SIMULATING CRYSTALLINE MEMBRANES

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We have simulated a simple model of crystalline membranes, using Monte Carlo methods, on lattice sizes up to 128^2. We verify the existence of a crumpling transition and show that, although no bare elastic constants are introduced, it nevertheless has a stable flat phase. We measure the critical properties of this flat phase and find a good agreement with theoretical predictions. In particular we find for the *roughness exponent* $\zeta = 0.64(2)$ and a *negative* Poisson ratio for a crystalline membrane, $\sigma \approx -0.32$.

1 Introduction

Tethered or crystalline membranes, i.e. two-dimensional solid surfaces embedded in 3 dimensions, are of great theoretical interest as they exhibit a non-trivial phase structure; a transition between a *crumpled* and a *flat* phase. This is all the more interesting as the existence of a two-dimensional system with a continuous symmetry and a long-ranged order appears to violate the Mermin-Wagner theorem. This ordering is made possible by thermal fluctuations that infinitely enhance the bending rigidy of the membrane at long wavelengths, thus stabilizing the surface.

There are both biological and inorganic examples of crystalline membranes: the spectrin skeleton of red blood cells [1]; thin sheets of graphite-oxide in aqueous suspension [2]; and the rag-like structure found in MoS_2 [3].

To describe a (continuous) elastic surface, embedded in 3 dimensions, we use the Landau-Ginsburg-Wilson effective Hamiltonian

$$H_{eff} = \int \mathrm{d}^2\sigma \left[\frac{\kappa}{2} \left(\partial_\alpha \vec{\phi}_\alpha \right)^2 + \frac{t}{2} \vec{\phi}_\alpha \cdot \vec{\phi}_\alpha + u \left(\vec{\phi}_\alpha \cdot \vec{\phi}_\beta \right)^2 + v \left(\vec{\phi}_\alpha \cdot \vec{\phi}_\alpha \right)^2 \right], \quad (1)$$

where $\vec{\phi}_\alpha = \partial_\alpha \vec{r}$ is the order field and $\vec{r}(\sigma) \in \mathbf{R}^3$. If the surface is sufficiently

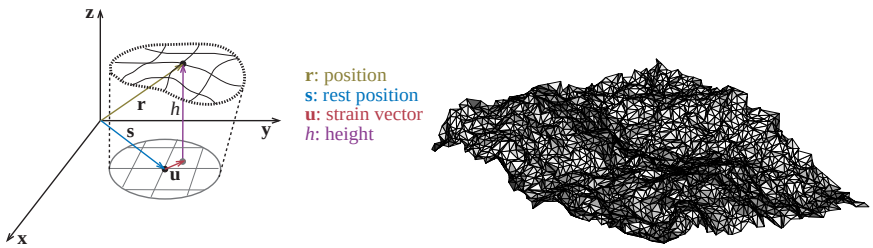

Figure 1: *Left:* The Monge representation of a crystalline membrane. *Right:* A snapshot of the surface in the flat phase ($\kappa = 1.1$) for $L = 46$.

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flat H_{eff} simplifies and can be written (in the Monge gauge, see Fig. 1) as

$$H_{\mathit{eff}} = \frac{1}{2}\int d^2\sigma \left[\kappa\,(\partial^2 h)^2 + 2\mu\, u_{\alpha\beta}^2 + \lambda\, u_{\gamma\gamma}^2\right] \tag{2}$$

where $u_{\alpha\beta} = \frac{1}{2}(\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha h \partial_\beta h)$ is the *strain tensor*, κ is the bending rigidity and μ, λ are the Lamé or elastic constants.

The model Eq. (2) has been investigated using ϵ-expansion [4] (AL) where it was found that the *whole* flat phase is critical, governed by an IR stable fixed point at infinite bending rigidity. In particular, the coupling constants acquire anomalous scaling dimensions: $\kappa_R(q) \sim q^{-\eta}$ and $\mu_R(q) \sim \lambda_R(q) \sim q^{\eta_u}$. The exponents η and η_u are related through scaling relations, together with the roughness exponent ζ which governs the scaling of the height-height correlation function; $\eta_u = 2 - 2\eta$ and $\zeta = (2-\eta)/2$. In addition to the ϵ-expansion this model has been studied in a large-d expansion [5], and by solving a set of self-consistent equations for the scaling exponents [6] (SCSA). The resulting exponents are compared to numerical simulations in Table 1.

2 Numerical simulations

For numerical investigations we need an appropriate discretization of a crystalline membrane. Conventionally this is done by a regular triangular lattice, with *fixed* connectivity, and a Hamiltonian containing two terms: a pair potential and a bending energy term. The former can be modelled as tethers between hard spheres or by introducing a repulsive potential between the nodes. Here we use much simpler approach, a Gaussian potential between neighboring nodes. The bending energy term is introduced explicitly as a ferromagnetic

interaction between normals on neighboring triangles:

$$H = \frac{1}{2}\sum_{<ij>}(\vec{r}_i - \vec{r}_j)^2 + \frac{\kappa}{2}\sum_{<ab>}(1 - \vec{n}_a \cdot \vec{n}_b) \tag{3}$$

where $\vec{r}_i$ is the position of node i and $\vec{n}_a$ is a normal to triangle a. Notice that the tethering potential has vanishing equilibrium length, hence no explicit elastic constants are introduced. For the surface to have a stable flat phase they must therefore be dynamically generated. Also, Eq. (4) defines a *phantom* surfaces, i.e. without self-avoidance. For the flat phase this is expected to be irrelevant, albeit the nature (existence) of the crumpling transition may depend on this.

We have simulated this model using Monte Carlo methods. As we are mostly interested in the flat phase, we choose to simulate a surface with free boundaries. This simplifies considerably the analysis of various observables such as correlation functions. We use lattice sizes ranging from 256 to 16394 nodes and update them with a local Metropolis algorithm. We performed 5×10^7 to 10^8 sweeps per volume and coupling — typically this gave 150 to 1000 independent configurations. For details of the simulations see [7].

3 Results

3.1 The crumpling transition

We have verified the existence of a crumpling transition in the model by measuring the specific heat at different values of the bending energy κ (Fig. 2). It displays a divergent peak at $\kappa_c \approx 0.79$ — preliminary estimate of the critical exponents yields $\alpha \approx 0.4$, indicating a $2nd$ order phase transition. To probe the nature of the two phases we looked at the *radius of gyration*, $R_g^2 = \langle \sum_i \vec{r}_i \cdot \vec{r}_j \rangle / N$, which measures the linear extend of the surface. Its scaling with system size, $R_g \sim N^{1/d_H}$, defines the Hausdorff dimension d_H. We find $d_H = 2.1(1)$ in the flat phase (as expected), while R_g grows logarithmically with volume in the crumpled phase.

3.2 The flat phase

To investigating the critical behavior of the flat phase we have measure the *height* and *phonon fluctuations* and the *normal-normal correlation function* — those give us ζ, η_u and η, respectively.

To measure the height fluctuations $\langle h^2 \rangle$ we need an estimate of the width of the surfaces. This is provided by the minimal eigenvalue of the *shape tensor*

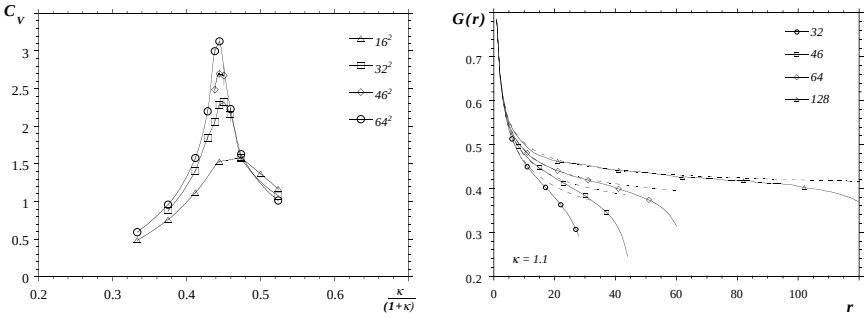

Figure 2: *Left:* The specific heat. *Right:* The normal-normal correlation function in the flat phase.

$S_{\alpha\beta} = \langle \sum_\sigma r_\alpha(\sigma) r_\beta(\sigma) \rangle_c$, $(\alpha, \beta = 1, 2, 3)$. The height fluctuation scale as $\langle h^2 \rangle \sim L^{2\zeta}$. At bending energy $\kappa = 1.1$ we find $\zeta = 0.64(2)$ (Table 1). Previous numerical simulations on similar models, have found values in the range 0.5 – 0.7 (see [7] for a comprehensive list).

The phonon fluctuations (the strain tensor) measures the deviation of the membrane from a rigid surface. We estimated those deviations by projecting the surface onto a flat plane, and comparing the projected node position to their rest value. It is trivial to show that $\langle |\vec{u}| \rangle \sim L^{\eta_u}$. Our measurements give $\eta_u = 0.50(1)$, implying $\eta \approx 0.75$.

Finally the normal-normal correlation function. In the flat phase we expect it to have a non-zero asymptote, $\langle \vec{n}_\sigma \cdot \vec{n}_o \rangle \sim C + c/r^\eta$, implying a long-range order in the surface. Here r is a geodesic distance between the center o and node σ. Since we use free boundaries, the surface is not translationally invariant and we only measure the correlations from the center. This is shown in Fig. 2 for $\kappa = 1.1$. Our best fit to the data implies $\eta \approx 0.62$.

3.3 The Poisson ratio

In addition to the anomalous scaling of the coupling constants, one of the most dramatic effect of fluctuations on a crystalline membrane is the prediction of a *negative* Poisson ratio σ. The Poisson ratio measures the in-plane transverse response of the surface when it is stretched in the longitudinal direction. For conventional matter, which shrinks in the transverse direction, it is defined to be positive. Analytical calculations predict for a crystalline membrane: $\sigma = -1/3$ (SCSA [6]) or $\sigma = -1/5$ (AL [4]). The unusual sign of σ is due to entropic suppression of the height fluctuations when stress is applied [8].

Table 1: Theoretical predictions and numerical results for the exponents governing the critical behavior of the flat phase.

	ζ	η_u	$\nu = 2/d_H$	η
AL	13/25 or 0.52	2/25 or 0.08	1	24/25 or 0.96
Large-d	2/3	2/3	1	2/3
SCSA	0.590	0.358	1	0.821
MC	0.64(2)	0.50(1)	0.95(5)	0.62

The Poisson ratio can be defined in terms of correlation functions at zero external stress using linear response theory [9]:

$$\sigma \;=\; -\,\frac{\langle u_{xx}u_{yy}\rangle_c}{\langle u_{yy}^2\rangle_c} \;=\; -\,\frac{\langle g_{xx}g_{yy}\rangle_c}{\langle g_{yy}^2\rangle_c} \tag{4}$$

where $g_{ij} = \partial_i\vec{r}\partial_j\vec{r}$ is the induced metric ($u_{ij} = g_{ij} - \delta_{ij}$). Our best estimate of the Poisson ratio, for $\kappa = 1.1$ and $N = 128^2$, is $\sigma = -0.32(2)$, in good agreement with the predictions from [6]. Earlier numerical simulations [10], on the other hand, found $\sigma = -0.15(1)$. Although it is hard to compare directly those simulations with ours, due to different simulations methods and discretization, this is a significant discrepancy. A possible explanation is that very small lattice are used in [10] — certainly we see big finite size effects in our simulations.

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