Glass phase in anisotropic surface model for membranes

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Abstract. A Finsler geometric surface model for membranes is studied by using the Monte Carlo simulation technique on connection-fixed triangle lattices with sphere topology. An in-plane three-dimensional unit vector $\sigma$ is assumed to be the in-plane tilt variable of the surface. The interaction with $\sigma$ is described by the XY-model Hamiltonian. Since this variable $\sigma$ is considered as a vector field on the surface, a Finsler metric is defined by using $\sigma$. We find that the model has three different phases. They change from the paramagnetic phase to the ferromagnetic and to the glass phases when the strength of the $XY$ interaction increases. Both the paramagnetic and the glass phases are characterized by random configuration of $\sigma$; the variable $\sigma$ randomly fluctuates in the paramagnetic phase while it is randomly frozen in the glass phase. We also find that the surface becomes spherical in both phases. On the contrary, in the ferromagnetic phase the surface shape becomes tubular or discotic due to the anisotropic bending rigidity and surface tension coefficient, which are dynamically generated by ordered configurations of $\sigma$.

1. Introduction

Anisotropic shape can be seen in biological membranes such as liposomes and vesicles [1] or in liquid crystal elastomers (LCEs) membranes [2, 3]. In those membranes, the strength of the surface force such as the surface tension $\gamma$ and bending rigidity $\kappa$ is expected to be dependent on whether these molecules are aligned or not. Indeed, the surface anisotropy can be obtained by modifying the bending rigidity $\kappa$ to be dependent on the internal direction of surface in the Ginzburg-Landau or Helfrich-Polyakov (HP) model for membranes [4, 5]. However, the modification of $\kappa$ in those models by hand gives only a constant $\kappa$ over the surface although it should depend on the direction.

Another technique to make $\kappa$ anisotropic is to assume a Finsler metric on the surface [6, 7]. In this approach, $\kappa$ depends not only on the direction but also on the position on the surface. Since the Finsler geometric model is defined in a continuous form, its treatment such as the discretization is not always uniquely determined. In the anisotropic model of Ref. [6], we assumed that (i) the tilt variable $\sigma$ belongs to $S^2$: unit sphere, and its tangential components are used as a vector field to define the Finsler metric, (ii) the Heisenberg spin model Hamiltonian $S_0$ is assumed for $\sigma$, (iii) the Finsler metric $g^{F}_{\alpha\beta}$ is constructed by deforming the Euclidean metric.
\( \delta_{ab}, \) (iv) \( g^R_{ab} \) is assumed for both the bond potential \( S_1 \) and the bending energy \( S_2 \), while \( \delta_{ab} \) is assumed for \( S_0 \).

In this presentation, we show the results obtained for the model, which is different from the one in [6]. It is defined as follows: (i) \( \sigma \in S^1 \): \( \sigma \) has the unit length, it belongs to the tangential plane and its values are assigned to the vertices, (ii) the XY model Hamiltonian \( S_0 \) is assumed for \( \sigma \), (iii) \( g^F_{ab} \) is constructed by modifying the induced metric \( g_{ab} = \partial_a X^\mu \partial_b X^\mu \), (iv) \( g^R_{ab} \) is assumed not only for \( S_1 \) and \( S_2 \) but also for \( S_0 \).

2. Model

The model is defined on the triangulated surface in \( \mathbb{R}^3 \), which is characterized by the three numbers \( (N, N_B, N_T) \), which are the total numbers of vertices, bonds and triangles.

![Figure 1](image-url)

**Figure 1.** (a) Edge vectors \( \vec{\ell}_i \) and internal angles \( \phi_i \) of a triangle in \( \mathbb{R}^3 \), (b) a triangle 123 and the three neighboring triangles, and (c) the parameters \( v_{ij} \) defined by Eq. (4).

The Hamiltonian is given by

\[
S(X, \sigma) = \lambda S_0 + S_1 + \kappa S_2, \tag{1}
\]

where \( S_0 \) is an energy for the directors (or tilts) \( \sigma_i \). The \( \sigma_i \) has values in \( S^1 \), which is the unit circle on the tangential plane at the vertex \( i \). The tangential plane is defined such that the unit normal vector \( \hat{n}_i \) at the vertex \( i \) is given by \( \hat{n}_i = \mathbf{N}_i / |\mathbf{N}_i| \), \( \mathbf{N}_i = \sum_j \mathbf{n}_j a_j \), where \( \mathbf{n}_j \) and \( a_j \) are the unit normal vector and the area of the triangle \( j \) linked to the vertex \( i \).

The internal energy \( S_0 \), the Gaussian bond potential \( S_1 \) and the bending energy \( S_2 \) are defined as follows:

\[
S_0 = \frac{1}{6} \sum_\Delta S_{0\Delta} / a_\Delta, \quad S_1 = \frac{1}{6} \sum_\Delta S_{1\Delta} / a_\Delta, \quad S_2 = \frac{1}{6} \sum_\Delta S_{2\Delta} / a_\Delta,
\]

\[
S_{0\Delta} = \left( v_{12} v_{13}^{-1} \ell_2^2 + v_{21} v_{23}^{-1} \ell_3^2 \right) (1 - \sigma_1 \cdot \sigma_2) + \left( v_{23} v_{21}^{-1} \ell_1^2 + v_{32} v_{31}^{-1} \ell_2^2 \right) (1 - \sigma_2 \cdot \sigma_3)
+ \left( v_{13} v_{12}^{-1} \ell_1^2 + v_{31} v_{32}^{-1} \ell_3^2 \right) (1 - \sigma_3 \cdot \sigma_1) \\
- \ell_1 \cdot \ell_2 \cdot (\sigma_2 - \sigma_1) \cdot (\sigma_3 - \sigma_1) - \ell_2 \cdot \ell_3 \cdot (\sigma_1 - \sigma_3) \cdot (\sigma_2 - \sigma_3)
- \ell_3 \cdot \ell_1 \cdot (\sigma_3 - \sigma_2) \cdot (\sigma_1 - \sigma_2),
\]

\[
S_{1\Delta} = \gamma_{1} \ell_1^2 \ell_2^2 + \gamma_{2} \ell_2^2 \ell_3^2 + \gamma_{3} \ell_3^2 \ell_1^2 - 2 \left( \ell_1^2 \ell_2^2 \cos^2 \phi_3 + \ell_2^2 \ell_3^2 \cos^2 \phi_1 + \ell_3^2 \ell_1^2 \cos^2 \phi_2 \right), \tag{2}
\]

\[
S_{2\Delta} = \kappa_1 \ell_1^2 (1 - \mathbf{n}_0 \cdot \mathbf{n}_1) + \kappa_2 \ell_2^2 (1 - \mathbf{n}_0 \cdot \mathbf{n}_2) + \kappa_3 \ell_3^2 (1 - \mathbf{n}_0 \cdot \mathbf{n}_3)
- \ell_1 \cdot \ell_2 \cdot (\mathbf{n}_0 - \mathbf{n}_1) \cdot (\mathbf{n}_0 - \mathbf{n}_2) - \ell_2 \cdot \ell_3 \cdot (\mathbf{n}_0 - \mathbf{n}_2) \cdot (\mathbf{n}_0 - \mathbf{n}_3)
- \ell_3 \cdot \ell_1 \cdot (\mathbf{n}_0 - \mathbf{n}_3) \cdot (\mathbf{n}_0 - \mathbf{n}_1),
\]

where \( 2 \cos^2 \phi_3 \) in \( S_{1\Delta} \) can also be written as \( 2 \cos^2 \phi_3 = (\ell_1^2 + \ell_2^2 - \ell_3^2) / \ell_1 \ell_2 \). The symbols \( \ell_i (i = 1, 2, 3) \) are the edge lengths of \( \Delta \), and \( \mathbf{n}_i (i = 0, 1, 2, 3) \) denote the unit normal vectors of
triangles (Fig. 1(b)). The symbol \(a_\Delta\) is the area of triangle \(\Delta\) defined by \(a_\Delta = (1/2)\ell_1\ell_2\sin\phi_3 = (1/2)\ell_3\ell_1\sin\phi_2 = (1/2)\ell_2\ell_3\sin\phi_1\). The symbol \(\sum_\Delta\) denotes the sum over all \(\Delta\). The coefficients \(\gamma_i\) and \(\kappa_i\) in Eq. (2) are defined by

\[
\gamma_1 = v_{13}v_{12}^{-1} + v_{12}v_{13}^{-1}, \quad \gamma_2 = v_{32}v_{31}^{-1} + v_{31}v_{32}^{-1}, \quad \gamma_3 = v_{21}v_{23}^{-1} + v_{23}v_{21}^{-1},
\]

\[
\kappa_1 = v_{13}v_{12}^{-1} + v_{12}v_{13}^{-1}, \quad \kappa_2 = v_{12}v_{32}^{-1} + v_{13}v_{31}^{-1}, \quad \kappa_3 = v_{21}v_{23}^{-1} + v_{31}v_{32}^{-1}.
\] (3)

The parameters \(v_{ij}\) are given by

\[
v_{ij} = 1 + [\sigma_{ij}], \quad \sigma_{ij} = N_v |\vec{s}_i \cdot \mathbf{t}_{ij}|,
\] (4)

where \([x]\) represents \(\text{Max}\{n \in \mathbb{Z}| n \leq x\}\), \(N_v = 100\), and \(\mathbf{t}_{ij}\) is the unit tangential vector from the vertex \(i\) to the vertex \(j\). The partition function \(Z\) is given by

\[
Z(\lambda, \kappa) = \sum_\sigma \mathcal{F} \prod_{i=1}^{\mathcal{N}} dX_i \exp[-S(X, \sigma)],
\]

where \(\mathcal{F} \prod_{i=1}^{\mathcal{N}} dX_i\) is the multiple three-dimensional integrations, that are performed by fixing the center of mass of the surface to the origin of \(\mathbb{R}^3\), and \(\sum_\sigma\) denotes the sum over tilt variables.

The assumed Finsler metric \(g_{ab}^F\) is given by

\[
g_{ab}^F = \left(\ell_1^2v_{12}^{-2}, \ell_1^{-1}.\ell_2v_{12}^{-1}v_{13}^{-1}, \ell_2^2v_{13}^{-2}\right),
\]

which reduces to the discrete induced metric if \(v_{ij} = 1\) for all \(ij\). The discrete Hamiltonians \(S_0\), \(S_1\) and \(S_2\) in Eq. (2) with the coefficients in Eq. (3) are obtained from the continuous Hamiltonians just like in the model of Ref. [6].

3. Monte Carlo results

![Figure 2](image-url)

**Figure 2.** Snapshots for (a) \(\lambda = 0.2\) (sphere), (b) \(\lambda = 1.5\) (tube), (c) \(\lambda = 3\) (disk), (d) \(\lambda = 17\) (glass). \(N = 5762\), \(b = 300\), and \(N_v = 100\). The view point of the lower snapshot is rotated about \(\pi/4\) around the vertical axis of the upper one. Red brushes denote the in-plane variable \(\sigma\).

We show snapshots for \(\lambda = 0.2\), \(\lambda = 1.5\), \(\lambda = 3\), and \(\lambda = 17\) (Figs.2(a)-2(d)), where the first one belongs to the high temperature phase and the remaining three belong to the low temperature phase. The random configurations in (a) and (d) correspond to the high temperature and the glass configurations, respectively. The magnetization \(M/N\) defined by \(M/N = (1/N)\sum_i \sigma_i = (1/N)\left|\sum_i \sigma_i^x, \sum_i \sigma_i^y, \sum_i \sigma_i^z\right|\) reflects whether the spin variables spatially align or not (Fig. 3(a)). To the contrary, the following \([M]/N\) can reflect whether the spins timely align or not (Fig. 3(b)):

\[
[M]/N = (1/N)\left|\sum_i M_i\right|,
\]

\[
M_i = \frac{1}{n_s}\left|\sum_n \sigma_i^x(n), \sum_n \sigma_i^y(n), \sum_n \sigma_i^z(n)\right|
\] (5)
where $n_s = \sum_{n=1}^{n_s} 1$ and $\frac{1}{n_s} \sum_{n=1}^{n_s}$ is the time series average of samples $\{\sigma_i(n)\}$, which is obtained at the vertex $i$ with the Monte Carlo (MC) time $n$. The magnetization $M/N$ is numerically obtained by performing the lattice average firstly and the time average finally, while $[M]/N$ is obtained with the time average firstly and with the lattice average finally. We expect $M/N \rightarrow 0$ if $\sigma_i$ is spatially random, while $[M]/N \rightarrow 0$ if $\sigma_i$ is timely random. Thus, the glass phase is characterized by $M/N \rightarrow 0$ and $[M]/N \rightarrow 1$. The glass phase is expected for $\lambda \geq 15$ (Figs. 3(a), (b)). In the high temperature phase, we see $M/N \rightarrow 0$ and $[M]/N \rightarrow 0$, which implies that $\sigma$ is random both spatially and timely. In the low temperature phase for $\lambda \geq 1.5$, $[M]/N \rightarrow 1$ is expected because $\sigma$ is timely unchanged or aligned whenever the surface is in the tube or disk configuration, while $M/N \rightarrow 1$ ($M/N \rightarrow 0$) is expected in the tube (disk) configuration.

At the phase boundary between the glass and disk/tube phases, $S_0/N_T$ and the maximal (minimal) linear extension $L_1$ ($L_3$) appear to change discontinuously, where $L_1$ is the maximal surface length along the line going through the center of surface, while $L_2$ is the maximal diameter of the sectional ellipse which is perpendicular to the line corresponding to $L_1$, and $L_3$ is the ellipse diameter at the line vertical to both of the lines corresponding to $L_1$ and $L_2$. We see $L_1 \simeq L_2 \simeq L_3$ in the glass phase (Fig. 3(d)), which implies that the surface is spherical in this phase. The surface shape in the disk/tube phase seems to be dependent on the initial condition in contrast to the model in Ref. [6].

The glass phase of the model is expected to be not stable but quasi-stable. Indeed, the mean field analysis of the Finsler XY model defined by $S = \lambda S_0$ with $\ell_i = 1$ on the regular square lattice indicates that the free energy has a quasi-stable state corresponding to the glass phase. This will be reported elsewhere. The author (HK) acknowledges Hideo Sekino in Toyohashi University of Technology for comments.

References
[1] H.-G. Döbereiner and U. Seifert, Europhys. Lett. 36, 325 (1996).
[2] Xiangjun Xing, Ranjan Mukhopadhyay, T. C. Lubensky, and Leo Radzihovsky, Phys. Rev. E. 68 (2003) 021108(1-17).
[3] Xiangjun Xing and Leo Radzihovsky, Annals of Phys. 323 (2008) 105.
[4] L. Radzihovsky, in Statistical Mechanics of Membranes and Surfaces, Second Edition, edited by D. Nelson, T. Piran, and S. Weinberg, (World Scientific, 2004) p.275.
[5] M. Bowick and A. Traveset, Phys. Rep. 344 (2001) 255.
[6] H. Koibuchi "A Finsler geometric model for membranes on triangulated surfaces", ic-msquare2102, Journal of Physics Conference Series Vol. 410 (2013) 012056 (4 pages).
[7] H. Koibuchi and H. Sekino, "Monte Carlo studies of a Finsler geometric surface model", Physica A (in press), http://arxiv.org/abs/1208.1806.