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Self-avoiding tethered membranes embedded into high dimensions

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Abstract. — The equilibrium structure of self-avoiding two-dimensional tethered membranes embedded in a space of dimension $d > 2$ are studied using molecular dynamics simulations for $3 \leq d \leq 8$. For embedding dimension $d \geq 5$, the membranes crumple while they remain flat for $d \leq 4$. In the crumpled phase, the radius of gyration $R_g$ increases as $L^\nu$, where $L$ is the linear size of the uncrumpled surface, and $\nu$ is significantly larger than the simple Flory estimate $\nu_F = 4/(d + 2)$. For $d = 4$, the membrane remains flat, even in the presence of site-dilution, indicating that as for $d = 3$, random site-dilution alone is not sufficient to produce crumpling of two-dimensional membranes.

1. Introduction.

The statistical properties of objects of arbitrary fractal connectivity embedded in a space of dimension $d$ has been the subject of great interest in recent years [1]. Besides the well-known example of linear polymers, other systems which have been investigated recently are swollen gelation/percolation clusters generated near the percolation threshold $p_c$ [2], Sierpinski gaskets [3,4] and two-dimensional tethered membranes [5,6]. Cates [1] was the first to use the term ‘polymeric fractals’ to describe the class of fractals which are made of flexible polymer chains at short length scales but which have an arbitrary self-similar connectivity at large distances. Such fractals are interesting because they are expected to have no inherent rigidity. Because such systems are locally very flexible, after they are allowed to relax and take on their equilibrium shape, they very often have a very different fractal dimension than they had when they were first constructed. Cates [1] worked out a Flory-level theory [7] in the presence of excluded volume interactions to determine an estimate for the swollen fractal dimension $d_f$ which relates the mass or number of monomers $N$ of the fractal to the size $R_g$, $R_g^{d_f} \sim N$ in the presence of excluded volume interactions. By balancing the elastic (entropic) free energy of the ‘phantom’ object without self-avoidance with the mean field estimate of the excluded volume interaction, he showed that $d_f$ depends only on
the spectral dimension $\tilde{d}$ [8] and the dimension of space $d$

$$d_t = \frac{(d + 2)\tilde{d}}{(\tilde{d} + 2)}$$

Kantor et al. [5] derived a similar result for $D$-dimensional manifolds ($D$ integer) such as linear polymers ($D = 1$), tethered surfaces ($D = 2$) and gels ($D = 3$). In this case the spectral dimension and the the dimension of the manifold are equivalent ($\tilde{d} = D$). For networks with regular connectivity, the exact value of $d_t$ depends only on the value of $D$ and the embedding dimension $d$ [5]. However for networks with irregular connectivity, particularly for objects which are inherently fractal and cannot be expressed in terms of a Euclidean metric, it is not clear whether the exact value of $d_t$ depends only on $\tilde{d}$ or on other details such as topological constraints [1].

Despite the fact that the Flory argument is only a simple mean field theory, it is known to work very well for a number cases, often producing estimates for $d_t$ which differ from the exact result by only a few percent or less for $d < d_{uc}$. Here $d_{uc} = 4\tilde{d}/(2 - \tilde{d})$ [1,9,10,11] is the upper critical dimension above which self-avoidance becomes irrelevant. Examples where the Flory theory, equation (1), works extremely well include linear polymers ($\tilde{d} = 1$) for $d \leq d_{uc} = 4$, gelation/percolation clusters ($\tilde{d} \approx 4/3$ in all dimensions [8]) embedded into $d = 3$ [2,12,13] and triangular Sierpiński gaskets ($\tilde{d} = 2\ln 3/\ln 5 \approx 1.365$ [14]) embedded into dimension $3 \leq d \leq d_{uc} \approx 8.6$ [4]. The Flory result for percolation/gelation clusters is expected to be a good approximation for all $d \leq d_{uc} = 8$, but it has only been checked in $d = 3$. In the two cases I am aware of which do not satisfy equation (1), an additional bending rigidity is believed to be present. These are the Sierpiński gasket in $d = 2$ [23] and two-dimensional tethered membranes ($D = \tilde{d} = 2$) in $d = 3$. While the early simulations [5] suggested that tethered membranes satisfy equation (1), later, more detailed work found that they remain flat [15-18] and do not crumple. This result was initially very surprising since renormalization group calculations [5-11] also suggested that the flat phase was unstable. The lack of a crumpling transition in $d = 3$ has recently been explained in terms of an implicit bending rigidity which is induced by the self-avoidance requirement even when no such term is present in the microscopic Hamiltonian [18]. If bending rigidity is relevant, then one cannot expect the Flory theory to work. Recently Boal et al. [18] studied rather small tethered membranes ($L < 17$) embedded in $d = 4$ and 5 dimensions and suggested the existence of a new ‘rough’ phase, in which the membranes were neither flat nor crumpled. However in this paper, I will show that simulations on much larger systems suggest that tethered membranes actually crumple for $d \geq 5$ and that the value of $d_t$ is significantly smaller than predicted by equation (1). In $d = 4$, the membranes remain flat.

It is interesting to consider in more detail why some systems, in particular those for which the spectral dimension is close to 1, crumple and others do not. Abraham and Nelson [18] suggest that a bending rigidity proportional to the temperature is generated for entropic reasons by the excluded volume interactions. They found that second neighbor interactions alone are sufficient to produce a flat phase even when further neighbor interactions are turned off. In a separate study, they [20] also found that a network of flexible linear polymers that are crosslinked to form a two-dimensional tethered membrane also remains flat even though this object is very flexible locally [21]. This suggests that the interactions inducing the bending rigidity whatever they are must be relevant under renormalization. Had this not been the case, then above a critical length of the linear polymer chain, the induced bending rigidity would fall below the critical value necessary to keep the membranes flat [22] and the membrane would crumple. To understand why excluded volume interactions do not generate a comparable bending rigidity for percolation/gelation clusters near $p_c$ or Sierpiński gaskets, it is informative to consider the relevancy of higher interaction terms in the Hamiltonian. Since renormalization group approaches explicitly take into account
the two-body repulsive interactions, it seems reasonable to assume that higher order terms are responsible for generating the implicit bending rigidity that keeps a tethered membrane flat. At least within Flory theory [10,23] it is straightforward to determine for a given value of $\bar{d}$ and $d$ whether the $n$-body interaction $v_n$ is relevant or not. According to the Flory theory [10,23]

$$\bar{d} = \frac{2(n-1)d}{2n + d},$$  \hspace{1cm} (2)

is the line where $n$-body interactions $v_n$ become relevant. Two-body terms are irrelevant for $d > d_{ac} = 4\bar{d}/(\bar{d} - 2)$ as mentioned above. Three-body terms are irrelevant for $\bar{d} > 4d/(6 + d)$. For 'polymeric fractals' [21] embedded into 3-dimensions, three-body terms are irrelevant for $\bar{d} < 4/3$.

This explains why there is no induced bending rigidity for linear chains and percolation/gelation clusters near $p_c$. Since the value of $\bar{d}$ for Sierpiński gaskets is close to 4/3, it is not too surprising that they crumple. It may also explain why these systems approximately satisfy equation (1) so well.

For tethered membranes, however, Flory theory suggests that four-body interactions are relevant below 4-dimensions and three-body terms are relevant below 6-dimensions and must be taken into account [23]. In fact, in $d = 3, 3-$, 4- and 5-body interactions are relevant and 6-body terms are marginal according to Flory theory. If three-body terms are sufficient to generate an effective bending rigidity, then Flory theory would predict that above $d = 6$ membranes should crumple, while if four-body terms are necessary to generate the bending rigidity, then the crumpling would occur above $d = 4$. While there is no reason to take the Flory theory very seriously as to the exact dimension at which a tethered membrane will crumple, it does suggest that crumpled membranes may exist, albeit in dimensions higher than 3. In this paper, I present the results of a detailed molecular simulation in $3 \leq d \leq 8$ dimensions which show that for $d \geq 5$, tethered membranes do in fact crumple. Why the crossover is between $d = 4$ and 5 is not clear. In addition, I find that these crumpled membranes do not satisfy equation (1) very well. Though there is no real reason why the Flory theory should work as well for fractals with $\bar{d}$ near 1, it is somewhat surprising that equation (1) does not give a reasonable estimate for crumpled membranes in $5 \leq d \leq 8$. Renormalization group calculations [23] suggest that at least for tethered membranes, $d_f$ should satisfy equation (1) as $d \rightarrow \infty$. Additional simulations for objects with spectral dimensions between 4/3 and 2 would be very useful to clarify the crossover dimension $d$ from the flat to the crumpled phase.

In $d = 4$, I find that tethered membranes remain flat and do not crumple. As was done in $d = 3$ [13,20,24], it is interesting to introduce local flexibility into these highly connected membranes to check whether they crumple. In an earlier study, Murat and I [13] studied randomly site-diluted membranes in $d = 3$. We found that membranes simply roughen as the dilution is increased but remain flat until they fall apart at the percolation threshold. Piischke and Fourcade [24] found a similar result for bond-diluted membranes. In this paper, I show that site-diluted membranes also remain flat in $d = 4$. One convenient way to characterize the properties of diluted membranes is to measure the order parameter [22] defined by the ratio of the largest eigenvalue of the moment of inertia tensor $\lambda_d$ to its value in the initial flat configuration $\lambda^*_d$,

$$\phi = \frac{\lambda_d}{\lambda^*_d}.$$  \hspace{1cm} (3)

In $d = 3$, we found that $\phi$ decreased approximately linearly as $p$ decreased and reached a value of about 0.31 at $p_c^+$. In $d = 4$, I find that $\phi$ also decreases as $p$ decreases but the dependence is not as linear as in $d = 3$. At $p_c^+$, $\phi$ reaches a value of about 0.15, then $\phi$ drops discontinuously to zero. Thus as in $d = 3$, random site-dilution alone is not sufficient to produce a crumpled state. In light of the above discussion on the relevancy of higher order terms this result should not be too surprising.
The outline of the paper is as follows. In section 2, I describe the model and the molecular dynamics technique used to perform the simulations. In section 3, I present my results for the eigenvalues of the moment of inertia tensor, the radius of gyration and the static structure functions for two-dimensional tethered membranes embedded into dimensions up to 8. I will then present results for site-diluted membranes. In section 4, I will briefly summarize the results and indicate some future directions.

2. Model and method.

Each membrane consists of \( N \) monomers of mass \( m \) connected by anharmonic springs. The monomers interact through a shifted Lennard-Jones potential given by

\[
U^0(r) = \begin{cases} 
4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} + \frac{1}{4} \right] & \text{if } r \leq r_c; \\
0 & \text{if } r > r_c,
\end{cases}
\]

with \( r_c = 2^{1/6} \sigma \). This purely repulsive potential represents the excluded volume interactions that are dominant in the case of monomers immersed in a good solvent. For monomers which are tethered (nearest neighbors) there is an additional attractive interaction potential of the form \[25\]

\[
U^{\text{bond}}(r) = \begin{cases} 
-0.5kR_0^2 \ln \left[ 1 - \left( \frac{r}{R_0} \right)^2 \right] & \text{if } r \leq R_0; \\
\infty & \text{if } r > R_0.
\end{cases}
\]

The parameters \( k = 30\epsilon / \sigma^2 \) and \( R_0 = 1.5\sigma \) are chosen to be the same as in [26]. Note that the form of the potential is somewhat different from those used by Kantor et al. [5], Plischke and Boal [15] and Abraham et al. [16] in that there exists no range of separation \( r \) in which the force vanishes. Also note that this potential does not include any explicit bending terms.

Denoting the total potential of monomer \( i \) by \( U_i \), the equation of motion for monomer \( i \) is given by

\[
m \frac{d^2 r_i}{dt^2} = -\nabla U_i - m\Gamma \frac{dr_i}{dt} + W_i(t).
\]

Here \( \Gamma \) is the bead friction which acts to couple the monomers to the heat bath. \( W_i(t) \) describes the random force acting on each bead. It can be written as a Gaussian white noise with

\[
\langle W_i(t) \cdot W_j(t') \rangle = \delta_{ij} \delta(t-t')6k_BT\Gamma,
\]

where \( T \) is the temperature and \( k_B \) is the Boltzmann constant. I have used \( \Gamma = \tau^{-1} \) and \( k_BT = 1.0\epsilon \). Here \( \tau = \sigma (m/\epsilon)^{1/2} \). The equations of motion are then solved using a velocity Verlet algorithm [27] with a time step \( \Delta t = 0.012\tau \) [28]. The program was vectorized for a supercomputer following the procedure described by Grest et al. [29] except that the periodic boundary conditions were removed and additional interactions between monomers which are tethered was added. The cell method was used to check whether non-tethered monomers were within the range of interaction by projecting the membrane into 3 dimensions. The axis of the 3-dimensional cube were chosen parallel to the eigenvectors \( \hat{u}_i \) \((d-2 < i < d)\) of the moment of inertia tensor with the largest three eigenvalues. Since the membrane can rotate during the course of the simulation, the direction of the cube was updated every 100 time steps. A similar procedure was used by Boal et al. [19] in their simulations for \( d > 3 \) except that they projected the membrane onto an infinitely long cylinder. The cpu time per step increased approximately linearly with \( dN \). For the tethered
membrane of size $N = 2437$ embedded into $d = 5$, 1 million timesteps took about 17 hours of cpu time on our Cray XMP 14/32e. With this choice of parameters, the average bond length between nearest neighbors that are tethered is found to be $0.97a$. Further details of the method can be found elsewhere [26].

The simulations were performed on two-dimensional triangular arrays of monomers in which all the nearest neighbors were tethered. The shape of these finite systems were in the form of a hexagonal sheet of linear dimension $L$. Values of $L$ in the range $13 \leq L \leq 57$ were studied for embedding dimensions $3 \leq d \leq 6$ while for $d = 8$ the largest system studied was $L = 43$. For these membranes the number of sites, $N$, is given by $N = (3L^2 + 1)/4$. For $d = 4$, simulations were also carried out on site-diluted membranes with an occupation fraction $p > p_c = 0.5$. In this case all but the largest cluster was eliminated and $N$ was in the range $1676 \leq N \leq 3070$. Typically $0.5 - 1.0 \times 10^6$ time steps were needed to equilibrate the systems. The equilibration of all the systems were checked by monitoring the autocorrelation function of the radius of gyration of the membranes. The simulations were then run for $1.5 - 2.0 \times 10^6$ time steps after equilibration. Note that due to the larger time step used here compared to our earlier simulations on tethered membranes in $d = 3$ [13], the total length of the runs are about twice as long.

To analyze our results we calculated several quantities. Every 100 steps the inertia matrix, its eigenvalues $\lambda_i (\lambda_1 < \lambda_2 \ldots < \lambda_d)$ and the radius of gyration squared, $R_g^2$, given by their sum were calculated. These quantities were also used to check the equilibration of the system through their autocorrelation. In the crumpled phase, all $d$ eigenvalues are expected to scale as $L^{2\nu}$, where $\nu = 2/d_4$. In the flat phase, the largest two eigenvalues should scale as $L^{2\nu||}$ with $\nu|| = 1$, while the $(d - 2)$ smallest eigenvalues should scale as $L^{2c}$.

The spherically averaged structure factor, $S(q)$, given by

$$S(q) = \frac{1}{N} \left\langle \sum_{i,j} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle,$$  

was also calculated. The angle brackets represent a configurational average typically taken every 10000 time steps. For each $q = |q|$, I averaged over 30 random orientations. In the scaling regime, $S(q) \sim q^{-d_i}$. As pointed out by Pilschke and Boal [15], it is also important to consider the anisotropic scattering intensity, $S_i(q)$, where the q's are restricted to be parallel to the eigenvector $\hat{e}_i$ of the inertia matrix corresponding to the eigenvalue $\lambda_i$. Since the topologically planar membranes have $\lambda_d \sim \lambda_{d-1} >> \lambda_i$ ($i \leq d - 2$), instead of simply measuring $S_d(q)$ and $S_{d-1}(q)$ separately, it is useful to measure

$$S_{||}(q) = \frac{1}{N} \left\langle \sum_{i,j} e^{i\mathbf{q} \cdot \mathbf{e}_i \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle,$$  

such that $q_{||}$ is parallel to $a_d \hat{e}_d + a_{d-1} \hat{e}_{d-1}$, where $a_i$ are random numbers. For $d \geq 4$, I also calculated $S_{12}(q)$, which is equivalent to $S_{||}(q)$, except that $q$ is parallel to $a_1 \hat{e}_1 + a_2 \hat{e}_2$. For these latter two quantities, I averaged over 30 random orientations for each $q = |q|$, thereby improving the statistics compared to $S_i(q)$. $S_{12}(q)$ and $S_{||}(q)$ were found to give equivalent results. As will be shown in the next two sections, these anisotropic scattering functions are very useful in demonstrating that for $d \leq 4$, the tethered membranes are anisotropic and flat, while for larger dimensions, they are isotropic and crumpled.
3. Results.

One simple way to distinguish the flat phase from the crumpled phase is to examine the eigenvalues of the moment of inertia matrix and the mean-square radius of gyration given by the sum of its eigenvalues. In figure 1, results for the eigenvalues of the moment of inertia tensor $\lambda_i$ versus $L$ for tethered membranes embedded in $d = 4, 5$ and 6 dimensions are presented. The lines are least square fits to the data for $13 \leq L \leq 57$. In $d = 4$, I find that the largest two eigenvalues scale as $\lambda_1 \sim L^{2\eta\parallel}$, with $\eta\parallel = 0.95 \pm 0.05$, consistent with the membrane being flat. The two smallest eigenvalues scale as $L^{2\zeta}$, with $\zeta = 0.84 \pm 0.05$. As seen from figure 1a, the magnitude of the eigenvalues, $\lambda_4 \sim \lambda_3 \gg \lambda_2 \sim \lambda_1$, are also consistent what one would expect for a flat membrane. However, the behavior of the eigenvalues is significantly different for $d \geq 5$ as seen in figures 1b and c. In this case, as for $d = 8$ (not shown), the $d$ eigenvalues scale with approximately the same slope. From fits to the data, $\nu = 0.85 \pm 0.05$ in $d = 5$, $0.74 \pm 0.04$ in $d = 6$ and $0.60 \pm 0.05$ in $d = 8$. In figure 2, results for the mean square radius of gyration $\langle R_g^2 \rangle$ versus $L$ for membranes embedded into dimension $d$, $3 \leq d \leq 8$, are shown. For $d = 3$ and 4, $\langle R_g^2 \rangle \sim L^2$ as one expects for the flat phase. However for larger values of $d$, the slope decreases as $d$ increases. Fits to the data give results for $\nu$ consistent with those obtained from scaling $\lambda_d$ as one would expect. While these results give the first clear evidence that the membranes crumple for $d \geq 5$, one should not
take these estimates of the exponents too seriously. From earlier experience in \( d = 3 \) [16,19,30] it was found that values for \( \zeta \) determined from scaling of \( \lambda_1 \) varied widely, from about 0.65 to 0.80. More reliable estimates were obtained by finite size scaling of the anisotropic structure function \( S_1(q) \) which will be discussed below.

![Figure 2](image2.png)

**Fig. 2.** — Radius of gyration \( \langle R_g^2 \rangle \) versus \( L \) for membranes embedded into dimension \( d, 3 \leq d \leq 8 \).

![Figure 3](image3.png)

**Fig. 3.** — The spherically averaged structure function \( S(q) \) for the largest membrane studied \( (N=2437 \text{ for } d=4, 5 \text{ and } 6 \text{ and } N=1387 \text{ for } d=8) \) versus \( q \).

The spherically averaged structure function \( S(q) \) is shown in figure 3 for the largest membrane studied, \( N=2437 \) for \( d=4, 5 \) and 6 and \( N=1387 \) for \( d=8 \). In the scaling regime, \( q_{\min} = 2\pi/R_g < q < 2\pi/3 \approx 2, S(q) \sim q^{-d_f}. \) The most accurate way to determine \( d_f \) from data of this type is to replot \( q^{d_f}S(q) \) versus \( q \) on a log-log plot for different values of \( d_f \). In the scaling regime, data for different values of \( L \) should overlap. \( d_f \) can then be obtained from those values which give
Fig. 4. — The spherically averaged structure function $S(q)$ ($\times$), the in-plane structure function $S_{\parallel}(q)$ ($\ast$) and $S_{12}(q)$ ($\circ$) for $D=2$ tethered membranes in a) $d = 4$, b) $d = 5$ and c) $d = 6$ dimensions for $N=2437$. 
a reasonably flat set of curves in the scaling regime. Following this procedure, reasonable fits to 
the data were obtained with $d_f = 2.2$ in $d = 4$, $2.4$ in $d = 5$, $2.8$ in $d = 6$ and $3.3$ in $d = 8$. 
The error in $d_f$ is approximately ±0.1. Since $\nu = 2/d_f$ for tethered membranes, these results give 
$\nu = 0.91$, $0.83$, $0.71$ and $0.61$ for $d = 4$, $5$, $6$ and $8$, respectively. In the flat phase, the membrane 
is not isotropic and $S(q)$ is a mixture of scattering contributions parallel and perpendicular to the 
plane of the membrane. Thus it is not surprising that $d_f$ is slightly larger than 2 in $d = 4$. This is 
seen more clearly in figure 4a, where $q^2S(q)$ is shown for $N = 2437$. As discussed by Abraham and 
Nelson [18], the kink and extra structure in $S(q)$ for a flat membrane is related to the different 
scaling regimes for scattering in the plane of the membrane and perpendicular to it. For $d \geq 5$, 
the results for $\nu$ are consistent with those obtained from the scaling of $\lambda_i$.

Because the flat phase is anisotropic, it is very useful to consider scattering functions for orien-
ted membranes. One convenient way to do this is to measure the in-plane structure function 
$S_{||}(q)$ given by equation (9). In $d = 3$, the fluctuations perpendicular to the plane of the mem-
brane in the flat phase were studied by choosing $q \parallel \hat{e}_1$, $S_1(q)$ [15,18,19]. For $d \geq 4$, one can also 
study $S_i(q)$ ($i \leq d - 2$), or average over a number of $q$'s, as long as they are all perpendicular to 
both $\hat{e}_2$ and $\hat{e}_{d-1}$. In order to improve statistics, it is useful to determine $S_{12}(q)$, in which $q$ 
was chosen to be in the plane formed by $\hat{e}_1$ and $\hat{e}_2$. Results for $S(q)$, $S_1(q)$ and $S_{12}(q)$ are shown 
in figure 4 for a $L=57$ ($N=2437$) membrane in $d = 4$, 5 and 6. The three scattering functions 
behave very differently and converge only for $q$-values which correspond to the length of a single 
 bond. The oscillations in $S_{||}(q)$ arise from the scattering off a 2d planar object with a relatively 
sharp interface. This effect has been discussed in detail by Abraham and Nelson [18] for tethered 
membranes in $d = 3$. Note that these oscillations even occur for $d \geq 5$, where the membranes 
are crumpled and not flat. This is because the membrane still has a well defined characteristic 
size and shape when projected onto the plane determined by the two largest eigenvectors of the 
moment of inertia matrix. This projected membrane is roughly the shape of a disk ($\lambda_d \sim \lambda_{d-1}$) 
and as a result oscillations in the 'in-plane' scattering occur. As shown in figure 5, the first and 
deepest minimum occurs for $qL \approx 10$ as in $d = 3$ [18,19]. However the larger the value of $d$, 
the fewer of these oscillations are present and they come less well-defined. In $d = 8$, only a small 
shoulder remains in $S_{||}(q)$ with not well developed minimum.

The clearest evidence that the membranes are crumpled for $d \geq 5$ comes from finite size scaling 
of the partial scattering functions $S_i(q)$, $S_{||}(q)$ and $S_{12}(q)$. In the flat phase $S_i(q)/N = \Phi_i(qL^n)$ 
with $n = 1$, while $S_i(q)/N \sim S_{12}(q)/N = \Phi_2(qL^2)$ ($i \leq d - 2$). However in the crumpled 
phase all of these structure functions should scale as $qL^\zeta$. In figures 5 and 6, I show the structure 
factors plotted in the scaling form for 4 values of $L$ in the range $21 \leq L \leq 57$ for $d = 4$, 5 and 6. 
Results for $S_1(q)$ show a similar scaling with the essentially the same exponent $\zeta$ as determined 
from $S_{12}(q)$. In $d = 4$, the results clearly support the conclusion that the membrane is flat. The 
value of $\zeta$ is $0.77 \pm 0.04$ while $\nu = 1$ near 1. In $d = 5$, $\zeta$ and $\nu$ differ slightly but are 
the same within their error bars. In $d = 6$ and 8, the two exponents agree very well. A summary 
of the exponents obtained from scaling $S_{||}(q)$ and $S_{12}(q)$ are given in table I. The error bars are 
subjectively determined by reploting figures 5 and 6 for several values of the exponents and qual-
itatively determining which give the best fit. For flat membranes, the in-plane structure function 
$S_{||}(q)$ should not satisfy the scaling relation over a wide range of intermediate wavevectors [18]. 
This is clearly seen in figure 5a.

The exponents determined from the scaling plots of various structure factors are shown in figure 
7. Also shown is the prediction of the Flory theory, $\nu = 2/d_f = 4/(d + 2)$. For $d = 3$, simulations 
on finite membranes of the type studied here found $\zeta = 0.64 \pm 0.04$ [18,30,31]. Two more recent 
studies [32] suggest that this value is too high and the actual value is closer to 0.5. The difference 
being attributed to a crossover effect due partially to the open boundary conditions. However, 
there remains some question as to whether the breaking of rotation invariance which occurs when
Table I. — Values for the critical exponents $\zeta$ and $\nu_\parallel$ for $3 \leq d \leq 8$ for two-dimensional tethered membranes as determined from the scaling of $S_{\parallel}(q)$ and $S_{12}(q)$ ($S_1(q)$ in $d = 3$). Results for $d = 3$ from reference [18,31].

<table>
<thead>
<tr>
<th>$d$</th>
<th>$\zeta$</th>
<th>$\nu_\parallel$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.64 ± 0.04</td>
<td>1.0</td>
</tr>
<tr>
<td>4</td>
<td>0.77 ± 0.04</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>0.77 ± 0.03</td>
<td>0.82 ± 0.05</td>
</tr>
<tr>
<td>6</td>
<td>0.69 ± 0.03</td>
<td>0.69 ± 0.05</td>
</tr>
<tr>
<td>8</td>
<td>0.60 ± 0.03</td>
<td>0.60 ± 0.03</td>
</tr>
</tbody>
</table>

Fig. 5. — The in-plane structure function $S_{\parallel}(q)/N$ versus $q L^{\nu_\parallel}$ for 4 values of $L$ in the range $21 \leq L \leq 57$ for a) $d = 4$, b) $d = 5$ and c) $d = 6$. The values for $\nu_\parallel$ are given in table I.

one introduces periodic boundary conditions does not reduce the size of the height fluctuations and change $\zeta$. At this time, the precise value of $\zeta$ in $d = 3$ remains an open question. To first order in $1/d$ [33], $\zeta = (1 - 1/d) + O(1/d^2)$, which is in remarkable agreement with the simulation results in both $d = 3$ and 4 for membranes with free boundaries. While this agreement may only be coincidence, it is intriguing. In figure 7, I have used 0.64 for $\zeta$, since this is the value which has been measured for comparable finite size systems with free boundary conditions as used in the present study. While the free ends may effect the value for $\zeta$ in the critical phase, they are less likely to effect the behavior of the system in the crumpled phase or the crossover dimension between the
Fig. 6. — The structure function $S_{12}(q)/N$ versus $qL^\zeta$ for various values of $L$ in the range $21 \leq L \leq 57$ for a) $d = 4$, b) $d = 5$ and c) $d = 6$. The values for $\zeta$ are given in table I.

Fig. 7. — The exponents $\zeta$ (o) and $\nu_{||}$ (●) as a function of the embedding dimension $d$ determined from the scaling of $S(q)$, $S_{12}(q)$ and $S_{||}(q)$. For $d \geq 5$, $\nu = \nu_{||} = \zeta$, indicating that the membranes are isotropic. The Flory exponent $\nu_F = 4/(d + 2)$ is shown for comparison.
flat and crumpled phases. One interesting point to note is that in the crumpled phase, the values of $\nu$ are significantly larger than predicted by the simple Flory theory. In terms of their fractal dimension, this means that the crumpled membranes are flatter or less crumpled, then predicted by equation (1). From the large $d$ expansion [23], one expects that the $\nu$ should approach $\nu_F$ as $d \to \infty$. This unexpected large derivation from the Flory prediction, which does not occur for polymeric fractals with smaller values of $\bar{d}$, is presumably related to the fact that $d$ and $d_{uc}$ are well separated for tethered membranes compared to systems with $\bar{d}$ near $1$.

In reference 13, Murat and I studied the properties of site-diluted tethered membranes in $d = 3$. We found that site-dilution alone was not sufficient to produce a crumpled membrane, though it did have the effect of producing a rougher membrane. For the triangular lattice used in the present simulations, the value of the order parameter $\phi$ was quite large, 0.85, in $d = 3$ for non-diluted membranes ($p = 1$). The introduction of disorder reduced this value to about 0.31 before the membranes fell apart at $p_c$. Because of the extra degrees of freedom in $d = 4$, the value of $\phi$ is significantly reduced even for $p = 1$. Thus it seemed reasonable to explore the possibility that additional site-dilution may have the desired effect of producing a crumpled phase in 4-dimensions even though it is not sufficient to do so in $d = 3$. In figure 8, I plot $\phi$ for a number of samples in both 3 and 4 dimensions. Since it is possible to only study a few samples for each value of $p$ due to the slow equilibration of the membranes, the exact magnitude of the finite size corrections to $\phi$ is not known, though I do not expect them to be large since the samples are reasonably large. For each value of $p$ typically 2-3 samples was used to determine $\phi$. In $d = 3$, there was very little sample to sample variation in the value of $\phi$ for each value of $p$ while in $d = 4$ the fluctuations were much larger. As expected $\phi$ decreases as $p$ decreases, but does not go to zero for $p > p_c$ in either $d = 3$ or 4. Since site-dilution alone cannot affect the relevancy of the higher order interactions $u_n$ for $p > p_c$, it not surprising that these membranes remained flat.


In this paper, I have shown from extensive molecular dynamics simulations that two-dimensional tethered membranes remain flat when embedded into 4-dimensions but crumple in higher dimensions. These results suggest that the induced bending rigidity which keeps these membranes flat in $d = 3$ is also present in 4-dimensions. If one assumes that this bending rigidity is generated...
by higher order interaction terms, then it is possible to interpret the transition from a flat state to a crumpled state in terms of whether these higher order terms are relevant or not. A simple Flory theory suggests that the four-body interaction terms are irrelevant above 4 dimensions and three-body terms above 6. Depending whether three-body terms alone are sufficient to generate the required bending rigidity or four-body terms are needed, Flory theory predicts \( d = 4 \) or 6 as the dimension above which the membrane should crumple. The fact that the transition occurs for \( d < 6 \) is consistent with the measured value of \( \nu \) in the crumpled phase being larger than Flory theory predicts [34]. The larger the value of \( \nu \), the smaller the fractal dimension \( d_r \). This leads to fewer interactions, as the crumpled state is less compact than predicted by equation (1), suggesting that the crossover dimension being less than 6 and \( \nu > \nu_F \) are related. However, why the crossover dimension is between \( d = 4 \) and 5 remains an open question.

![Phase diagram](image)

**Fig. 9.** — Phase diagram for polymeric fractals. The crosses represent data for linear polymers \( \tilde{d} = 1 \), the squares are for Sierpiński gaskets [3,4] and the circles are for two-dimensional tethered membranes. The open symbols are in the flat phase while the closed symbols and crosses are in the crumpled phase. The dashed line separates the flat and crumpled phase. SA stands for self-avoidance which is irrelevant in the lower right of the diagram.

In figure 9, a phase diagram for ‘polymeric fractals’ [21] determined from all available data is shown. This plot is similar to one recently published by Levinson [4] except that his contains an intermediate ‘rough’ phase \( \zeta < \nu_\parallel < 1 \), which Boal et al. [19] found for small membranes \( L \leq 17 \) in \( d = 4 \) and 5. The present simulations on much larger systems suggest that this phase does not exist. Tethered membranes in \( d = 4 \) are flat while those in \( d = 5 \) are crumpled. Combining results for linear polymers, triangular Sierpiński gaskets and tethered membranes, one sees that the phase diagram is quite rich. There is a flat phase in between the stretched regime and the crumpled regime. The crumpled regime is divided into two regions, one where self avoidance (SA) is relevant and the other where it is not. Additional data for other values of \( \tilde{d} \) would be very useful to fill out this phase diagram. Systems with values of \( \tilde{d} > 2 \), for example gels, embedded in \( d > 3 \) would be useful to examine the phase boundary between the flat and crumpled regimes. Systems with \( \tilde{d} \) in the range 4/3 to 2, would be very helpful in understanding why Flory theory is a good approximation for \( \nu \) for values of \( \tilde{d} \) near 1, but not so good for \( \tilde{d} = 2 \). I plan to carry out some of these studies in the future.
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References

[21] Since tethered membranes made in the form of a two-dimensional network of flexible linear polymers also remain flat [20], it is appropriate to use the term 'polymeric fractal' to also describe this system. Therefore in this paper, I will use the generic term 'polymeric fractals' to describe all simply connected objects which are embedded into dimension d, from linear polymer chains and percolation/gelation clusters to two-dimensional tethered membranes and three-dimensional gels.
[28] In our previous simulations of tethered membranes [13] the equations of motion were integrated with a fifth-order predictor-corrector algorithm with a smaller time step $\Delta t = 0.0067 \tau$. K. Kremer and G.S. Grest (unpublished) have found that in the presence of the heat bath, it is possible to use a much larger time step using the velocity Verlet rather than the predictor-corrector algorithm.
[34] Levinson E., private communication.