Self-Avoiding Surfaces, Topology, and Lattice Animals

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With Monte Carlo simulation we study closed self-avoiding surfaces (SAS) of arbitrary genus on a cubic lattice. The gyration radius and entropic exponents are $\nu = 0.506 \pm 0.005$ and $\theta = 1.50 \pm 0.06$, respectively. Thus, SAS behave like lattice animals (LA) or branched polymers at criticality. This result, contradicting previous conjectures, is due to a mechanism of geometrical redundancy, which is tested by exact renormalization on a hierarchical vesicle model. By mapping SAS into restricted interacting site LA, we conjecture $\nu_\Theta = \frac{1}{2}$, $\phi_\Theta = 1$, and $\theta_\Theta = \frac{3}{2}$ at the LA theta point.

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The importance of random surfaces is well established in many areas of condensed matter and high-energy physics. These fields range from cell biophysics [1] to string [2] and lattice gauge theories [3]. In this Letter we consider a much-studied [4] model of lattice self-avoiding surfaces (SAS), which also bears interestingly on the physics of vesicles (close membranes like red blood cells) [5]. SAS are constructed by gluing together plaquettes of a cubic lattice; they are closed and do not self-intersect: Every lattice edge belongs to either zero or two plaquettes. Plaquette overlaps are forbidden; i.e., each lattice plaquette enters the SAS only once. While vertex overlaps are allowed, they are not real connections, and the corresponding vertex is counted twice in computing the topological characteristic χ, given by the number of plaquettes plus vertices minus edges. The number of handles, H, is related to χ by $\chi = 2 - 2H$.

A major issue in SAS statistics is identifying what determines the universality class of critical behavior when, like in vesicle models, suitable fugacities K and e^p (p is an osmotic pressure, see below) control average area and enclosed volume, respectively. Topological properties connected to the intrinsic geometry of surfaces, like χ, are prime candidates. SAS with H restricted to be zero are now known [6] to behave like branched polymers (BP), in that thin ramified tubular configurations dominate the asymptotic limit.

Recent arguments [7] proposed that, at $p=0$ ("flaccid" vesicle regime), SAS with arbitrary fluctuating H should belong to a class different from that of the above SAS constrained to be homeomorphic to the sphere ($H=0$): The vesicles should suddenly either inflate or condense, changing fractal properties drastically as soon as the constraint is released [8]. Such behavior is inconsistent with analogies to lattice animals (LA), i.e., polymers without the BP constraint forbidding cycles. Presuming handles are formed by thin tubules, analogous to LA cycles, the dense character of SAS corresponds to behavior found in cycle LA only when a cycle-enhancing fugacity exceeds the theta threshold [9]. Indeed, we shall show that in $d=3$ SAS do conform to the analogy with cycle LA uninfluenced by such fugacity; the argument in Ref. [7] fails because of the vanishing of a scaling amplitude, the analog of which is nonzero in $d=2$. In this Letter we further clarify the relationship between LA and SAS in $d=3$ and find the dependence of the critical exponents on H for ensembles with a constrained number of handles. We also find an exact mapping from a version of our SAS model to an interacting site LA problem. Hence, a recent argument for the Θ-point exponents of $d=2$ LA [10] can be extended to $d=3$.

Consider first the following generating function (model 1):

$$G(K,p) \propto \sum_S |S|^m K^{|S|} e^{pV(S)}, \tag{1}$$

where the sum is over surfaces, S, with unrestricted H, area $|S|$, and enclosed volume $V(S)$, and m is chosen big enough (e.g., $m=2$) to ensure critical divergence of G and of grand-canonical averages of interest. G is implicitly normalized to be a quantity per lattice site. Here p is the internal minus the external pressure over $k_B T$. For $p \le 0$, one expects singular behaviors of the form

$$G(K,p) \underset{K \to K_c(p)^-}{\sim} [K_c(p) - K]^{\theta - m - 1} \tag{2}$$

and

$$\langle R \rangle_{K,p} = \frac{\sum_S |S|^m K^{|S|} e^{pV(S)} R(S)}{G} \underset{K \to K_c(p)^-}{\sim} [K_c(p) - K]^{-\nu}, \tag{3}$$

for the average grand-canonical radius. In Eq. (3) $R(S)$ represents the radius of gyration with respect to the center of mass of S.

We determined θ and ν using a novel Monte Carlo (MC) strategy based on an oct-tree data structure. Its predecessor [6] was designed for the case of vesicles with $H=0$. With the present code, we can test cases having either an unrestricted or a restricted number of handles.

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Genus is monitored by local checks on the oct-tree after each MC step (MCS). The trial move adds or removes a cube with at least one face in S. Any genus-changing move can disconnect the surface, even one *adding* a cube: "Corking" a bottle disconnects its inner and outer surfaces. Connectivity is a global property: To see if such a step is allowed, we must check the whole surface in our code by traversing the *graph* defined by the plaquettes. Steps with a connectivity check require time $O(|S|)$ vs $O(1)$ for ordinary steps. Hence, instead of the previous $O(k)$ running time for a calculation of k MCS on a surface with $H=0$, the general case requires much longer time $O(k\langle|S|\rangle \mathrm{Prob}(\Delta H \neq 0))$.

Model 2 generalizes model 1 by allowing edge overlaps, with appropriate double counting. (Vertices can then count up to 4 times in computing χ.) The corresponding G in Eq. (1) acquires an important new physical meaning: It is directly related to the generating function of site LA interacting at each edge joining occupied sites. To verify this assertion, one can place an animal site at the center of each elementary cube enclosed by S. Denoting the number of sites by $n=V$ and the number of edges connecting nearest-neighbor sites by l, we have $6n=2l+|S|$ and can write

$$\overline{G} \propto \sum_S K^{|S|} e^{pV(S)} = \sum_S K^{6n-2l} e^{pn} \equiv \sum_{\text{animals}} \lambda^n \mu^l \tag{4}$$

with $\lambda = e^p K^6$ and $\mu = K^{-2}$ representing the site fugacity and edge Boltzmann factors, respectively. $\overline{G}$ embodies a model of site LA, which is expected to display Θ-point collapse [9]. This particular LA model forbids surface disconnections, i.e., internal hollows. This computationally important restriction should leave universal properties unchanged; e.g., holes appear irrelevant for $d=2$ LA at the Θ point [10]. Since $G=(K\partial/\partial K)^m \overline{G}$, $\overline{G}$ and G must have the same singularity structure: The LA and the vesicle problems must have the same critical singularities.

G and $\overline{G}$ are not defined once $p>0$. If $K_c(0)>0$, then one expects the line segment with $p=0$ and $K \le K_c(0)$ to constitute a locus of droplet (first-order) singularities for the problem [11] (cf. Fig. 1). We focus below on the critical behavior for $p=0$ as $K \to K_c(0)^-$, and the crossover from this regime to the deflated ($p<0$) one.

Proceeding as in Ref. [6], we obtained ν, the exponent for the radius of gyration, fitting both Eq. (3) and the canonical law

$$\langle R \rangle_N = \frac{\sum_{|S|=N} R(S)}{\sum_{|S|=N} 1} \underset{N\to\infty}{\sim} N^{\nu} \tag{5}$$

for both models 1 and 2. Data are displayed in the lower pair of log-log plots in Fig. 2. From either the canonical or grand-canonical fit, we obtained $\nu = 0.506 \pm 0.005$ for model 1. Model 2 converges to the asymptotic regime more slowly; a straightforward MC analysis gives $\nu = 0.48 \pm 0.01$. These values clearly suggest the accepted ν of $\frac{1}{2}$ for BP and LA in $d=3$ [12]. Further evidence that SAS with arbitrary χ (or H) belong to the universality class of LA comes from determinations of θ and $K_c(0)$. These quantities are best obtained from plots of $\langle|S|\rangle^{-1}$ vs K, noting

$$\langle|S|\rangle_{p=0,K} = K\frac{\partial \ln G}{\partial K} \underset{K\to K_c(0)^-}{\sim} K_c(0)\frac{m+1-\theta}{K_c(0)-K}. \tag{6}$$

Our result $\theta = 1.50 \pm 0.06$ for model 1 agrees fully with the value $\frac{3}{2}$ expected for BP and LA in $d=3$ [12]. The result for model 2, $\theta = 1.7 \pm 0.1$, again suffers from poor-

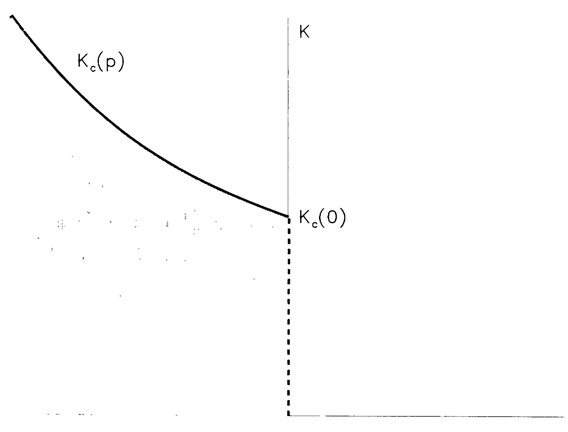

FIG. 1. Schematic plot of the K vs p phase diagram. Only in the shaded region is G convergent. $(K_c(0),0)$ maps into $(\mu_\Theta = 3.19, \lambda_\Theta = 0.03)$ of the LA problem. $K_c(p) - K_c(0) \propto |p|$ for small $p<0$, consistent with $\phi = \phi_\Theta = 1$. Along the dashed vertical segment $p=0$, $K \le K_c(0)$, there is a locus of droplet singularities.

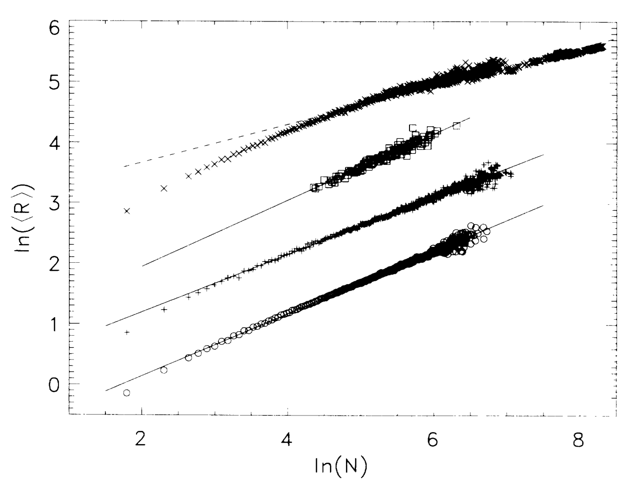

FIG. 2. Log-log plot of the canonical mean radius of gyration $\langle R \rangle_N$ vs N, at $p=0$. For model 1 (○), at $K=0.568$, and for model 2 (+), at $K=0.556$, displaced up by 1.0, the straight lines illustrate the fits given in the text. In contrast to these runs at $L=1.0$, the upper two sets of data are from runs at high handle fugacity $L=16.0$, for model 1 at $K=0.5615$. If the handle number is *fixed*, in the depicted case (□) at $H=2$, ν is still about $\frac{1}{2}$. (The data are displaced up by 2.0.) If H is *unrestricted* (×), ν appears to cross over to a value closer to $1/d$: The dashed line has a slope of 0.32. (These data are displaced up by 3.0.)

er convergence. $K_c(0)=0.577\pm0.004$ for model 1 is only slightly smaller than the corresponding critical coupling for SAS with $H=0$ (0.578 ± 0.005 [6]). This result is reminiscent of LA compared to BP. The critical fugacity of LA, which are allowed to have nonzero cyclomatic number (corresponding to $H\geq 0$ for SAS), is only slightly, but definitely, lower than that of BP [13]. For model 2, $K_c=0.560\pm0.004$.

We also estimated the asymptotic behavior of the volume-to-surface ratio $\langle V\rangle_N/N$, where $\langle V\rangle_N$ denotes the average volume enclosed by SAS with N plaquettes [as in Eq. (5), with V replacing R]. For example, for model 1 we find numerically that the ratio approaches a constant (~ 0.306) as $N\to\infty$. *This and the preceding results are inconsistent with expectations from Ref. [7]* where, for model 1, the existence was established of a relevant exponent $y=d=3$, associated with a scaling field $v\propto p$, to leading order, at the fixed point describing $p=0$ critical behavior. This exponent should control the crossover to the deflated regime. Specifically, simple scaling considerations lead to

$$\langle V\rangle_{p=0,K}\sim \left.\frac{\partial \ln G_S}{\delta p}\right|_{p=0}\underset{K\to K_c(0)^-}{\propto}\left.\frac{\partial \ln G_S}{\partial v}\right|_{u,\bar u\neq 0,v=0}[K_c(0)-K]^{-\phi}, \tag{7}$$

where G_S is the singular part of G, $\phi=y\nu$, and u is the corresponding scaling field. Here $\bar u=b^{1/\nu}u\propto b^{1/\nu}(K_c-K)$, where b is a length rescaling factor. Equation (7) means that the region enclosed by critical SAS should be "dense," i.e., have fractal dimension $\bar d=y=3$. Similar [14] and other methods [15] showed that $d=2$ self-avoiding rings (SAR) are in fact dense. From Eq. (7) and since $N\sim[K_c(0)-K]^{-1}$, we expect

$$\langle V\rangle_N/N\underset{N\to\infty}{\sim}N^{\phi-1}=N^{y\nu-1}.$$

In grand-canonical analyses of both models 1 and 2, $\langle V\rangle_N/N$ approaches a constant asymptotically, implying $\phi=1$ and, thence, $y=\nu^{-1}\simeq 2$, not 3.

The reason that SAS need not be dense is that the renormalization-group (RG) argument leading to $\phi=y\nu=3\nu$ fails if $\partial G_S/\partial v$ vanishes. The scaling term on the right-hand side of Eq. (7) then has zero amplitude, and the $y=3$ exponent does not influence critical behavior. This result again conforms with the picture that SAS with arbitrary H consist essentially of thin tubules, which aggregate to form LA. A scaling field $v\propto p$ should still be associated with the exact exponent $y=3$ [7]; only the assumption of a nonzero amplitude in Eq. (7) appears unwarranted in hindsight. When $\partial\ln G_S/\partial v|_{\bar u\neq 0,v=0}=0$, this derivative should be replaced in Eq. (7) by $\partial\ln G_S/\partial u|_{\bar u\neq 0,v=0}$ and y by $1/\nu$, yielding again $\phi=1$. This gives the dominant contribution to $\langle V\rangle$ if u and v are the only relevant scaling fields, since clearly u also depends on p. The vanishing amplitude in the leading singular behavior of $\langle V\rangle_N$ is particularly surprising since its analog for $d=2$ vesicles must be nonzero [14,15].

To gain insight into why $\partial G_S/\partial v$ might vanish, we studied by exact RG methods a vesicle model (a static ringlike one-tolerant trail) on a $d=2$ Sierpinski gasket [16,17]. As the attractive interaction (for double visits of sites) varies, the ring passes through a sequence of three critical regimes [16], including one in which the enclosed area is proportional to the perimeter and lacks the fractal dimension $\bar d$ of the underlying gasket (corresponding to $d=3$ in the SAS case). We verified that, while the linearized RG transformation at the corresponding fixed point has an exponent $y=\bar d$, the singular generating function does not depend on the corresponding scaling field; hence, $\bar d$ does not affect scaling behavior. Similar behavior occurs for our SAS, at least in model 1. For the other two regimes, in contrast, the vesicle is dense, and the dimension $y=\bar d$ also associated with the respective fixed points plays a role, reminiscent of SAR in $d=2$ [17]. Presumably such scaling-field independence occurs in geometrical critical phenomena whenever the scaling behavior can be explained by models which are in some sense stripped-down versions of the original one. Our SAS, once coarse grained, have the same scaling properties as LA, which are constructed, e.g., from lattice edges rather than plaquette tubules with finite cross sections. The dependence of various singular quantities on a field like v may well disappear in all regimes which show critical LA behavior. Thus, models 1 and, most likely, 2 exhibit what we call "geometrical redundancy" [18], leading to a decrease in the number of parameters on which the *singular* quantities directly depend. *Redundancy occurs in SAS but not SAR because ramified configurations dominate only for SAS. To assess in general when it occurs, one must know more about singular quantities than is available from linearized RG transformations.*

For LA the exponent θ depends on the cyclomatic number, c, in ensembles with a fixed number of cycles: Specifically, $\theta_c=\theta-c$ [19]. Moreover, once c is fixed, the critical edge fugacity assumes the value of the $c=0$ case [20]. To see if θ depends similarly on H for SAS, we performed extensive runs for model 1 at different K's, both with the restriction $H=1$ and $H=2$. In order to sample surfaces with $H>0$ more efficiently, we modified G by inserting in Eq. (1) a factor $L^{H(S)}$, with handle fugacity $L>1$ to enhance loop formation. With *H fixed* but arbitrary, ν does not change appreciably compared to the case of $L=1$ and unrestricted topology. Similar to LA, $K_c(0)$ is insensitive to H: For $H=1$ and $H=2$, $K_c(0)=0.578\pm0.006$ and $K_c(0)=0.579\pm0.008$, respectively, both very close to the $H=0$ value [6]. However, fits of Eq. (6) gave $\theta_{H=1}=-0.5\pm0.5$ and $\theta_{H=2}=-2.3\pm1.0$; in spite of the relatively large errors, these two results (and $\theta_{H=0}$ earlier) are clearly not consistent with the above relationship for LA with H simply replacing c.

This dependence of θ on H at $p=0$ seems to be the only peculiar effect of topology on SAS critical exponents.

On the other hand, the similarity with cycle LA suggests that, as L increases, the SAS should undergo a Θ collapse into a dense configuration. As shown in Fig. 2, at high L and *unrestricted* (fluctuating) H, ν appears to take on a value close to $1/d$. We are currently testing whether the transition still belongs to the Θ-point universality class of cycle LA in $d=3$, about which we can conversely learn more from our results for model 2 at $p=0$ and $L=1$: Starting with the mapping implied by Eq. (4), following arguments similar to those in Ref. [10], we find that the point $(K,p)=(K_c(0),0)$ is also multicritical for our LA problem. Moreover, since $(K<K_c(0),0)$ is a line of droplet singularities, we identify $(K_c(0),0)$ with the tricritical Θ point (cf. Fig. 1). The two scaling fields u and v, expressed now in terms of $\Delta\lambda$ and $\Delta\mu$, i.e., the deviations from the tricritical point, serve as the relevant fields of the Θ fixed point. Since we obviously expect $\bar{G}_S$ to be independent of v, like G_S, our results for model 2 suggest the conjecture $\nu_\Theta=\frac{1}{2}$ and $\phi_\Theta=1$ for our $d=3$ cycle LA. If singularities are controlled by u only, its dimension determines ν_Θ, and the crossover exponent ϕ_Θ must be unity, like ϕ above, with the critical fugacity $\lambda_c(\mu)$ varying linearly with $\Delta\mu$ near the Θ point (cf. Fig. 1). Hence, at the Θ point in $d=3$, our restricted LA should have the same exponent ν (viz. $\frac{1}{2}$) as these LA [21], as well as ordinary BP and LA [12], display in the swollen regime. Furthermore, MC analysis of $\langle V\rangle$ as a function of λ, for $\lambda\to\lambda_\Theta^-$ and $\mu=\mu_\Theta$, yields $\theta_\Theta=1.7\pm0.1$, fully consistent with the θ obtained for model 2 via Eq. (6). We expect both θ's to assume the LA value of $\frac{3}{2}$ [12]. Presuming internal hollows are irrelevant for universal properties, we conjecture that the Θ-point exponents have the same values for unrestricted cycle LA. Nonuniversal quantities like λ_Θ and μ_Θ will, of course, depend (weakly) on the restriction. From our mapping we deduce $\lambda_\Theta=0.031\pm0.002$ and $\mu_\Theta=3.19\pm0.05$. Numerical estimates of ϕ_Θ for unrestricted LA, even though disparate [22], are near our prediction.

In summary, we have shown here that closed SAS with arbitrary genus behave like LA at $p=0$, in spite of the presence of a scaling field with dimension $y=d=3$. Since the singular quantities turn out to be independent of this field, the interiors of SAS should not be dense. This redundancy mechanism should operate whenever the critical behavior of a geometrical object can be explained in terms of a model constituting a sort of shrunk version of the original one. Finally, we found, consistent with LA, evidence for collapse of SAS to a dense phase at high enough handle fugacity. We located the Θ point for a restricted cycle LA in $d=3$ and conjectured $\nu_\Theta=\frac{1}{2}$, $\phi_\Theta=1$, and $\theta_\Theta=\frac{3}{2}$, even for unrestricted LA.

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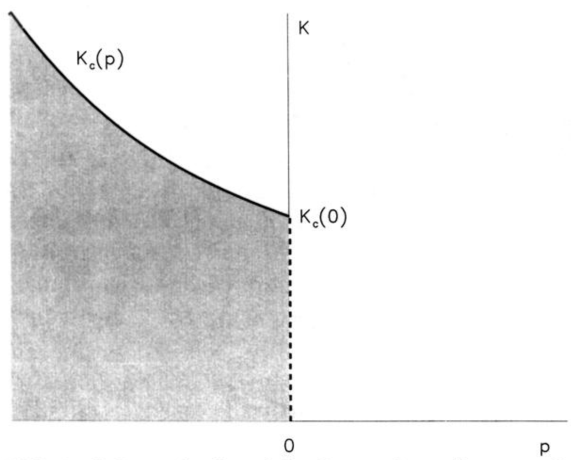

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