

First-order transition of tethered membranes in three-dimensional space

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We study a model of phantom tethered membranes, embedded in three-dimensional space, by extensive Monte Carlo simulations. The membranes have hexagonal lattice structure where each monomer is interacting with six nearest-neighbors (NN). Tethering interaction between NN, as well as curvature penalty between NN triangles are taken into account. This model is new in the sense that NN interactions are taken into account by a truncated Lennard-Jones potential including both repulsive and attractive parts. The main result of our study is that the system undergoes a *first-order crumpling transition* from low-temperature flat phase to high-temperature crumpled phase, in contrast with early numerical results on models of tethered membranes.

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I. INTRODUCTION

Statistical mechanics of membranes is a rich subject and has been studied since about twenty years. Motivations to obtain a full understanding of the behavior of these complex systems are enforced by many experimental realizations. For recent reviews, see Refs. [1] and [2]. See also Ref. [3] for many introducing and pedagogical courses on the subject.

Membranes are two-dimensional fluctuating systems of monomers. According to their physical properties, membranes can be “fluid” or “tethered.” Fluid membranes consist of freely moving monomers, i.e., with Hamiltonian depending only on the shape of membranes. On the contrary, monomers in tethered membranes are tied together by a tethering potential and their connectivity is fixed. In addition, a membrane can be self-avoiding if intersections with itself are forbidden. Otherwise, it is a phantom membrane. In this paper, we focus our attention on a model of tethered membranes with external curvature energy without self-avoidance.

Any realistic model should include self-avoiding interactions. But phase diagrams of phantom membranes are rich and contribute to understand the behavior of self-avoiding membranes [4,5]. It is now firmly established that phantom membranes undergo a crumpling transition between a flat and a crumpled phase. The flat phase possesses long-range orientational order between the normal to the surfaces whereas the crumpled phase is totally disordered. However, the nature of the crumpling transition is still puzzling. Renormalization group (RG) calculations [6] with a Landau continuous model [7] predict a discontinuous phase transition when the dimension d of the embedding space is lower than 219, including the physical case $d=3$. This continuous model describes membranes as D -dimensional manifolds with internal flat coordinates σ , embedded in a d -dimensional (euclidean) space, where the position of σ is denoted by $\mathbf{r}(\sigma)$. Tangents $\mathbf{t}_\alpha = \partial\mathbf{r}/\partial x^\alpha$ are identified as the order parameter of the crumpling transition, i.e.,

$$\langle \mathbf{t}_\alpha \rangle = 0 \quad \text{in the crumpled phase} \\ \neq 0 \quad \text{in the flat phase.}$$

Following a standard method, a free energy functional F is built for the $\{\mathbf{r}(\sigma)\}$ by a Landau-Ginzburg expansion in \mathbf{t}_α . Moreover, rotational invariance is required. This leads to

$$F\{\mathbf{r}(\sigma)\} = \int d^D\sigma \frac{t}{2} (\partial_\alpha \mathbf{r})^2 + \frac{\kappa}{2} (\partial_\alpha \partial_\alpha \mathbf{r})^2 + u (\partial_\alpha \partial_\beta \mathbf{r})^2 \\ + v (\partial_\alpha \mathbf{r} \partial_\alpha \mathbf{r})^2 + \frac{b}{2} \int d^D\sigma_1 \int d^D\sigma_2 \delta^{(d)}(\mathbf{r}(\sigma_1) \\ - \mathbf{r}(\sigma_2)).$$

κ is the bending rigidity, coupled to the square of the extrinsic curvature. t , u , and v are harmonic and anharmonic elastic coefficients. b is the coupling constant for self-avoiding energy. Higher-order terms in the expansion are expected to be irrelevant in the infrared limit.

In the phantom case ($b=0$), continuous crumpling transition is expected by mean-field arguments for $t=0$. Taking into account the fluctuations, long distance behavior can be obtained *via* renormalization group technics, using an $\epsilon=4-D$ expansion. The authors of Ref. [6] calculated the β functions to the lowest order in ϵ . They found no stable fixed point for d (the dimension of the embedding space) less than $d_c \simeq 219$, interpreting this as a weak fluctuation-driven first-order phase transition. However, this prediction may not be reliable in the physical case ($d=3, D=2$) corresponding to $\epsilon=2$.

On the other hand, numerical simulations of lattice models [8–18], large d expansion [19] and calculations based on truncations [20] of the Schwinger-Dyson equations are consistent with a continuous phase transition.

In this paper, we try to shed light on this contradiction with an extensive Monte Carlo (MC) study on a model of phantom tethered membranes with bending rigidity. As it turns out, our results show that the crumpling transition within our model is of first order in agreement with the RG prediction of [6].

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Section II is devoted to a description of the model. Our method is described in Sec. III and the results are shown in Sec. IV. Concluding remarks are given in the last section.

II. THE MODEL

We consider a two-dimensional (2D) lattice of monomers connected in hexagonal structure, and embedded in the physical 3d euclidean space. The tethering potential between nearest-neighbor (NN) monomers is a truncated Lennard-Jones (LJ) potential. The curvature energy is a standard normal-normal interaction between NN triangles. The distance between NN monomers is not allowed to be larger than an upper bound distance R_{max} . Otherwise, in the absence of R_{max} , monomers are no longer effectively tethered at high temperature and the system becomes a gas. In order to keep essential features of the LJ potential, R_{max} must be sufficiently larger than r_0 , the NN distance corresponding to the minimum of the potential, so that R_{max} lies in the flat asymptotic region of the potential. However, to have an actual tethered membrane, R_{max} should not be too large as discussed above. Moreover, equilibration times increase as R_{max} increases, since NN distances are then allowed to grow more and more.

The system is described by the Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} U(r_{ij}) - K \sum_{\langle \alpha \beta \rangle} \mathbf{n}_\alpha \cdot \mathbf{n}_\beta. \quad (1)$$

The first sum is performed on pairs of NN monomers $\langle i, j \rangle$ only, and the second one is restricted to pairs of NN triangles $\langle \alpha, \beta \rangle$. Tethering interaction between NN monomers labeled by i and j depends only on their distance r_{ij} in the 3d embedding space and is described by $U(r_{ij})$,

$$U(r_{ij}) = U_o \left[\left(\frac{r_o}{r_{ij}} \right)^{12} - 2 \left(\frac{r_o}{r_{ij}} \right)^6 \right] \text{ if } r_{ij} < R_{max} \\ = 0 \text{ if } r_{ij} \geq R_{max}, \quad (2)$$

with $r_{ij} = \|\mathbf{r}_i - \mathbf{r}_j\|$, \mathbf{r}_i and \mathbf{r}_j being the position vectors in the 3d space. r_o is the equilibrium distance between NN monomers. The second term in Eq. (1) is the external curvature energy, with K the bending rigidity. The 3d-vector \mathbf{n}_α is defined as the normal unit vector of the α th triangle formed by three NN monomers. Note that \mathbf{n}_α is defined for a counterclockwise oriented triangle.

The phase space of the model depends on three parameters. We fix two of them, namely U_o and K , and look for temperature-dependent properties.

III. NUMERICAL METHOD

We consider a membrane of linear size L . The total number of monomers is $N = L \times L$. We choose $U_o = 3$ and $K = 1$. A more extensive study would require to explore the complete phase space, but these particular values already give interesting results. In the following, $K = 1$ is taken as unit of energy. We take also $k_B = 1$ (Boltzmann constant) to simplify the temperature unit. The NN distance in the ground

state is taken to be the unit of distance, i.e., $r_o = 1$, and the upper bound $R_{max} = 4$. We use free boundary conditions, at constant pressure in our simulations.

The following algorithm was used. Starting from the ground state where monomers are on the hexagonal lattice sites, we heat the system to a temperature T . We equilibrate the system at variable volume. The local equilibration is done as follows: we take a monomer and move it to a nearby random position in a cubic box of volume δ^3 around its position, in the 3d space. This position is accepted if it lowers the energy. Otherwise it is accepted with a probability according to the Metropolis algorithm. We repeat this for all monomers: we say we achieve one MC step/monomer. We choose $\delta \approx 0.1$ to have an acceptance of the order of 50%.

We define the following physical quantities - averaged total energy $\langle E \rangle$, averaged normal vector $\langle n \rangle$, averaged NN distance $\langle d \rangle$, radius of gyration R_g with the following standard definitions:

$$\langle E \rangle = \langle \mathcal{H} \rangle, \quad (3)$$

$$\langle n \rangle = \frac{1}{2(L-1)^2} \left\langle \left| \sum_{\alpha} \mathbf{n}_{\alpha} \right| \right\rangle, \quad (4)$$

$$\langle d \rangle = \frac{1}{(3L-1)(L-1)} \sum_{\langle i, j \rangle} \langle r_{ij} \rangle, \quad (5)$$

$$R_g^2 = \frac{1}{2L^4} \sum_{i, j} \langle (\mathbf{r}_i - \mathbf{r}_j)^2 \rangle, \quad (6)$$

where $\langle \dots \rangle$ indicates thermal average and the sum in $\langle d \rangle$ is performed only on NN links.

All the results described below are obtained after thermalization of the system. This requires about $10^6 - 10^7$ MC steps/monomer, depending on the temperature. After thermalization, measures are done on $10^6 - 10^7$ MC steps/monomer, depending also on the temperature.

Error bars are calculated using a standard jack-knife algorithm.

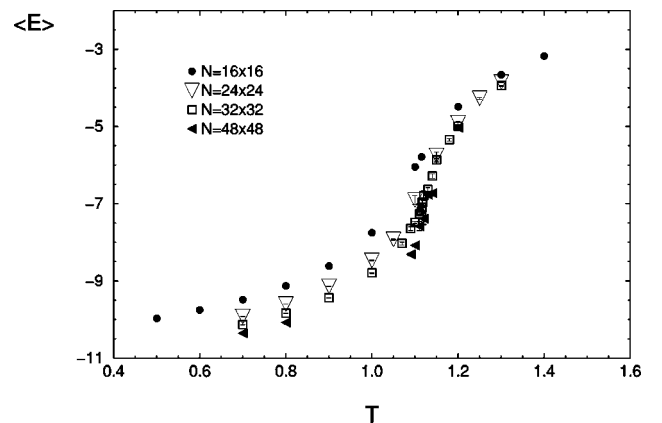


FIG. 1. Averaged energy versus temperature, for $N = 16 \times 16$, 24×24 , 32×32 , and 48×48 .

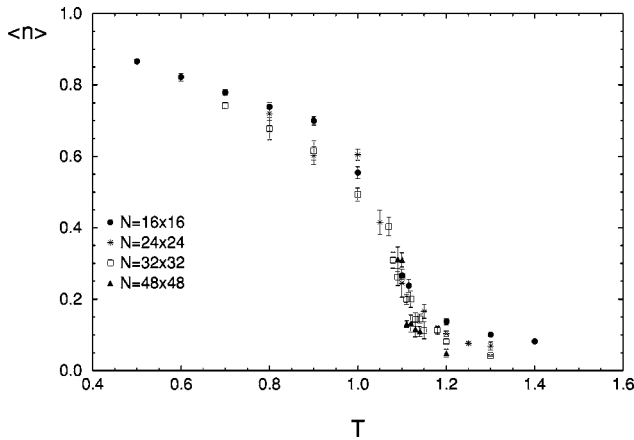


FIG. 2. $\langle n \rangle$ versus T , for $N=16 \times 16$, 24×24 , 32×32 , and 48×48 .

IV. RESULTS AND ANALYSIS

At low temperature, equilibrium configurations are configurations of minimum energy. This means that NN distance must be close to r_o , the minimum of the LJ potential, and that NN normals must be parallel to minimize curvature energy. So, equilibrium states correspond to a flat state, with $\langle n \rangle \approx 1$ and $R_g \approx L$. It is an ordered phase.

At high temperature, maximal entropy configurations correspond to crumpled states, where the membrane is compact and occupies a very small volume in the embedding space. It is a completely disordered phase, with $\langle n \rangle = 0$ and $R_g \ll L$.

Between low and high temperatures, a crumpling phase transition is expected. In this work, we study the nature of this transition to see whether it is continuous or not.

As a first point, we measured $\langle E \rangle$, $\langle n \rangle$, $\langle d \rangle$ and R_g versus temperature for sizes $N=16 \times 16$, $N=24 \times 24$, $N=32 \times 32$, and $N=48 \times 48$. Results are shown in Figs. 1, 2, 3, and 4.

It turned out that equilibration times are very large for this system. So, as we were interested in critical properties, we concentrated our work on the temperature region around the phase transition, especially for $N=48 \times 48$. Figures 1, 2, 3, and 4 clearly show a phase transition between a flat and a

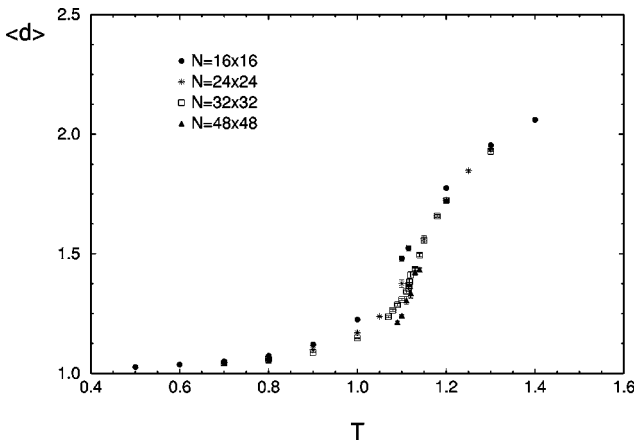


FIG. 3. Averaged NN distance $\langle d \rangle$ versus T , for $N=16 \times 16$, 24×24 , 32×32 , and 48×48 .

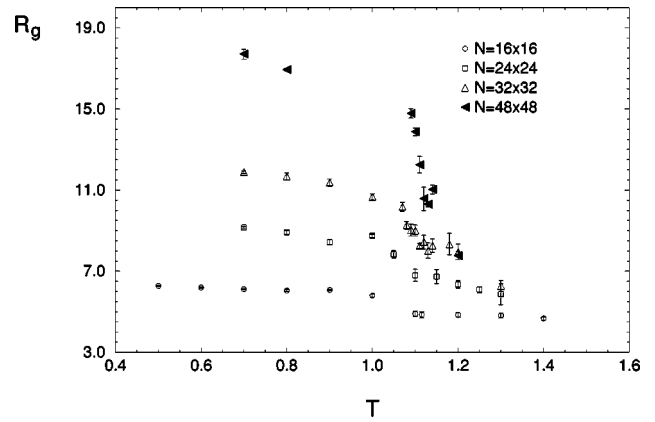


FIG. 4. Averaged gyration radius R_g versus T , for $N=16 \times 16$, 24×24 , 32×32 , and 48×48 .

crumpled phase at $T \approx 1.1$: there is a sharp jump of $\langle E \rangle$ from the low- T flat phase to the high- T crumpled phase. Note that the slope of $\langle E \rangle$ increases with size in the transition region. The order parameter $\langle n \rangle$ drops from a finite value (this value would clearly tend to 1 as T tends to zero) to a vanishing value, as expected for an order-disorder transition.

At the transition, R_g falls from a finite value dependent of the linear size L to a small value more or less independent of L . This corresponds to the scaling $R_g \sim L^\nu$, with $\nu = 1$ in the flat phase and $\nu = 0$ (indeed, a logarithmic dependence) in the crumpled phase. It should be noticed that the NN distance remains finite in the crumpled phase, which means that monomers actually still form a tethered membrane even in the high-temperature phase as discussed earlier.

The second purpose of our work was to determine whether the transition is continuous or not. A standard method, when using numerical simulations, consists in a finite size scaling analysis of the maximum of the specific heat C_v . For a second-order phase transition, it is expected to grow as the linear system size. For a discontinuous transition, there are in principle discontinuities in thermodynamic quantities. However, for small systems, a discontinuous phase transition can appear to be continuous if the correla-

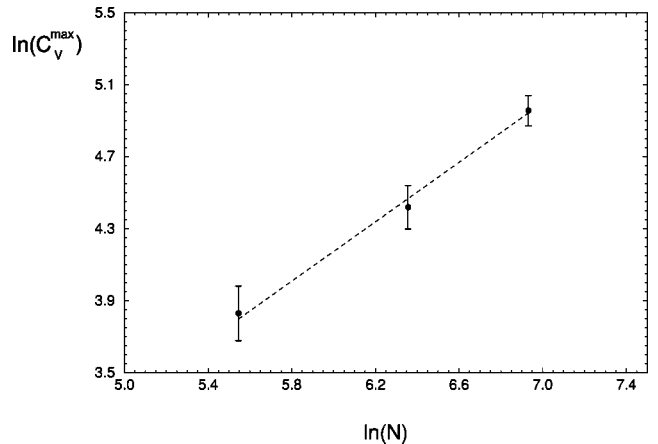


FIG. 5. C_v^{max} versus N in logarithmic coordinates, for $N=16 \times 16$, $N=24 \times 24$, and $N=32 \times 32$. The dashed line is the best fit.

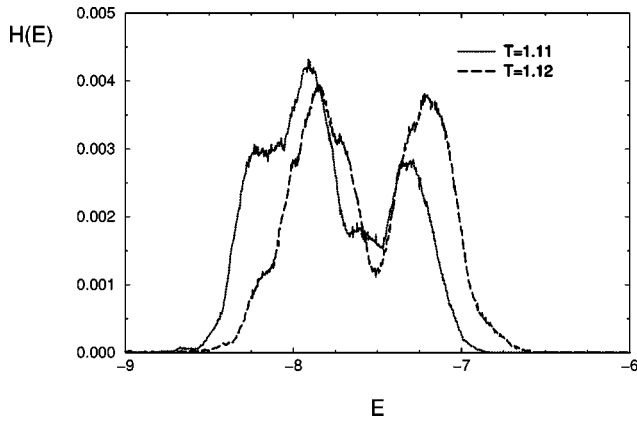


FIG. 6. Normalized histogram for the energy, for $N=48 \times 48$. The double-peak structure shows the first-order character of the phase transition in the critical region ($T=1.11$ and $T=1.12$).

tion length is greater than the linear size of the system. In that case, C_v^{max} is expected to grow as the size of the system [21].

We measured C_v^{max} for $N=16 \times 16$, $N=24 \times 24$, and $N=32 \times 32$ using the histogram technique [22]. For these small sizes, energy histograms have a single peak for all temperatures we explored around the transition (multihistogram method). They are found more or less Gaussian.

In Fig. 5, we plot C_v^{max} versus N in logarithmic scale. Fitting these data, we obtain $C_v^{max} \sim N^x$ with $x=0.83(12)$. This value is far from the value $x=0.5$ expected for a continuous transition. It is closer to 1, the theoretical value for a first-order transition as discussed above. At this stage, in view of this, we conjecture that the transition is of first order. As seen below this conjecture is confirmed by histograms made for a larger size.

In order to check further the first-order character of the transition, we increase L . For large L , if the transition is of first order, the energy histogram should show a structure of multiple peaks corresponding to the coexistence of ordered and disordered phases at the transition. The system would go back and forth between these phases resulting in a double-peak energy histogram. Taking $L=48$, we indeed observed this double-peak histogram in the region $T \approx 1.1$, as shown in Fig. 6. Note that above and below the critical region, this double-peak structure is absent, as shown in Fig. 7. This is a very strong signal which confirms the first-order character of the crumpling transition found earlier by finite-size scaling of C_v^{max} .

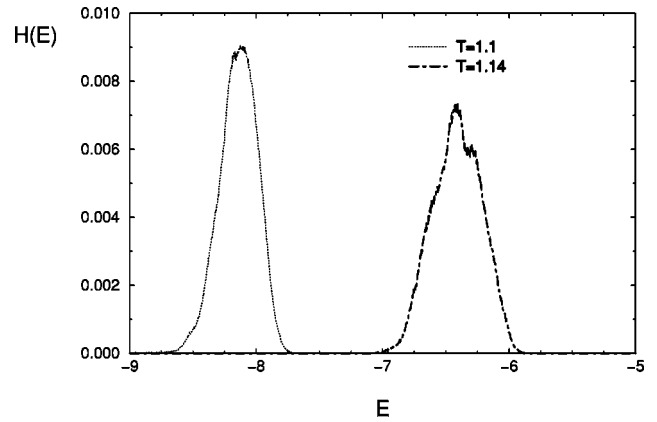


FIG. 7. Normalized histogram for the energy, for $N=48 \times 48$: the single-peak structure above ($T=1.14$) and below ($T=1.1$) the critical region.

V. CONCLUSION

We have studied the crumpling phase transition by MC simulation of a model of tethered membranes with LJ potential energy and bending rigidity. We have shown clearly the first-order nature of the phase transition between flat and crumpled phases, in contrast with earlier simulations using Gaussian tethering interaction. Note that these early MC results [8–18] and also analytical calculations [19,20] show a *continuous* phase transition for models which do not include anharmonic excitations. We believe that the anharmonic nature of the LJ potential used in our model to some extent contributes to the first-order transition observed here. We did not vary in this work the value of bending rigidity K . Let us mention however that for $K=0$, there is no flat phase, the membrane is crumpled at all T .

It would be interesting to include self-avoidance between non-nearest-neighbors in our model. However, it seems that in that case the precise form of NN potential is irrelevant: for repulsive self-avoidance between non-nearest-neighbors the membrane is always flat regardless of the form of the potential between NN, even in the absence of bending rigidity. [8,9,23,24] This is interpreted as an effective bending rigidity induced by excluded volume effect. This can be overcome by an attractive interaction between non nearest-neighbors in addition to the repulsive self-avoiding interaction, leading to the folding of the membrane at low T and a flat phase at high T [25]. Including such repulsive and attractive interactions between non-nearest-neighbors in our model is a formidable task which is left for future investigations.

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