

Monte Carlo simulation of bond-diluted tethered membranes

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We simulate bond-diluted self-avoiding tethered membranes of linear size $L=7$ to 41. For any $p > p_c$ we find only the flat phase. The three eigenvalues of the inertia tensor (λ_3 the largest, λ_1 the smallest eigenvalue) scale with system size according to $\lambda_j \sim L^{2\nu_j}$ with $\nu_3(p) = \nu_2(p) = 1.0$ and $\nu_1(p) \approx \frac{2}{3}$ for all $p > p_c$. Our data indicate that at the percolation concentration the system is isotropically crumpled with fractal dimension indistinguishable from the Flory prediction. The cross-over between the isotropically crumpled and flat fixed point is also studied.

The statistical properties of polymerized and liquid membranes, free to fluctuate in d -dimensional space have been widely discussed in the past few years. One particularly simple system, the tethered membrane model introduced by Kantor, Kardar, and Nelson,¹ has been intensively studied both by numerical¹⁻⁶ and analytical techniques.^{1,7-11} This model, in which particles are connected in a fixed topology (e.g., a hexagonal or square network), is the generalization of the corresponding ($D=1$) bead and chain polymer model to dimension $D=2$ and serves as a prototype model for polymerized membranes. In contrast to linear polymers,¹² for which simulations, renormalization group studies, and Flory mean field theory all predict a "crumpled" phase, there is no such consistency in the case of tethered membranes.

A number of different numerical simulations have been carried out for tethered membranes and the results of the largest and most recent ones^{3,5,6} support the original conclusion of Plischke and Boal² that two-dimensional self-avoiding tethered membranes are flat rather than crumpled when embedded in three-dimensional space. The properties of the flat phase are nevertheless interesting. The shape of the membrane is characterized by the three eigenvalues of the inertia tensor and it is found^{2,3} that the two largest eigenvalues have the property $\lambda_{2,3} \sim L^2$, where L is the characteristic size of the stretched membrane, whereas the smallest eigenvalue scales as $\lambda_1 \sim L^{2\nu_1}$ with $\nu_1 \approx 0.67$. This result indicates that tethered membranes, albeit flat, are rough in the thermodynamic limit ($L \rightarrow \infty$).

Tethered membranes belong to the class of crystalline surfaces. Liquid membranes, found for example in microemulsions, form a different class and there is general agreement¹³ that liquid membranes are characterized by a finite persistence length and are, therefore, crumpled in the thermodynamic limit. One important difference between liquid and crystalline membranes is the nature of the elastic constants. In a liquid membrane, the shear modulus vanishes whereas a solid membrane, at least when confined to a plane, will have nonzero shear and bulk moduli. When free to fluctuate, nonlinear coupling between the in-plane and out-of-plane modes of a crystalline membrane leads to a stiffening of the membrane,⁸

stabilizing the flat phase.

It is well known¹⁴ that randomly diluted networks with central forces between the particles undergo a "rigidity percolation" transition at a concentration p_R , which, for hexagonal networks, is well above the geometric percolation concentration p_c . At this rigidity percolation point, the elastic constants of the network vanish and remain zero for all concentrations $p_c < p < p_R$. The reason for this is the geometrical nature of the backbone (as defined in the context of percolation) at and below the rigidity percolation point. When the system is constrained to lie in a plane, the rigid structure results from loops or triangles which are present at all length scales for $p > p_R$. For $p < p_R$ there are not enough loops to provide stiffness, and all elastic constants vanish. Therefore one may expect the in-plane modes of the bond-diluted membrane (for $p < p_R$) to be of a different nature than those of an undiluted membrane. One of our motivations in undertaking this work was to investigate whether or not this change in the elastic properties results in a crumpled phase of the fluctuating membrane.

Recently, Grest and Murat¹⁵ carried out molecular-dynamics calculations for site-diluted tethered membranes both above and below the threshold for rigidity percolation. They found no evidence for a crumpled phase for any concentration $p > p_c$. This may be due to the fact that the renormalized elastic constants of the undiluted network vanish at long wavelength due to the aforementioned coupling between in-plane and out-of-plane modes. Thus the effect of rigidity percolation may be a subtle one¹⁶ which is not yet evident in the simulations of Ref. 15 or, indeed, in the ones reported here.

We have carried out Monte Carlo simulations for bond-diluted tethered membranes in the concentration range $0.4 \leq p$. For the hexagonal networks studied here, geometric percolation occurs at $p_c = 2 \sin(\pi/18) \approx 0.3473$ and rigidity percolation occurs at $p_R \approx 0.65$.¹⁴ Thus there is a substantial range of concentrations for which one should be able to observe the effects of vanishing rigidity.

The details of the simulations are as follows. A hexagonal cluster of "diameter" L containing $N = (3L^2 + 1)/4$ particles and $3(3L - 5)(L + 1)/4$ bonds is excised from

an infinite hexagonal lattice. A fraction $(1-p)$ of the nearest-neighbor bonds is then randomly removed and the largest connected cluster identified. The particles in the remaining clusters are discarded and the largest cluster is then equilibrated by a standard Metropolis Monte Carlo procedure. Tethering is enforced either by a flexible string of maximum extension $3^{1/2}$ in units of particle diameter, or by the modified 6-12 potential of Ref. 3. Particles more than one lattice spacing apart on the network interact either through a hard sphere potential (case 1) or through a 6-12 potential, cut off at the point of zero force. The results of the two sets of calculations are equivalent and we support only on the more extensive simulations with hard-core potentials.

In these simulations, clusters of size $L = 7$ to 41 were used and in all cases the result were averaged over a number of realizations of the bond-cutting process. For the smallest clusters ($L = 7$), 50–150 different diluted networks are simulated; for the largest clusters ($L = 41$) computational limitations only allowed the simulation of three realizations. A measure of the equilibration time of linear polymers is the Rouse time, $\tau_R = N/s^2$, where N is the number of particles in the chain and s the length of a Monte Carlo step. Although the relaxation time of tethered membranes seems to scale with a higher power of N ,^{1,4} the Rouse time has commonly been used^{1,2,4} as a crude measure of the equilibration time for Monte Carlo calculations. Here we have used $N(p=1)/s^2$ Monte Carlo steps as our unit of time but have also calculated autocorrelation functions⁴ of the quantities of interest in order to verify that we had a significant number of statistically independent configurations. These autocorrelation functions decay roughly exponentially with time with a time constant which, for our system sizes, is of the order of 10–20 “Rouse times.” In all cases, the data were obtained from runs which were at least 1000 Rouse times in length after the initial transient and several clusters of size $L = 25$ were simulated for 10 000 Rouse times as a check that the shorter runs yielded averages characteristic of equilibrium.

As in previous work,^{2–4} the inertia tensor of the system was diagonalized for each configuration in the data set and the eigenvalues ordered according to size with λ_1 the smallest, λ_3 the largest. We assume that as $L \rightarrow \infty$, these eigenvalues scale as $\lambda_j \sim L^{2\nu_j}$ and determine as effective exponent $\nu_{j,\text{eff}}(L_1, L_2)$ from the formula

$$\nu_{j,\text{eff}}(L_1, L_2) = \frac{1}{2} \frac{\ln[\lambda_j(L_2)/\lambda_j(L_1)]}{\ln(L_2/L_1)}. \quad (1)$$

The data for λ_1 and λ_3 are quite noisy and the effective

exponents for these eigenvalues are not well converged. Conversely, the second eigenvalue, λ_2 , does not fluctuate nearly as much, either for a particular cluster or for different realizations of clusters at a given concentration of bonds. Table I shows the effective exponent $\nu_{2,\text{eff}}$ for a range of concentrations and for different values of L_1 and L_2 . Since ν_j cannot be larger than 1 for any $p > p_c$, we conjecture that $\nu_2 = 1.0$ for all $p > p_c$. Moreover, $\nu_3 \geq \nu_2$ and it therefore seems that the scaling exponents of the two largest eigenvalues are constant, i.e., $\nu_2(p) = \nu_3(p) = 1.0$ for all $p > p_c$. This conclusion is consistent with the results reported in Ref. 15. As mentioned above, the data for λ_1 show large fluctuations and it is difficult to determine the exponent ν_1 with any precision. However, the data are at least consistent with $\nu_1(p) = \nu_1 \approx 0.67$.

At the bond percolation point the infinite connected cluster has Hausdorff dimension $D = \frac{91}{48} < 2$ and is expected to be crumpled. This isotropically crumpled phase has been seen in the simulations of Grest and Murat.¹⁵ The Flory theory for self-avoiding networks predicts¹⁷ that the fractal dimension of the crumpled network will be

$$d_f = \frac{(d+2)d_s}{d_s+2} \quad (2)$$

where $d_s \approx \frac{4}{3}$ is the spectral dimension of the percolating cluster.¹⁸ For $d = 3$, we therefore obtain $d_f = 2$ as the Flory prediction at $p = p_c$. All of the preceding results are consistent with the picture that the equilibrium behavior of tethered membranes is controlled by two fixed points (in the renormalization group sense). We have, therefore, attempted to study the crossover from the unstable crumpled fixed point to the flat-phase fixed point.

We define $N(p)$ to be the “mass” of the largest cluster at concentration p . At $p = p_c$ the system crumples and the three eigenvalues of the inertia tensor scale with the mass with the same exponent $2/d_f$. As one crosses over from the crumpled to the flat-phase fixed point, the three eigenvalues are characterized by scaling functions whose arguments are given by the ratios of length scales entering into the problem. In this case, aside from L , there are at least two (possibly related) length scales, namely, the percolation correlation length and the normal-normal correlation length of the flat phase. This correlation length is finite at $p = 1$ and presumably diverges at p_c as some power of $p - p_c$. For the range of concentrations simulated here, the percolation correlation length is quite small and it is presumably the normal-normal correlation length which enters into the scaling functions. Our simulations are not large enough to enable us to determine

TABLE I. The effective exponent $\nu_{2,\text{eff}}(L_1, L_2)$, defined in Eq. (1), for tethered membranes with various concentrations p of nearest-neighbor bonds.

| $p = 1.0$ | | | $p = 0.6$ | | | $p = 0.5$ | | | $p = 0.45$ | | |
|-----------|-------|----------------------|-----------|-------|----------------------|-----------|-------|----------------------|------------|-------|----------------------|
| L_1 | L_2 | $\nu_{2,\text{eff}}$ | L_1 | L_2 | $\nu_{2,\text{eff}}$ | L_1 | L_2 | $\nu_{2,\text{eff}}$ | L_1 | L_2 | $\nu_{2,\text{eff}}$ |
| 7 | 11 | 0.96 | 7 | 11 | 0.93 | 7 | 11 | 0.92 | 7 | 11 | 0.98 |
| 11 | 19 | 1.02 | 11 | 15 | 1.00 | 11 | 15 | 0.99 | 11 | 17 | 0.96 |
| 19 | 25 | 0.97 | 15 | 25 | 0.96 | 15 | 25 | 0.95 | 17 | 25 | 1.00 |
| | | | 25 | 41 | 1.02 | 25 | 41 | 1.04 | | | |

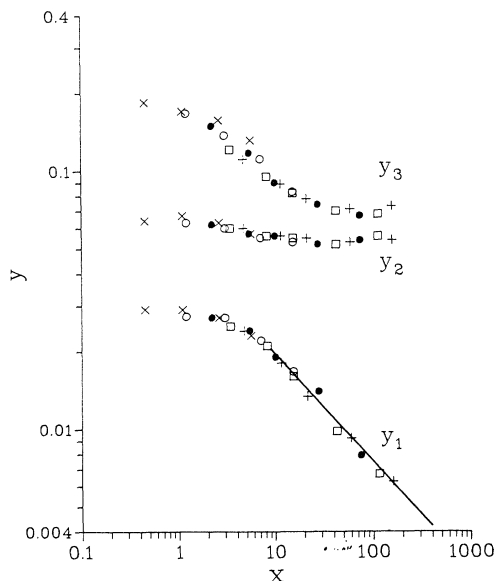


FIG. 1. Plot of the scaling functions $y_j(x) = \lambda_j(p)/N(p)$ as function of the scaling variable $x = N(1)(p - p_c)^\phi$ for $\phi = 1.5$ and where $N(1)$ is the number of particles in the undiluted network. Crosses: $p = 0.4$; circles: $p = 0.45$; solid dots, $p = 0.50$; squares, $p = 0.60$; plus signs: $p = 0.65$.

how this length depends on $p - p_c$ and we therefore fit our data to the following phenomenological scaling form:

$$\lambda_j(p) = [N(p)]^{2/d_f} y_j [N(1)(p - p_c)^\phi]. \quad (3)$$

The crossover exponent ϕ , as well as the fractal dimension d_f , should be determined from the data. However, the present data are not extensive or well converged

enough to permit a convincing two-parameter fit. We define the variable $x = N(1)(p - p_c)^\phi$ and find that $\phi \approx 1.5$ provides a reasonable collapse of the data when the fractal dimension is taken to be the Flory value $d_f = 2$ (see Fig. 1). The scaling functions y_j should then have the asymptotic form $y_j(x) \rightarrow \text{const}$ as $x \rightarrow 0$, for all j , and $y_{2,3}(x) \rightarrow \text{const}$ as $x \rightarrow \infty$, whereas $y_1(x) \sim x^{-1+\nu_1}$ for large x . Figure 1 shows the functions $y_j = \lambda_j/N(p)$ as function of the variable x . Although x is never particularly small for the range of concentrations simulated, the three scaling functions certainly seem to approach a constant for small x . In the case of y_1 there is a distinct break in the data near $x \approx 10$ and the solid line which is drawn by eye has slope -0.4 , yielding $\nu_1 = 0.6$ for the flat phase of the tethered membrane, in reasonable agreement with the previously determined value of 0.67. The almost complete independence of x of the function y_2 is, of course, the reason for the excellent convergence of the effective exponent ν_2 seen in Table I.

In summary, the calculations reported here are consistent with the following simple picture of the equilibrium behavior of tethered self-avoiding membranes. Bond-diluted self-avoiding tethered membranes are in the flat phase for all concentrations above the bond percolation concentration. At percolation the fractal dimension of the infinite cluster is close to 2, the value predicted by Flory theory, and the membrane is isotropically crumpled.

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