta, \mu) = \sum_{c \in \mathcal{C}} \exp[-\beta s(c) + \mu \chi(c)]. \tag{9}$$

Now positive (negative) μ will enhance (suppress) the Euler characteristic, and we expect the transition temperature β_{tr} to become a function of the parameter μ. For the Monte Carlo simulation the Boltzmann factors [Eq. (3)] have to be modified appropriately. The results of a series of Monte Carlo runs are collected in Fig. 3 for three and four dimensions. Also, in three dimensions, the vanishing of the Euler characteristic at the critical temperature [cf. Eq. (8)] holds true for all values of μ. Let us remark that model II might also be interesting from the quantum field theory point of view, since for small N the U(N) lattice gauge model's partition function is approximately given by (cf. Maritan and Omero,[11] and Durhuus, Fröhlich, and Jonsson[11])

$$Z \approx \sum_{c \in \mathcal{C}} \left(\frac{N}{g^2} \right)^s N^{\chi}.$$

Another topological quantity which is intrinsic and locally computable can be expressed in terms of the numbers of connected components n_{comp} and handles

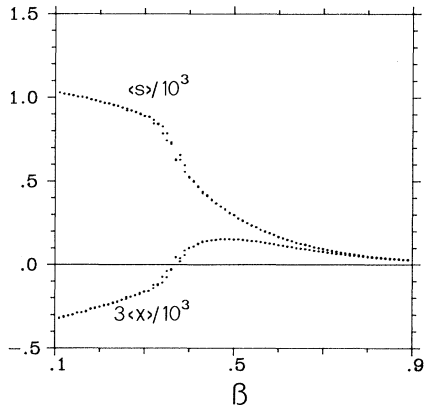

FIG. 1. Monte Carlo results for model I on a 10^3 lattice obtained in a β cycle. The average surface $\langle s \rangle$ and Euler characteristic $\langle \chi \rangle$ values are taken over 500 configurations, each obtained after three complete sweeps through the lattice. The rapid decrease of $\langle s \rangle$ but absence of a hysteresis loop show evidence for a second-order phase transition at $\beta_{tr} = 0.36$. For low temperatures $\langle s \rangle \approx 3\langle \chi \rangle$, since per unit cube $s = 6$ and $\chi = 2$.

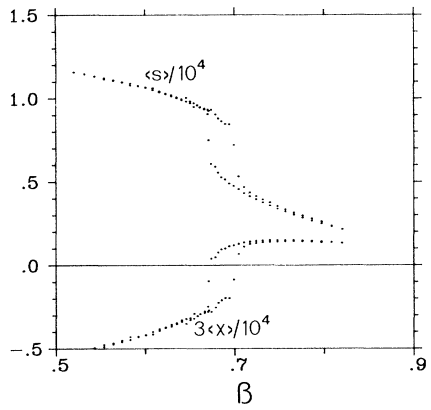

FIG. 2. Monte Carlo results for model I on a 10^4 lattice obtained in a β cycle. The average values for $\langle s \rangle$ and $\langle \chi \rangle$ are taken over 1000 configurations. The hysteresis loops are interpreted to result from relaxations and show evidence for a first-order phase transition at $\beta_{tr} = 0.68$ and a latent heat of $\Delta s/10^4 = 0.45$.

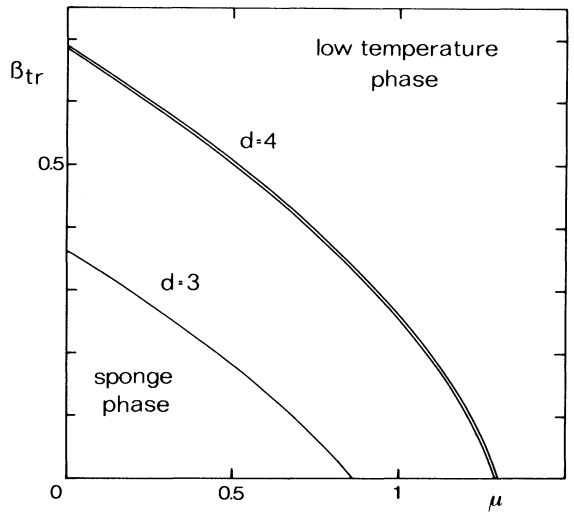

FIG. 3. Phase diagram for model II in three and four dimensions showing the transition lines which separate the low-temperature phase from the disordered sponge phase. We observe second-order transitions in three dimensions and first-order transitions (double lines) in four dimensions.

n_{hand} for closed self-avoiding surfaces,

$$\psi = 2(n_{\text{comp}} - n_{\text{hand}}). \tag{10}$$

For "strictly self-avoiding" surfaces, i.e., without contact points, ψ is equal to the Euler characteristic χ. But if contact points are permitted, the following relation holds:

$$\psi = \chi + n_{\text{contact points}}, \tag{11}$$

since surfaces which touch at a contact point are considered not to be connected at this point. Therefore ψ is the natural quantity for our self-avoiding surfaces and we consider a third model with new interesting features,

$$Z_{\text{III}}(\beta,\lambda) = \sum_{c \in \mathcal{C}} \exp[-\beta s(c) + \lambda \psi(c)]. \tag{12}$$

Since the average number of contact points will be small for small λ, we expect model III not to deviate substantially from model II in that regime. For positive increasing λ, however, there will be a further enhancement of contact points. Therefore, we expect in three dimensions for large λ the existence of a new ground state consisting of simple cubes (or "droplets"), each touching eight others at its corners. This is the dense packing of self-avoiding (along edges) closed surfaces. In our Monte Carlo simulations we indeed observe this droplet phase which is separated from the other two phases by a line of first-order transitions, as shown in the diagrams of Figs. 4(a) and 4(b) for three and four dimensions, respectively. The triple points are found to be approximately at

$$\begin{aligned} (\beta,\lambda)_{\text{trip}} &= (0.00, 0.75) \quad \text{for} \quad d=3, \\ (\beta,\lambda)_{\text{trip}} &= (0.27, 0.80) \quad \text{for} \quad d=4. \end{aligned} \tag{13}$$

It is instructive to see three phases showing up in Monte Carlo simulations for a "λ cycle" with β slightly above β_{trip}. Figure 5 presents $\langle s \rangle$ and $\langle \chi \rangle$ for a measurement in four dimensions along the dashed line in Fig. 4(b).

We would like to point out that in our simulations

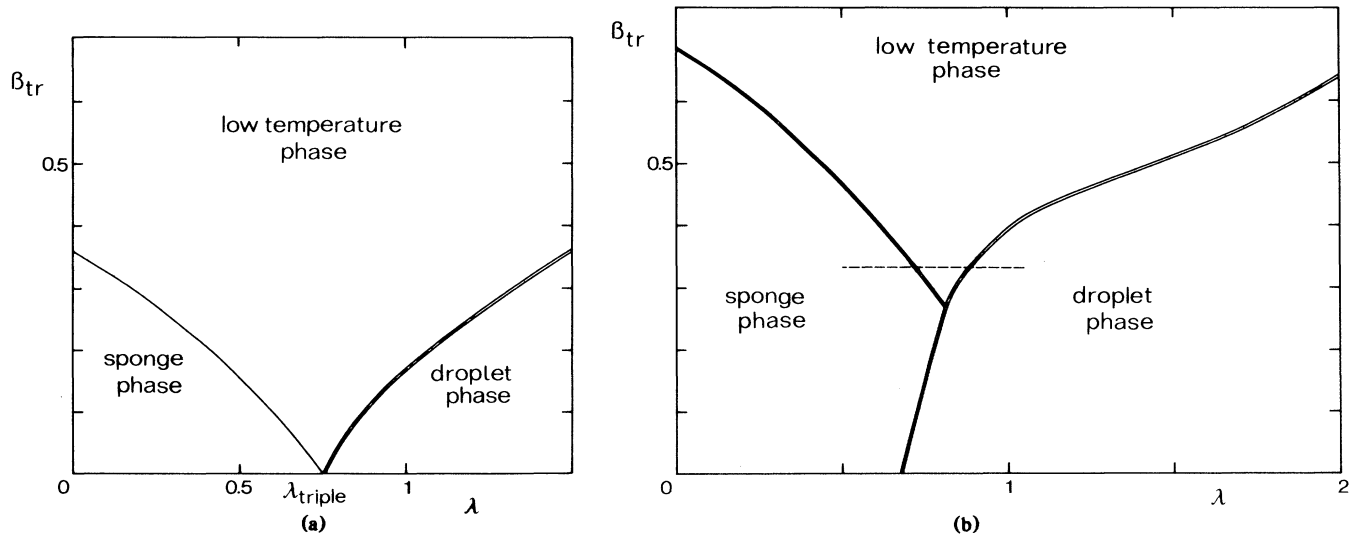

FIG. 4. Phase diagram for model III in (a) three and (b) four dimensions showing three phases, transition lines, and the triple points.

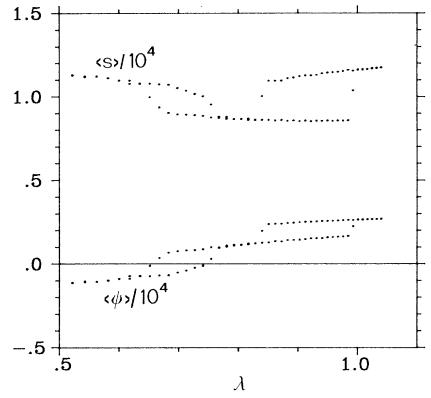

FIG. 5. Monte Carlo results for model III in four dimensions. The average surface $\langle s\rangle$ and $\langle\psi\rangle = 2\langle n_{\rm comp} - n_{\rm hand}\rangle$ were obtained at $\beta = 0.33$ in a λ cycle along the dashed line in Fig. 4(b) through all three phases. The hysteresis loops correspond to the two first-order transitions: sponge → low-temperature → droplet phase.

the existence of the third antiferromagneticlike phase (droplet phase) does not depend on an additional attractive force as was introduced, e.g., by Sterling and Greensite,[7] but it is sort of a hard-core effect. It is generated essentially by the self-avoidance requirement of the surfaces which for large λ and β are almost exclusively unit cubes (with $s = 6$). In fact, we may rewrite the partition function as

$$Z_{\rm III} = \sum_{c \in \mathscr{C}} \exp(-\sigma n_{\rm comp} - \beta s' - 2\lambda n_{\rm hand}), \qquad (14)$$

where $s' = s - 6n_{\rm comp}$ and $\sigma = 6\beta - 2\lambda$. For large λ and β and $\sigma = {\rm const}$, s' and $n_{\rm hand}$ will be suppressed, and we can approximate

$$Z_{\rm III} \simeq \sum_{c \in \mathscr{C}} \exp(-\sigma n_{\rm comp}). \qquad (15)$$

Thus that part of the corresponding transition line should approximately be given by $\sigma_{\rm tr} = 6\beta_{\rm tr} - 2\lambda_{\rm tr} \approx {\rm const}$, which is in good agreement with our Monte Carlo results, where we find

$$\sigma_{\rm tr} = -0.05. \qquad (16)$$

In the case of self-avoiding closed surfaces in three dimensions, there exists a natural order parameter

$$m = (V_{\rm in} - V_{\rm ex})/(V_{\rm in} + V_{\rm ex}), \qquad (17)$$

since the surfaces can be thought to divide the whole lattice into "interior" and "exterior" parts, $V_{\rm in}$ and $V_{\rm ex}$, respectively. It vanishes at the critical temperature like

$$m \sim (T_c - T)^{\beta}, \qquad (18)$$

and is identically zero in the sponge phase. The latter phase is invariant under the exchange interior ⟷ exterior, whereas this symmetry is spontaneously broken in the other phases. We have determined the critical exponents (α, β, etc.), which will be reported elsewhere.[12]

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