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Short Communication

The Gaussian Approximation for Self-Avoiding Tethered Surfaces

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Abstract. — We analyze the generalized Edwards model for self-avoiding tethered surfaces using a gaussian variational approximation. We find surfaces are crumpled above four dimensions with an exponent \( \nu = 4/d \), which is in fairly good agreement with the most recent numerical simulations.

The role of self-avoidance in the statistical mechanics of tethered surfaces is poorly understood at present. A generalization of the Edwards hamiltonian provides a field theoretic model for the problem, however the upper critical dimension is infinite, making an epsilon expansion inaccessible. The situation improves if one considers fluctuating manifolds of dimension different from two and there have been a number of renormalization group calculations performed in this setting. Unfortunately, the relevance of this work to two dimensional manifolds is unclear.

An alternative approach is to generalize the Flory approximation. If we denote by \( R \) the characteristic linear size of the embedded surface and by \( t \) the intrinsic size of the surface, we may define an exponent describing the surface's fractal character by

\[
R \sim t^{\nu} \quad t \to \infty.
\]  

The generalized Flory approximation predicts

\[
\nu_F = \frac{4}{d + 2},
\]

where \( d \) is the dimension of the embedding space. A generalization of the self-consistent field method for polymers also gives (2). We see in particular that Flory theory predicts a surface is crumpled above two dimensions. However, for polymers, the Flory approximation's success is the result of a cancellation between competing errors; there doesn't seem to be any a priori reason to expect Flory theory to work as well for surfaces. Indeed, large-scale numerical simulations suggest that self-avoiding tethered surfaces are flat in three dimensions. More recently, it has been found that surfaces crumple for dimensions above four, but with values of \( \nu \) different from (2).

In this paper we study the generalized Edwards model using a gaussian variational approximation. This technique was applied to polymers in and was recently applied with success.
to a somewhat different problem in [8]. We find fairly good agreement with the results from [6]: surfaces are crumpled above four dimensions with an exponent $\nu = 4/d$.

The Hamiltonian for the generalized Edwards model is given by [1]

$$ \mathcal{H} = \frac{1}{2} \int d^2 t \sum_{i=1}^{d} \nabla^2 x^i(t) \cdot \nabla x^i(t) + v \int d^2 t \int d^2 t' \delta^d(\mathbf{z}(t) - \mathbf{z}(t')) $$

where $\mathbf{z}(t)$ maps the surface to $d$-dimensional Euclidean space.

We approximate $\mathcal{H}$ with the most general possible (translation-invariant) Gaussian Hamiltonian, which we write in Fourier space as

$$ \mathcal{H}_0 = \int \frac{d^2 k}{(2\pi)^2} \sum_i x^i(k) g(k) x^i(-k), \quad (3) $$

and define averages with respect to $\mathcal{H}$ and $\mathcal{H}_0$ by

$$ \langle \mathcal{O} \rangle \equiv \int D\mathbf{x} \; e^{-\mathcal{H} \mathcal{O}} $$
$$ \langle \mathcal{O} \rangle_0 \equiv \int D\mathbf{x} \; e^{-\mathcal{H}_0 \mathcal{O}} $$

$$ \mathcal{Z} \equiv \langle 1 \rangle \quad \mathcal{F} \equiv -\log \mathcal{Z} $$
$$ \mathcal{Z}_0 \equiv \langle 1 \rangle_0 \quad \mathcal{F}_0 \equiv -\log \mathcal{Z}_0. $$

From a simple convexity argument we have

$$ \frac{1}{\mathcal{Z}_0} \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 + \mathcal{F}_0 \geq \mathcal{F}. \quad (4) $$

Thus, to find the optimal $g(k)$ we must minimize the left hand side of (4) with respect to $g(k)$. (We are simply minimizing the free energy using a Gaussian probability distribution [7],[4],[8].)

Note that (3) is explicitly invariant under rotations in the embedding space. Thus, should any flat phase appear, it will be averaged over all possible orientations and the average value $\langle \mathbf{z}(t) \rangle$ will vanish.

The left hand side of (4) is easy to calculate since it only involves Gaussian integrals. We find

$$ \frac{1}{\mathcal{Z}_0} \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 + \mathcal{F}_0 = A \left[ \int \frac{d^2 k}{(2\pi)^2} \left( \frac{k^2}{2g(k)} - 1 \right) + \frac{v}{(2\pi)^d} \int d^2 t \left( \frac{1}{K(t)} \right)^{d/2} \right. $$

$$ \left. - \frac{d^2 k}{(2\pi)^2} \log g(k) \right] $$

$$ \tag{5} $$

where $A$ is the area of the surface and

$$ K(t) = \frac{1}{2d \mathcal{Z}_0} ((\mathbf{z}(t) - \mathbf{z}(0))^2)_0 = \int \frac{d^2 k}{(2\pi)^2} \frac{1 - \cos \mathbf{k} \cdot \mathbf{t}}{g(k)}. \quad (6) $$

Taking the variational derivative of (5) with respect to $g(k)$ and setting the result equal to zero we find

$$ g(k) = k^2 - \frac{dv}{2^d \pi^{d/2}} \int d^2 t K(t)^{-1-d/2} (1 - \cos \mathbf{k} \cdot \mathbf{t}). \quad (7) $$
The exponent \( \nu \) defined in (1) may be extracted from the large \( t \) behavior of \( K(t) \)

\[
K(t) \sim t^{2 \nu_G} \quad t \to \infty,
\]

which is fixed by (6) and (7). The analysis of equations (6) and (7) follows the treatment in [7],[4] with only minor modifications and we refer the reader to these references for details. One easily finds

\[
\nu_G = 4/d \quad d > 4
\]

with logarithmic corrections appearing for \( d = 4 \). Thus, the gaussian approximation predicts above four dimensions the surface is crumpled with \( \nu \) approaching one (flat phase) as the dimension approaches four. Note that the approximation gives exact results in the limit \( d \to \infty \). Also, both Flory theory and the epsilon expansion [2] predict \( \nu \sim 4/d \) for \( d \to \infty \). Below we list the results from the most recent numerical simulations [6]\(^1\) and compare them with the Flory and Gaussian predictions.

<table>
<thead>
<tr>
<th>( d )</th>
<th>( \nu ) ([6])</th>
<th>( \nu_F )</th>
<th>( \nu_G )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.0</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.0</td>
<td>0.666</td>
<td>1 (with log corrections)</td>
</tr>
<tr>
<td>5</td>
<td>0.82 ± 0.05</td>
<td>0.571</td>
<td>0.80</td>
</tr>
<tr>
<td>6</td>
<td>0.69 ± 0.05</td>
<td>0.50</td>
<td>0.666</td>
</tr>
<tr>
<td>8</td>
<td>0.60 ± 0.03</td>
<td>0.40</td>
<td>0.50</td>
</tr>
</tbody>
</table>

It seems clear that the Gaussian approximation does a better job than the Flory approximation in determining the exponent \( \nu \). Note that the reverse is true for polymers [4] where the Flory value of \( \nu_F = 3/d + 2 \) is much better than the Gaussian result \( \nu_G = 2/d \).

The primary defect in the Gaussian approximation is that it should take account of the entropy exactly and the repulsive energy only approximately [4]. As a result, since the free energy is not at its true minimum, the repulsive energy is over-estimated and the swelling is too large. Thus, we expect the Gaussian prediction for \( \nu \) to be an upper bound. This is manifestly the case for polymers.

The Gaussian approximation may be further criticized because other critical exponents are fixed at incorrect values (at least for polymers) irrespective of the Gaussian trial probability [4]. If we define the probability for contact between points a distance \( r \) apart by

\[
P(r) = \frac{1}{Z} \left( \delta^d(r - \bar{x}(t_1) + \bar{x}(t_2)) \right)
\]

then in the limit\(^2\)

\[
|t_1 - t_2| \sim R^{1/\nu},
\]

with \( R \) the characteristic size of the surface, we have

\[
P(r) = f(r/R)/R^d.
\]

The exponent \( \theta \) is defined by

\[
f(y) \sim y^\theta \quad y \to 0
\]

\(^1\) We take for \( \nu \) the exponent describing the scaling of the in-plane structure function [6].

\(^2\) Strictly speaking we should distinguish between the cases in which the contact points are far apart but in the bulk and when one or both points are near the boundary [4],[9].
and for polymers in three dimensions, numerical simulations give \[4\]

\[ \theta \approx 0.275. \]

For the Gaussian distribution (3) one may easily compute (8) for either polymers or surfaces. In both cases one finds

\[ P_G(r) = \frac{\exp(-r^2/4R^2)}{2^d\pi^{d/2}R^d} \quad R \equiv K(t_1 - t_2) \]

and thus

\[ \theta_G = 0. \]

This is a great failure for polymers, however the correct value of \(\theta\) for self-avoiding tethered surfaces is unknown. Nevertheless, the apparent success of the Gaussian approximation does not require that the correct value of \(\theta\) is small. Rather, the computation of \(\nu_G\) could involve a fortuitous suppression of errors as is known to occur for old theories of polymers, which predict both the Flory value for \(\nu\) (which is quite close to the correct value) and \(\theta = 0\) (which is wrong) \[4\].

Clearly, more analytical and numerical work is needed before we can assess the utility of the gaussian approximation and possible corrections to it in describing self-avoiding tethered surfaces.

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References


