Phase Transition in Tensionless Surfaces

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Abstract

We will study the critical behavior of the discrete bilaplacian model. This model describes the growth of tensionless surfaces. Tensionless surfaces are very important, for example, in molecular beam epitaxial and in biological membranes. We will describe previous analytical and numerical results. Finally we will show recent numerical simulations which can be described by a single Kosterlitz-Thouless (KT) phase transition between a continuum massless bilaplacian behavior and a massive one.

1 Introduction

Tensionless surfaces appear in different and important fields in Science. For instance, in Biology the lipid membranes are practically tensionless membranes and in process of growth of surfaces as the Molecular beam Epitaxy, the surface behaves without surface tension.

This paper is devoted to study the critical behavior of a model which describes tensionless surfaces. In the next two sections we will deduce the main equations and describe with a bit of detail some examples. Nextly we will set up some notation and in the following section we will report analytical results. In the last two sections we will summarize previous numerical simulations, our numerical results and the conclusions.

1.1 Tensionless surfaces [1]

The free energy of a surface ($F = \mu N - pV + \sigma A$) can be written on a more general way:

$$F = (\frac{\mu}{v} - p) \int \int dx\, dy\, h(x,y) + \int \int dx\, dy\, \phi(h_x, h_y)\ .$$

μ is the chemical potential, $v = V/N$, $h(x,y)$ is the height of the surface at the point of coordinates (x,y), p is the pressure, $\phi(h_x, h_y) = \sigma(h_x, h_y)\sqrt{1 + h_x^2 + h_y^2}$, σ being the surface tension and A is the area.

Working a constant pressure, we can study the influence of a) the chemical potential and b) the surface tension in the growth of a surface.

The main effect of the chemical potential is to induce diffusion on the surface from regions with higher chemical potential to regions with lower chemical potential. The current (only on the surface) is then

$$\boldsymbol{j} = -D_s \nabla \mu$$

and the continuity equation (the number of particles is constant)

$$\frac{\partial h}{\partial t} = -\nabla \boldsymbol{j}\ .$$

Hence

$$\frac{\partial h}{\partial t} = D_s \nabla^2 \mu = -\kappa (\nabla^2)^2 h$$

with $\kappa > 0$.

Now, we will study the surface tension. Supposing that the chemical potential of the vapor is uniform μ_0, there will be evaporation in places where $\mu > \mu_0$. We can assume that the variation of the height with time is linear with the chemical potential difference:

$$\frac{\partial h}{\partial t} \propto -(\mu - \mu_0)$$

and so

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h$$

with $\nu > 0$.

Taking into account evaporation, surface diffusion and thermal fluctuations we can write the following Langevin equation

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h - \kappa (\nabla^2)^2 h + \eta(\boldsymbol{r}, t)$$

where $\eta(\boldsymbol{r}, t)$ is a Gaussian noise, which is the generalized continuum bilaplacian model. [1] By putting $\nu = 0$ we obtain a model for continuum tensionless surfaces.

1.2 Examples

One example of tensionless surface is the lipid membrane [2]. The fluid of lipids which conform the membrane is above its melting point and so the lipids can move inside the membrane. Recently Gov and Safran [3] have introduced the following equation to modelize the action of the elastic cytoskeleton on the fluid membrane:

$$\kappa(\nabla^2)^2\chi(r) + V(r)\chi(r) = 0 \ ,$$

where $\chi(r) = \langle h(r) \rangle$ (Mean Field approximation), and V introduces into the model the pinning of the surface by the cytoskeleton.

The second example of tensionless surfaces is the molecular beam epitaxy (MBE) which is a process of a high interest in technology. In most MBE process there are not evaporation, e.g in Nickel, but in GaAs, arsenic evaporates.

Finally, the third example is the two dimensional melting. Nelson [6] proposed the discrete bilaplacian as a model for this melting.

2 The model and some observables

The Hamiltonian of the generalized discrete Laplacian model is

$$\mathcal{H} = \sum_{\boldsymbol{r}} \left(\nu[\nabla_d h(\boldsymbol{r})]^2 + \kappa[\nabla_d^2 h(\boldsymbol{r})]^2 \right) \ ,$$

where ∇_d is the discrete gradient and $h \in Z$. The discrete bilaplacian model is obtained by putting $\nu = 0$.

It is interesting to define two different correlation functions (or propagators). The first one, the normal correlation function is defined as

$$C(r) \equiv \langle (h(\boldsymbol{r}) - h(0))^2 \rangle \ ,$$

and the slope-slope correlation function is

$$C_d(s) \equiv \langle (\nabla_d h(\boldsymbol{r} + \boldsymbol{s}) - \nabla_d h(\boldsymbol{r}))^2 \rangle \ .$$

[1] We can take into account an external flux of particles, F, by performing the transformation $h \to h + Ft$.

In the continuum model (i.e. continuum heights) the previous two propagators behave in momentum space as $C(q) \propto 1/q^4$ and $C_d(q) \propto 1/q^2$ respectively.

Finally we define the specific heat, C, as

$$C = \frac{1}{V}\left(\langle H^2\rangle - \langle H\rangle^2\right) \ .$$

where $V = L^2$ is the volume of the lattice.

3 The Discrete Bilaplacian Model: Analytical Results

In this section we will describe, briefly, results obtained using three different analytical methods: mapping to a two dimensional vector Coulomb gas, Mean Field and Renormalization group (dynamics). Unfortunately the predictions of these three analytical approaches do not provide with the same results.

- Nelson Scenario [6]

  Nelson proposed the discrete bilaplacian as a model for the two dimensional melting. By using the Poisson summation formula the discrete bilaplacian can be written as a vector Coulomb gas. Taking into account the most relevant terms in the modified Coulomb gas a sequence of two KT transitions were found:

(1) $T > T_{c1}$: $C(r) \propto r^2 \log r$, $C_d(r) \propto \log r$. (Solid phase)
(2) $T_{c1} > T > T_{c2}$: $C(r) \propto \log r$, $C_d(r) \propto 1$. (Hexatic phase)
(3) $T < T_{c2}$: $C(r) \propto 1$, $C_d(r) \propto 1$. (Isotropic liquid phase)

- Mean Field Scenario [7]

  The starting point is the Bogoliubov-Feynman inequality:

$$\mathcal{F} \leq \mathcal{F}_0 + \langle \mathcal{H} - \mathcal{H}_0\rangle_0 \equiv \mathcal{F}_{\rm MF}$$
$$\mathcal{H}_0 \equiv \frac{T}{2}\sum_{\boldsymbol{q}} S^{-1}(\boldsymbol{q})\, h_{\boldsymbol{q}}\, h_{\boldsymbol{q}}$$

  And the propagator, $S(\boldsymbol{q})$, itself is the variational parameter. When particularizing the Mean Field free energy, $\mathcal{F}_{\rm MF}$, to two dimensions, a first order phase transition is found.

- Renormalization Group Scenario [8]

  The starting point is the Langevin equation and the model is renormalized using the scheme of Nozières-Gallet [9].

  Let us define $L_c(l) = \sqrt{\kappa(l)/\nu(l)}$, $l = \log b$, b being the scale factor in RG. The main results of this approach is that if $L < L_c(l)$ the surface is tensionless, otherwise the surface has tension surface. In addition, for large lattices ($l \to \infty$) the surface has always tension surface. So, there is no phase transition in the thermodynamic limit.

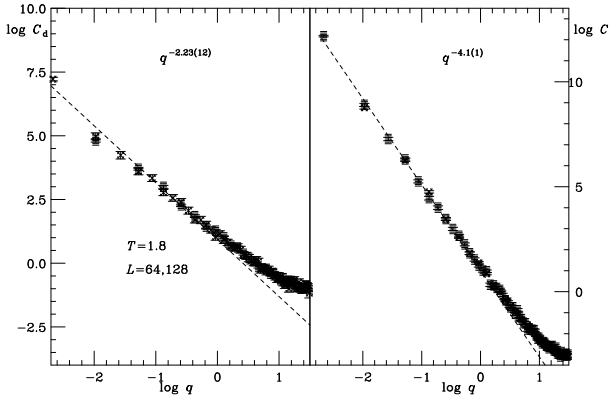

Fig. 1. Propagators. $T = 1.8$

4 The Discrete Bilaplacian Model: Numerical Results

Numerical simulations performed by Bruce [4] confirms the Nelson scenario with $T_{c1} = 2.2$ and $T_{c2} = 1.64$. However numerical simulations done by Janke and Kleinert [5] in a modified model would imply a first order phase transition in the discrete bilaplacian model at $T_c = 2.454$.

In the following we will check these two scenarios by computing the normal and slope propagators at $T = 1.8$. In figure (1) can be seen that both propagators follow the continuum bilaplacian prediction ($1/q^4$ and $1/q^2$ behaviors respectively), hence the Bruce and the Janke and Kleinert scenarios cannot be valid with the critical temperatures reported.

We have repeated the computation in the low temperature region $T = 1.5$. In figure (2) a dramatic change of behavior can be observed. The slope-slope propagator shows a bell shape and the normal propagator shows a plateau in the low momentum regime indicating a massive phase. We can explain these two behaviors assuming a massive continuum bilaplacian model, which has $1/(q^4 + m^4)$ as the normal propagator, where the mass m is the inverse of the correlation length of this phase. This behavior for the normal propagator implies a behavior $q^2/(q^4+m^4)$ for the slope-slope propagator, which presents the bell shape.

Notice that in figures (1) and (2) there are no finite size effects in the numerical precision: the $L = 64$ data and the $L = 128$ ones are compatibles in the statistical error.

We have studied the behavior of the specific heat. This observable shows a clear maximum as a function of the temperature for a given lattice size. We have plotted the value of that maximum as a function of the lattice size in figure (3). In the low L region a linear behavior has been found, but for large

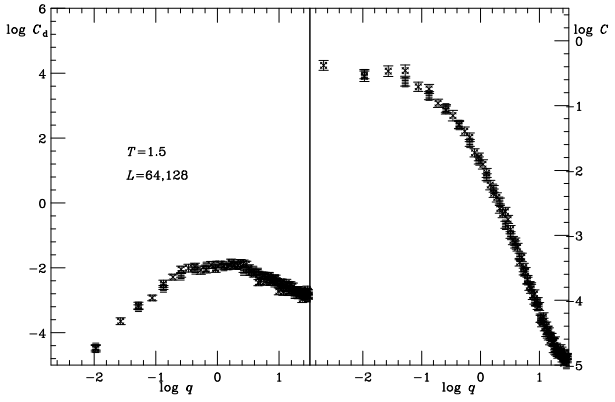

Fig. 2. Propagators. $T = 1.5$

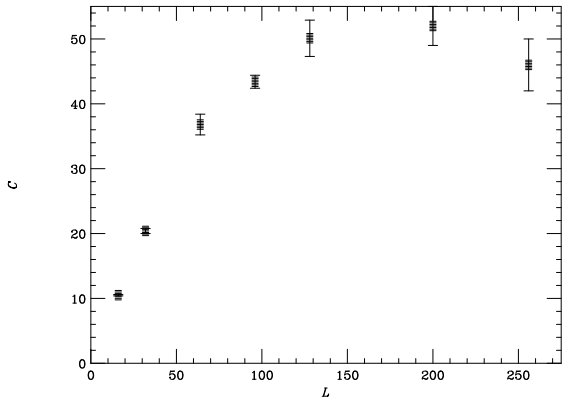

Fig. 3. Peak of specific heat as a function of L.

lattices a plateau has been achieved. This behavior resembles the behavior of the peak of the specific heat in a KT phase transition. With this behavior we can assume $\alpha \leq 0$: i.e. there is no divergence of the specific heat (α is the critical exponent which governs the divergence of the specific heat).

We can do a further analysis monitoring the dependence of the apparent critical temperature, $T_c(L)$ (defined as the temperature in which the specific heat shows the maximum for a given lattice size). This apparent critical temperature scales, in an ordinary second order phase transition, as [10]

$$T_c(L) = T_c + aL^{-1/\nu} \, .$$

In figure (4) we reported $T_c(L)$ against L and the fit to equation (4). We obtain $\nu = 0.70(7)$. However, this value of ν, assuming $\alpha \leq 0$; implies violation of hyperscaling. Hence, we try a fit motivated by the KT scenario [10]:

$$T_c(L) = T_c + \frac{a}{(\log L + b)^2} \, ,$$

where a and b are constants, and T_c is the bulk critical temperature. We show

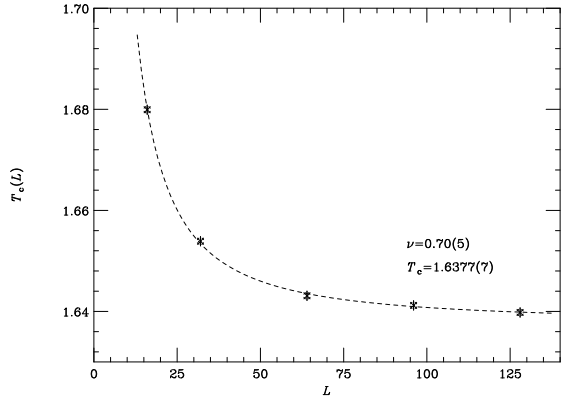

Fig. 4. $T_c(L)$ as a function of L. Fit to equation (4).

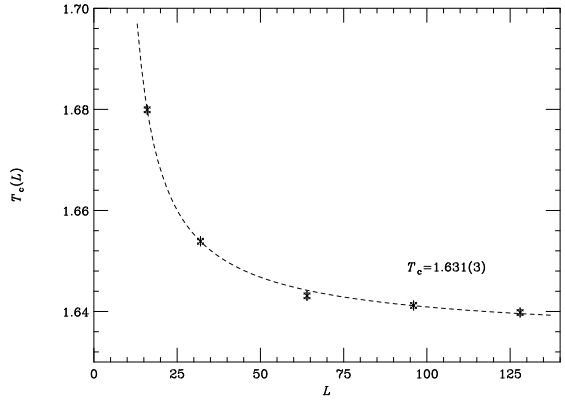

Fig. 5. $T_c(L)$ as a function of L. KT scenario: fit to equation (4).

in figure (5) this fit and the agreement is good.

However, the analysis of the order of the transition deserves further researches [11].

5 Conclusions

We summarize our main conclusions.

The system behaves in a continuum massless bilaplacian way at $T = 1.8$ so the Bruce and Janke and Kleinert results cannot be right.

The system undergoes a continuous phase transition near $T = 1.64$ (where the system develops a not diverging specific heat peak) between a hight temperature phase well describe by the bilaplacian and a low temperature one which can be described by a massive quartic propagator. Recently, we have obtained evidence that the propagators at $T = 1.64$ behave as at $T = 1.5$. In addition at $T = 1.7$ the propagators are still as at $T = 1.8$. Hence, a detailed study of

the region near $T \in (1.64, 1.7)$ is needed in order to discard completely the intermediate phase proposed by Nelson, the hexatic one (a detailed study will be reported elsewhere [11]).

A choice for the critical exponents $\alpha \leq 0$ and $\nu \simeq 0.7$ violates hyperscaling ($\alpha = 2 - \nu d$) in two dimensions, so we conjecture that the phase transition is in the KT universality class.

Acknowledgments

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