Scaling behavior of randomly triangulated self-avoiding surfaces

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The conformation and scaling properties of two-dimensional randomly triangulated self-avoiding surfaces embedded in three-dimensional space are studied using Monte Carlo methods. Results for the fractal dimension d_f and the spectral dimension d_s, as well as the ratios of the eigenvalues of the moment of inertia tensor (which characterize the mean shapes of the surfaces), are presented. It is shown that these surfaces belong to the self-avoiding branched polymer universality class.

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The statistical mechanics of tensionless two-dimensional membranes has recently attracted a great deal of attention [1,2]. Initially, this interest arose because of applications in the physics of microemulsions and biological membranes and vesicles. More recently, similar issues have been discussed in the context of string theories in high-energy physics.

Most biological membranes, as well as the surfactant monolayer membranes which provide the basic structural element for complex fluids, such as microemulsions, are found in the fluid phase, where the molecules can diffuse freely and their hydrocarbon tails are disordered. At length scales large compared to the size of individual molecules, these membranes can be modeled as self-avoiding, tensionless surfaces whose bending modes are controled by a bending rigidity κ. A fluid membrane of linear size L is expected to exhibit transverse fluctuations [3] of extension $L_\perp \sim (kT/\kappa)^{1/2}L$ on length scales small compared to the persistence length ξ_p [4]. These shape fluctuations lead to a monotonically decreasing scale-dependent effective rigidity [5,6]. At length scales $L \gg \xi_p$, this effective rigidity is negligibly small, and the membrane is expected to be in a *crumpled* state characterized by the absence of long-range orientational order of normals erected perpendicular to the local surface elements [2]. The structure of the crumpled state is characterized by the fractal dimension d_f [7], which relates the mass of the membrane to its radius of gyration, and the spectral dimension d_s [8–10], which describes the mean-square displacement of a Brownian particle diffusing within the membrane. The object of this paper is to determine the scaling behavior of self-avoiding fluid membranes with a fixed topology at length scales $L \gg \xi_p$. It is shown that these surfaces belong to the self-avoiding branched polymers universality class, with $d_f = 2$ and $d_s = 1.25 \pm 0.05$.

Our conclusions are based on a Monte Carlo study of a simple string-and-bead model for randomly triangulated two-dimensional surfaces of fixed topology embedded in three dimensions. The surface is modeled by a triangular network of N hard-sphere particles of diameter $\sigma = 1$ connected by tethers of maximum extent l_0. For a fixed triangulation, this model has been used extensively to study polymerized, or tethered, membranes [11]. To model a fluid membrane one must, in addition, sum over all possible triangulations, i.e., consider the triangulations as a dynamical field [12–25]. This can be accomplished using a two-step Monte Carlo procedure. First, one attempts to sequentially update the position vector of each monomer by a random increment in the cube $[-s,s]^3$. The move is accepted if it does not violate the constraints imposed by the finite tether length and hard-sphere self-avoidance. s is chosen so that approximately 50% of the updating attempts are accepted. Second, one attempts to flip N randomly chosen bonds. A bond flip consists of deleting a tether and constructing a new one between the two previously unconnected vertices of the two adjacent triangles. The flip is accepted with a probability given by the Boltzman factor [16] if all vertices have a minimum of three neighbors after the flip. We do not explicitly set an upper limit on the maximum number of neighbors. This bond-flipping procedure has been shown to be ergodic [12]. If, during a single time step, all links or bonds have the same probability of being flipped, this transformation also preserves detailed balance. We have checked that increasing the number of bond-flip attempts per sweep by a factor of 5 does not influence our results. Finally, note that one more term needs to be incorporated in the action. In order to ensure reparametrization invariance, the integration measure over the position field should have the form [12–14,17]

$$D\mathbf{r} = \prod_i q_i^{3/2} d^3 r_i \ , \tag{1}$$

where q_i is the coordination number of monomer i. We have absorbed the coordination number part of this measure into the action as a term

$$\beta \mathcal{H}_\sigma = -\alpha \sum_i \ln q_i \ , \tag{2}$$

where $\alpha = \frac{3}{2}$ [18].

Our simulations were carried out primarily on surfaces

of spherical topology consisting of N monomers using $l_0=\sqrt{2}$ and $s=0.1$. This choice of parameters ensures self-avoidance and leads to coordinate vector acceptance rates on the order of 0.48 and bond-flip acceptance rates of about 0.08. The procedure we employ conserves both the number of monomers and bonds. Some runs were performed on open membranes with free-edge boundary conditions. Since we do not flip boundary tethers, the open membranes we simulate have perimeters of fixed length.

In order to characterize the scaling behavior and conformation of the membrane we have determined the mean values of the eigenvalues λ_i $(i=1,2,3)$ of the (discretized) moment of inertia tensor [19]

$$\mathcal{T}_{\alpha\beta}=\frac{1}{N^2}\sum_{i,j}\frac{q_i q_j}{9}[r_i^\alpha-r_j^\alpha][r_i^\beta-r_j^\beta]\ , \tag{3}$$

as well as the anisotropies $\Gamma_i=\langle\lambda_i/\lambda_3\rangle$, $i=1,2$, where λ_3 is the largest eigenvalue of the moment of inertial tensor. The sum, $R_g^2=\sum_i\langle\lambda_i\rangle$, characterizes the extent of the membrane in the embedding space in terms of its surface area ($\sim N$). If the membrane is crumpled, one expects $R_g^2\sim N^\nu$, with an exponent $\nu<1$. Alternatively, one can use the fractal dimension d_f [7] to relate the mass N of the membrane to its size in the embedding space: $N\sim R_g^{d_f}$. These two indices are related by $\nu=2/d_f$. If the membrane is a fractal object, one would also expect the volume V of a vesicle to scale with N with another nontrivial fractal dimension d_V: $V\sim R_g^{d_V}$.

The anisotropies Γ_i characterize the mean shapes of the membrane. Although the overall ensemble average of the membranes we simulate must be spatially isotropic, it was noticed some time ago [20] that the mean shapes, referred, for example, to the object's own principle axes of gyration, are not. In fact, the values of Γ_i, like the exponents d_f and d_V, characterize the universality class of the object under consideration.

Figure 1 contains a plot of our data for the mean-squared radius of gyration R_g^2 and, for vesicles, the mean volume V versus the number of monomers. Averages were taken over 10^7 to 4×10^7 Monte Carlo steps per monomer. The data are consistent with $R_g^2\sim N^\nu$, with $\nu=1$, for both vesicles and open membranes. For vesicles, we need to go to larger system sizes to see scaling. In general, we find that the data for R_g^2 are "noisier" than for the mean volume V and that the data for V scale very nicely already for moderate values of N. These results imply $d_f=d_V=2$, values which characterize self-avoiding branched polymer behavior [21,22]. Furthermore, typical configurations, such as the one shown in Fig. 2, also exhibit the collapsed, treelike, ramified structure which characterizes this universality class. Note that many of the branches collapse to the minimum-allowed diameter (three-bond circumference for our algorithm).

Our results for the anisotropies $\Gamma_i=\langle\lambda_i/\lambda_3\rangle$, as well as the ratios of the mean values of the eigenvalues of the moment of inertia tensor $\Sigma_i=\langle\lambda_i\rangle/\langle\lambda_3\rangle$, are shown in Fig. 3. Only results for vesicles are presented because our data for open membranes showed significantly greater scatter. The finite-size corrections to these quantities can be seen to be rather small; furthermore, our data are consistent with a leading analytic correction term $(1/N)$, as is the case for branched polymers and lattice animals in two dimensions [20]. Assuming $\Gamma_i=\Gamma_i^\infty(1+\gamma_i/N+\cdots)$, we obtain $\Gamma_1^\infty=0.117\pm0.003$ and $\Gamma_2^\infty=0.335\pm0.006$. The Σ_i^∞ are several percent smaller. The crumpled vesicles are therefore prolate and more anisotropic than branched polymers in two dimensions. Although the Γ_i (and Σ_i) are the most direct measure of the anisotropy, there are no results available for these quantities with which to compare. For technical reasons, the shape of fractal clusters has generally been characterized in terms of expectation values of rotational-

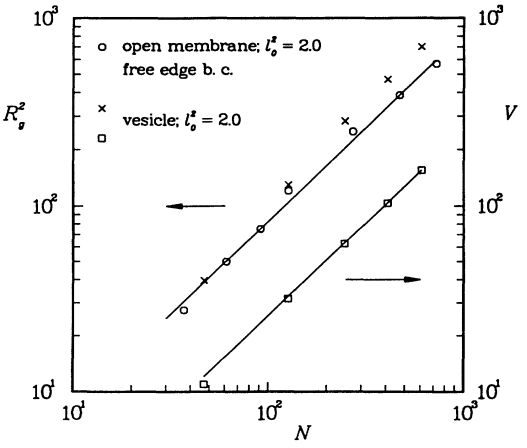

FIG. 1. Mean-squared radius of gyration R_g^2 and vesicle volume V vs number of monomers N. The solid lines are plots of $R_g^2\sim N$ and $V\sim N$.

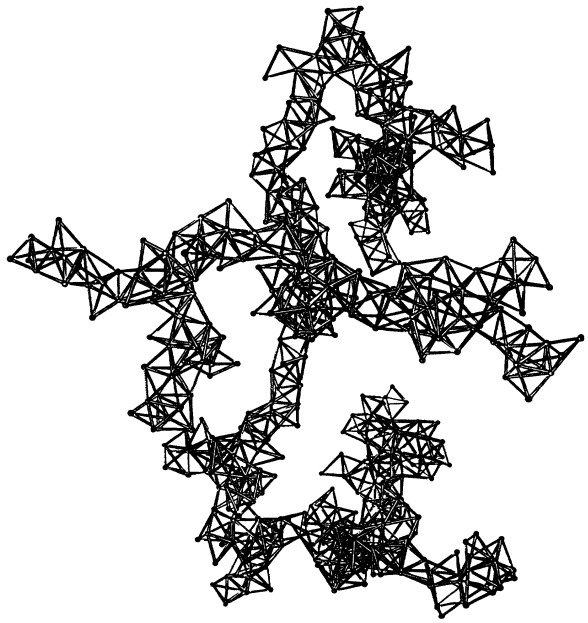

FIG. 2. Typical configuration of a vesicle with $N=607$ monomers.

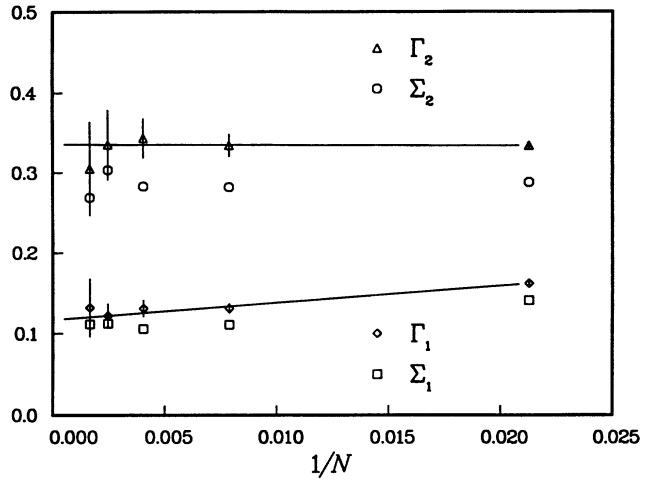

FIG. 3. Anisotropies $\Gamma_i=\langle\lambda_i/\lambda_3\rangle$ and $\Sigma_i=\langle\lambda_i\rangle/\langle\lambda_3\rangle$, $i=1,2$ vs $1/N$ for $N=47$, 127, 247, 407, and 607. The straight lines are fits to the data.

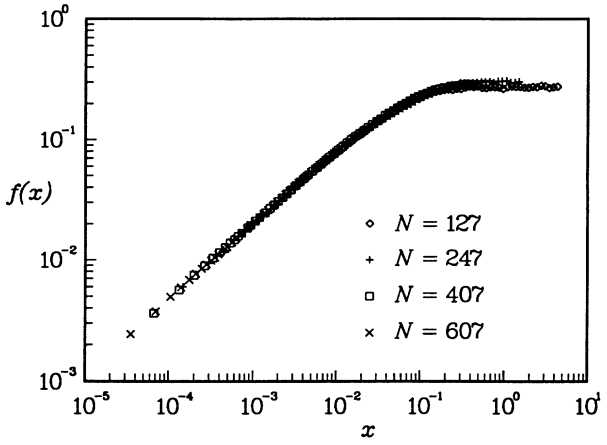

FIG. 4. The scaling function $f(x)=\langle[\mathbf{r}(t)-\mathbf{r}(0)]^2\rangle/N^{\nu}$ vs $x=t/N^{2/d_s}$, obtained using $\nu=1$ and $d_s=1.25$.

ly invariant polynomials of $\mathcal{T}_{\alpha\beta}$ [23,24]. Two quantities which have been analyzed are

$$\Delta_d=\frac{d}{d-1}\frac{\langle \mathrm{Tr}\hat{\mathcal{T}}^2\rangle}{\langle(\mathrm{Tr}\mathcal{T})^2\rangle}$$

and

$$S_d=\frac{d^2}{(d-1)(d-2)}\frac{\langle \mathrm{Tr}\hat{\mathcal{T}}^3\rangle}{\langle(\mathrm{Tr}\mathcal{T})^3\rangle}\ ,$$

where $\hat{\mathcal{T}}_{\alpha\beta}=\mathcal{T}_{\alpha\beta}-\bar{\lambda}\delta_{\alpha\beta}$, and $\bar{\lambda}=(1/d)\sum_{i=1}^{d}\lambda_i$. $0\le\Delta_d\le 1$ is a normalized measure of the anisotropy. The sign of $-[1/(d-1)^3]\le S_d\le 1$ determines whether the object is oblate ($S_d<0$), or prolate ($S_d>0$); its magnitude is a measure of the strength of the anisotropy. A linear regression analysis of our data for these quantities averaged over 2×10^7 Monte Carlo steps per monomer for $N=47$, 127, and 247 yields $\Delta_3=0.383\pm0.031$ and $S_3=0.248\pm0.033$, in excellent agreement with the results $\Delta_3=0.390\pm0.003$ and $S_3=0.27\pm0.01$ obtained by exact enumerations of lattice animal clusters in three dimensions [25].

Finally, we determine the spectral dimension d_s [8–10], which characterizes the connectivity of the random surface. The standard way to measure d_s is by averaging over random walks performed on a sufficient number of independent realizations of random surfaces of various size. The mean-square displacement after t steps of a random walk on a surface consisting of N monomers is expected to scale as [26,27]

$$\langle[\mathbf{r}(t)-\mathbf{r}(0)]^2\rangle=N^{\nu}f(t/N^{2/d_s})\ ,$$

where the scaling function $f(x)\sim x^{d_s/d_f}$ for $x\ll1$ and $f(x)=\text{const}$ for $x\gg1$. For $x\ll1$, the mean-squared displacement scales as t^{d_s/d_f}, while for $x\gg1$ it saturates at a value proportional to the mean-squared radius of gyration. The crossover time, $\tau\sim N^{2/d_s}$, is the mean time it takes for the walk to access all sites. The longest relaxation time τ_R in our simulations is the characteristic time it takes for a monomer to diffuse over the whole surface. It therefore also scales with the same exponent, namely, $\tau_R\sim N^{2/d_s}$.

In order to determine the spectral dimension, we have averaged $[\mathbf{r}(t)-\mathbf{r}(0)]^2$ over $2N$ walk on 22 independent realizations of vesicles of size $N=127$, 247, 407, and 607. Taking $\nu=1$, we find that the data for $\langle[\mathbf{r}(t)-\mathbf{r}(0)]^2>/N^{\nu}$ collapse on a universal scaling function for $d_s=1.25\pm0.05$ (see Fig. 4). This is in agreement with the best estimate we know of for branched polymers ($d_s=1.2$) [28].

All these results are consistent with the conclusion that randomly triangulated self-avoiding surfaces belong to the self-avoiding branched polymer universality class. This agrees with what was found for self-avoiding random surfaces constructed from elementary two-cells (plaquettes) on a three-dimensional simple-cubic lattice [29,30]. Since both discretizations yield the same scaling behavior, it is reasonable to assume that the predictions of these models provides an accurate description of the behavior in the continuum limit.

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