The Crumpling Transition of Dynamically Triangulated Random Surfaces

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Abstract

We present the crumpling transition in three-dimensional Euclidian space of dynamically triangulated random surfaces with edge extrinsic curvature and fixed topology of a sphere as well as simulations of a dynamically triangulated torus. We used longer runs than previous simulations and give new and more accurate estimates of critical exponents. Our data indicate a cusp singularity in the specific heat. The transition temperature, as well as the exponents are topology dependent.

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1 Introduction

In this paper we are concerned with the statistical mechanics of surfaces. A possible approach in space dimensions $D > 1$ is to discretize the surface using a triangulation [1-4]. For this we need to specify the Hamiltonian $H$. The surface $S$ is replaced by a simplicial triangulation $T$, specified by the number of nodes $N$, of links and triangles, and the $X$-coordinate field by the coordinates $X$ of the nodes. The metrical fluctuations of the manifold are modeled by summing over triangulations induced by link-flips [5-7]. The Hamiltonian is now choosen, such that the partition function is not dominated by configurations with spikes. In order to suppress these spikes one adds a term with extrinsic curvature. As a function of the extrinsic curvature the model shows a transition (crumpling transition) at finite rigidity of the surface [8-18].

In a previous paper, we discussed the extrinsic and intrinsic geometrical properties of dynamically triangulated random surfaces (for example the Hausdorff-dimension, spectral and spreading dimension) above, below and at the transition [32].

The partition function of the above model can be written as

$$Z_N = \int d^D X_0 \int \prod_{i=1}^{N-1} d^D X_i e^{-\mathcal{H}}$$

where the translational mode is integrated out. The Hamiltonian $\mathcal{H}$ is defined as

$$\mathcal{H} = \beta \cdot \sum_{\langle i,j \rangle} (X_i^\mu - X_j^\mu)^2 + \lambda \cdot \sum_{\Delta_i,\Delta_j} (1 - \hat{n}_{\Delta_i} \cdot \hat{n}_{\Delta_j}) - \alpha \cdot \sum_{i=0}^{N} \log \sigma_i$$

The Gaussian part of the Hamiltonian $\mathcal{H}_g$ is a sum over the positions $X$ in embedding Euclidian space of all nearest neighbours nodes, i.e. all links of the triangulation. We shall use $\beta = 1$ because of the rescaling invariance.

$\mathcal{H}_e$ is an edge extrinsic curvature term [19-26]. $\sum_{\Delta_i,\Delta_j}$ denotes a summation over all adjacent triangles which share an edge and $\hat{n}_{\Delta_i} \cdot \hat{n}_{\Delta_j}$ is the scalar product of the vectors normal to a triangle.

The third part of the Hamiltonian $\mathcal{H}_m$ is the discretization of the square root of the metric. $\sigma_i$ denotes the number of nearest neighbours of node $i$. $\alpha$ depends on the measure. We used $\alpha = D/2$ for the simulations in $D = 3$ dimensional embedding space.

Here we investigate such a model numerically (Monte Carlo simulations), applying finite-size scaling ideas. These ideas have proven successful in other contexts for the analysis of phase transitions. We expect that the above model shows a phase transition at some critical value of the coupling $\lambda$. There are several questions which we want to address: What is the order of the transition? If the transition is of second order, what are the exponents? Are the exponents topology dependent? Is the transition temperature topology dependent?
2 Simulation Method and Autocorrelations

First let us study the effect of the extrinsic curvature on the auto-correlation time of several observables, i.e., we are interested in the dynamics of a random surface induced by a Monte Carlo process. Such a study is of course a prerequisite for a detailed numerical study of the apparent transition which such surfaces undergo as a function of a bending rigidity. From our results which we present below we must conclude that extensive computer resources must be applied because of the very long relaxation times which even for moderate surface sizes can reach several tenths of thousands sweeps.

We want to look at the closed dynamically triangulated random surfaces without self-avoidance. As models for such surfaces we take the first two topologically closed surfaces: The sphere and the torus (c.f. Figure 1). The torus is specified by identifying edges of the parameter space \( \mathcal{P} \) whereas the sphere, because of its genus needs a slightly more complicated set-up procedure.

Figure 1: Shown are two examples of configurations of dynamically triangulated random surfaces. The left picture shows a sphere and the right part a torus.

What we are interested in is to calculate the auto-correlation function of an observable \( \mathcal{O} \) as a function of time

\[
\rho_{O}(t, N) = \frac{<\mathcal{O}(0)\mathcal{O}(t)>_{N} - <\mathcal{O}>^{2}_{N}}{<\mathcal{O}^{2}>_{N} - <\mathcal{O}>^{2}_{N}}
\]

and its dependence on the number of nodes \( N \) of the surface. From the auto-correlation function we are then able to extract the auto-correlation time \( \tau_{O}(N) \). This is done calculating the integrated auto-correlation function, i.e.,

\[
\tau_{int,O} = \frac{1}{2} \int_{-\infty}^{+\infty} dt \; \rho_{O}(t, N).
\]

We also compared the integrated auto-correlation time with the exponential correlation time and the statistical inefficiency, but found no disagreement within the errors. If the successively generated configurations can be considered as non-interacting beads as is done in the Rouse theory \([27, 28]\) we will find for example for the radius of gyration

\[
\tau_{R_{gyr}^{2}} \propto N
\]

and in general we expect

\[
\tau_{O} \propto N^{a}.
\]

To calculate observables such as the gaussian part \( \mathcal{H}_{g} \) of the Hamiltonian or the radius of gyration \( R_{gyr} \), we use the standard Monte Carlo algorithm \([29-31]\). Such an algorithm induces a stochastic dynamics and all our results apply only to such an induced dynamics. One Monte Carlo sweep is completed when each triangulation point was given the chance for a displacement from its previous position and the edges of the triangulation were given the chance to re-connected or flip to an...
orthogonal position (c.f. Figure 2). The flip operation implements the sum over all possible triangulation). This corresponds to one new configuration.

Table 1 summarizes our results for the exponent $a$ for the sphere. The exponents where extracted from the data of system sizes from 36 up to 288. At this point we should mention that the expected transition is at $\lambda_c \approx 1.5$. Out data was collected above and below the transition.

Above and below the transition the radius of gyration shows the Rouse behaviour. The gaussian part of the Hamiltonian shows clearly a dependence on the bending rigidity. Above the transition point the auto-correlation exponent changes to one and below it is almost zero. The same holds for the edge part of the Hamiltonian.

| $\lambda$ | $\tau_{H_{\text{gaussian}}}$ | $\tau_{H_{\text{edge}}}$ | $R_{\text{gyr}}^2$ | shift | flips |
|-----------|-------------------------------|---------------------------|---------------------|-------|-------|
| 0.00      | $0.2 \pm 0.3$                 | $0.2 \pm 0.2$             | $1.1 \pm 0.2$       | 0.51  | 0.76  |
| 1.00      | $0.1 \pm 0.3$                 | $0.4 \pm 0.2$             | $1.1 \pm 0.4$       | 0.51  | 0.36  |
| 1.75      | $1.0 \pm 0.1$                 | $0.8 \pm 0.2$             | $1.1 \pm 0.2$       | 0.47  | 0.28–0.34 |
| 3.00      | $1.0 \pm 0.1$                 | $1.0 \pm 0.1$             | $1.0 \pm 0.3$       | 0.50  | 0.23–0.33 |

Table 1: Table of the results for the exponent $a$ on the auto-correlation times of dynamically triangulated random sphere. $\lambda$ is the measure of the bending rigidity. Shift and flips give the acceptance probability for a displacement of a node and flip for an edge change.

Almost all of the observations for the spherical case carry over to the case of the torus.

3 Results of the Simulations

Finite size scaling assumes, that there is only one relevant linear length scale, which is compared to the correlation length. To apply finite size scaling to the crumpling transition of dynamically triangulated random surfaces (DTRS) one must therefore assume a single length scale determined by the number of nodes $N$ and the internal dimension $d$ of the surface

$$L \propto N^{1/d}.$$  

This internal dimension $d$ also depends on the external properties of the surface and $\lambda$.

So let us first look at the specific heat. If the transition is of second order we would have
\[ C(\lambda, L) = L^{\alpha/\nu} \hat{C} \left[ (\lambda - \lambda_c)L^{-\nu} \right] \]  
(8)

where \( \hat{C} \) is a scaling function, which depends on how one implements the surface. At the critical \( \lambda \) the scaling function is regular and the scaling hypothesis leads to

\[ C_N^{\text{max}} \propto AN^{\alpha/\nu d} + \ldots \]  
(9)

for the scaling of the peak in the specific heat. If we assume a first order transition then \( C_N^{\text{max}} \) diverges as \( L^d \) because of the \( \delta \)-distribution of \( C_{\infty}(T) \) \[33, 34, 35\].

An evaluation of the specific heat \( C \) of DTRS (neglecting the metric contribution \( H_m \)) gives the following expression

\[ C_{\text{all}} = \frac{D}{2} + \frac{\lambda^2}{N}(\langle H_e^2 \rangle - \langle H_e \rangle^2) \]  
(10)

The first part is related to the Gaussian Hamiltonian \( H_g \) and the second to the specific heat \( C \) of the edge extrinsic curvature \( H_e \). The specific heat for the edge extrinsic curvature is shown in Figure 3 for the two topologies considered. The interpolation was done by the method of Ferrenberg and Swendsen \[36, 37\] using histograms of \( H_e \).

**Figure 3:** Specific heat \( C \) (edge extrinsic curvature part) of the sphere (left part) and of the torus (right part).

**Figure 4:** Maximum of the specific heat \( C_N^{\text{max}} \) of the torus (\( \bigcirc \)) and the sphere (\( \Box \)).

Using the data of the specific heat obtained by applying the extrapolation method, we can get a very accurate estimate of the positions of the maxima and of the heights. Figure 3 shows \( C_N^{\text{max}} \) of the torus and the sphere. A change to \( L^d \) behaviour is very unlikely and for that reason the data strongly suggest a continuous phase transition in agreement with previous work \[8,14-17,38,39\]. From the data shown in Figure 4 we can obtain the following upper boundaries of critical exponents

\[ \text{Sphere: } \frac{\alpha}{\nu d} \leq 0.00 \pm 0.04 \quad \text{Torus: } \frac{\alpha}{\nu d} \leq 0.06 \pm 0.02 \]  
(11)

Using this simple method, we cannot distinguish a diverging specific heat with very small but positive \( \alpha \), a logarithmic divergence \( \alpha_s = 0 \) and a power law cusp \( \alpha_s < 0 \), where \( \alpha_s \) denotes the exponent of the singular part of the specific heat. We will use the abbreviation \( \alpha \) instead of \( \alpha_s \).

Following Fisher \[40\], these three cases may be distinguished with a fit of the form
\[ C(\Delta \lambda) = A \cdot \frac{1}{\alpha} (\Delta \lambda^{-\alpha} - 1) + B, \quad \Delta \lambda = \left| \lambda_c^N - \lambda \right| \] (12)

Figure 5 shows such fits for \( \alpha = 0.1 \) (power law), \( \alpha = -0.01 \) (near logarithmic) and \( \alpha = -1.2, -2.0 \) (power law cusp). The fits clearly favour a power law cusp of the specific heat with a large negative value of \( \alpha \), although we were not able to estimate the exponent \( \alpha \) precisely.

Figure 5: Plot of the specific heat \( C \) against \( x = \frac{1}{\alpha} (\Delta \lambda^{-\alpha} - 1) \) with \( \alpha = 0.1 \) (upper left), \( -0.01 \) (upper right), \( -1.2 \) (lower left) and \( \alpha = -2.0 \) (lower right).

Our results are in contrast to the estimates of Renken and Kogut \( \alpha/\nu d = 0.14(3) \) for the sphere. They assumed scaling above \( N = 72 \), but the more accurate data in Figure 4 shows that this assumption is not true. The decreasing slope in Figure 4 is also present in their Figure 5 \( \alpha/\nu d = 0.185(50) \), but they used a different discretization based on \( \phi^3 \) graphs with a flip acceptance rate of only \( O(1\%) \) at \( \lambda_c \approx 1.5 \) and larger correlation times of the edge extrinsic curvature than in our discretization.

Another possibility to determine the order of the transition is the cumulant \( \mathcal{V}_N \) of the edge extrinsic curvature

\[ \mathcal{V}_N := 1 - \frac{1}{3} \frac{\langle H_e^4 \rangle_N}{\langle H_e^2 \rangle_N^2}, \] (13)

which behaves quite differently at temperature driven first- and second-order transitions

\begin{align*}
1. \text{ and 2.order:} & \quad \mathcal{V}_N \big|_{\text{min}} \xrightarrow{N \to \infty} \frac{2}{3}, \quad T \neq T_c, \text{fixed} \quad (14) \\
2. \text{order:} & \quad \mathcal{V}_N \big|_{\text{min}} \xrightarrow{N \to \infty} \frac{2}{3}, \quad T = T_c(N) \quad (15) \\
1. \text{order:} & \quad \mathcal{V}_N \big|_{\text{min}} \xrightarrow{N \to \infty} 1 - \frac{2(E_+^4 + E_-^4)}{3(E_+^2 + E_-^2)^2}, \quad T = T_c(N) \quad (16)
\end{align*}

\( E_+ \) and \( E_- \) are the energies of the system above and below the transition. For a very weak first-order transition \( (E_+ \approx E_-) \) we also have \( \mathcal{V}_N \big|_{\text{min}} \approx 2/3 \).

We computed \( \mathcal{V}_N \) defined by equation (13) using again the method of Ferrenberg and Swendsen \( \alpha/\nu d = 0.14(3) \). The resulting figures show the predicted single peak minima with wings following equation (14). The finite size dependence of the minima of \( \mathcal{V}_N \big|_{\text{min}} \) shown in Figure 5 distinctly favours the asymptotic behaviour in equation (13) and therefore a continuous phase transition or a very weak first order transition.

In general, finite size scaling predicts also a shift \( \Delta \lambda = \lambda_c^N - \lambda_c^\infty \) of the effective transition ‘temperature’ \( \lambda_c^N \) proportional to \( N^{-1/\nu d} = L^{-d} \) for a first- and proportional to \( N^{-1/\nu} = L^{-1/\nu} \) for a second-order transition. Unfortunately \( \lambda_c^\infty \) of dynamically
triangulated random surfaces is not known. For that reason, we have to use a two-parameter fit with unknowns $\lambda_\infty$ and $\nu_d$. But we can improve the reliability of this fit, because we know more. First, the fit has to be a straight line (neglecting corrections to scaling) and we have $\lim_{N \to \infty} \Delta \lambda(N) = 0$. Second, the shift $\Delta \lambda(N)$ is different for the specific heat and the cumulant in general. Therefore the slope of the fitted lines will be different in general, but we still have $\lim_{N \to \infty} \Delta \lambda(N) = 0$ for both observables.

Figure 7: Best fit of $y = \Delta \lambda$ against $x = N^{-1/\nu_d}$ for the sphere (left part) and the torus (right part). (✸) denotes the specific heat $C$ data, (✷) those of the cumulant $\mathcal{V}$.

Figure 7 shows the best fits for the sphere and the torus. The estimates of the parameters are

$$\lambda_\infty^\circ = 1.51 \pm 0.04 \; , \; \nu_d = 3.2 \pm 0.5$$

(17)

for the sphere and

$$\lambda_\infty^\circ = 1.47 \pm 0.02 \; , \; \nu_d = 2.5 \pm 0.5$$

(18)

for the torus.

We turn now to the order parameter itself. Common practise is to take $\zeta = R/L$ ($R$ is the typical radius, $L$ the linear size of the membrane) to be a suitable order parameter [41-47]. Initially [17] it was also defined as $R_g(L) = \zeta L$ ($L \to \infty$), with the linear size $L$ of the hexagon and the radius of gyration $R_g^2 \propto \sum_{ij} \langle |X_i - X_j|^2 \rangle$. A suitable choice for the order parameter therefore is

$$\zeta := \frac{R^2}{N}$$

(19)

with

$$R^2 = \frac{1}{N(N-1)} \left\langle \sum_{i,j} \sigma_i \sigma_j (\vec{X}_i - \vec{X}_j)^2 \right\rangle$$

(20)

$\sigma_i$ denotes the number of nearest neighbours, i.e. the number of links connected to a node $i$. The associated susceptibility is

$$\chi_{R^2} := L^d \left( \langle \zeta^2 \rangle - \langle \zeta \rangle^2 \right) = \frac{1}{N} \left( \langle R^4 \rangle - \langle R^2 \rangle^2 \right)$$

(21)

Figure 8 shows the order parameter $\zeta$ and Figure 9 the susceptibility of the sphere. The results for the torus are similar.
Figure 8: Order parameter $\zeta = R^2/N$ of the sphere. Errors are smaller than symbol size.

Figure 9: Susceptibility $\chi_{R^2}$ of the sphere (Lines to guide the eye).

We also measured another possible order parameter $\zeta' = \langle R'^2 \rangle / N$,

$$\langle R'^2 \rangle = \frac{1}{N} \left\langle \sum_i \left( \vec{X}_i - \overline{\vec{X}} \right)^2 \right\rangle$$

which exhibits a small increase near the phase transition and a slower decay of $\zeta'$ for $\lambda \to 0$. The difference is caused by a change of the internal geometry near the phase transition [32].

With the data for the sphere in Figure 8 and the corresponding data of the torus one can estimate the critical exponent $\beta/\nu d$ of the order parameter assuming a second order transition. Here we use as the effective critical temperature the position of the peak of the specific heat $C_{\text{max}}$ (c.f. Figure 10).

Figure 10: Scaling of the radius of gyration squared $\langle R^2(N) \rangle$ at the position of the maximum of the specific heat $C_{\text{max}}$. (♢) denotes the data of the torus, (□) data of the sphere.

An estimate of $\beta/\nu d$ using

$$\langle R^2(N, \lambda_c^{\text{eff}}) \rangle \propto N^{\beta/(\nu d) + 1}$$

results in

Torus: $\beta/\nu d = 0.28 \pm 0.02$ , Sphere: $\beta/\nu d = 0.35 \pm 0.04$  \hspace{1cm} (23)

and with the values of $\nu d$ in equation (17) and (18)

Torus: $\beta = 0.7 \pm 0.2$ , Sphere: $\beta = 1.1 \pm 0.2$  \hspace{1cm} (24)

Figure 11 shows the scaling of the maxima of the susceptibility $\chi$ (equation (21), Figure 9).

The results are

Torus: $\gamma/\nu d = 0.62 \pm 0.06$ , Sphere: $\gamma/\nu d = 0.66 \pm 0.06$  \hspace{1cm} (25)

and, using the values of $\nu d$ in equation (17) and (18),

Torus: $\gamma = 1.6 \pm 0.5$ , Sphere: $\gamma = 2.1 \pm 0.5$  \hspace{1cm} (26)

With these large error bars and estimated values $\alpha \approx -1.5$ the results are almost compatible with the scaling relation.
Figure 11: *Scaling of the susceptibility* $\chi$ (equation (21), Fig. 9) *in the case of a torus* (✸) and a sphere (✷).

$$\alpha + 2\beta + \gamma = 2$$

(27)

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