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New evidence for super-roughening in crystalline surfaces with a disordered substrate

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Abstract. We study the behaviour of the Binder cumulant related to long-distance correlation functions of the discrete Gaussian model of disordered substrate crystalline surfaces. We exhibit numerical evidence that the non-Gaussian behaviour in the low- T region persists on large-length scales, in agreement with the broken phase being super-rough.

1. Introduction

The disordered discrete Gaussian model (that we will denote hereafter as a discrete model) is related to the two-dimensional random phase Sine–Gordon model (that we will denote as the continuum model). The two models belong to the same universality class, which includes different physical systems: for example it is supposed to describe crystalline surfaces growing upon a disordered substrate [1], as well as a two-dimensional randomly pinned arrays of flux lines with the magnetic field parallel to the superconducting plane [2].

The standard approach used to investigate this model is the renormalization group [1–4]. The application of the Mezard–Parisi variational approximation [5] (originally developed for models with continuous replica symmetry breaking) leads to a one-step replica broken solution [6], and because of that it is problematic [7]: still the main features found in the variational approach are very different from the ones found by using the standard renormalization group. The most evident difference is probably in the behaviour one expects in the broken phase for the height–height correlation function.

A considerable amount of work (see, for instance, [6–19]) has been devoted to the subject. In contrast to some former claims, the situation has been shown to be in agreement with the existence of a broken super-rough phase, as implied by the renormalization group approach, by the numerical simulations of [7, 19].

Recently very convincing further evidence for the system being super-rough down to $T = 0$ has been established in [20–22], by exact computations of the ground state of finite volume samples of the discrete model.

In this paper we focus on the non-Gaussian behaviour of the discrete model in the broken phase. We show that it persists on large length scales. This is definitely not compatible

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with the predictions of the variational theory[†]. In contrast, our data are well compatible with the behaviour suggested by the renormalization group computations.

Labelling with $\{d_i\}$ the integer-valued dynamical variables and by $\{\eta_i\}$ the quenched disorder, the Hamiltonian of the discrete model is

$$\mathcal{H}[\phi] \equiv \frac{\kappa}{2} \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 \quad \phi_i \equiv d_i + \eta_i \quad (1)$$

where the sum runs over first neighbouring sites of a bidimensional lattice. The model is related to the limit of coupling constant $\lambda \rightarrow \infty$ of the continuous model

$$\mathcal{H}[\phi] \equiv \frac{\kappa}{2} \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 - \lambda \sum_i \cos(2\pi(\phi_i - \eta_i)) \quad (2)$$

where now ϕ_i are the continuous dynamical variables.

The partition function is defined as

$$Z_\eta \equiv \sum e^{-\beta\mathcal{H}} \quad (3)$$

where $\beta = \frac{1}{T}$ is the inverse temperature of the problem.

A relevant observable quantity is the correlation function defined by

$$C(r, T) \equiv \overline{(\phi(\mathbf{r}_0) - \phi(\mathbf{r}_0 + \mathbf{r}))^2}. \quad (4)$$

In the high- T phase thermal fluctuations make the quenched disorder irrelevant. Both the renormalization group and the variational theory predict a Gaussian behaviour with a logarithmic growth of the height–height correlation function

$$C_{T>T_c}(r, T) \simeq \frac{T}{k\pi} \log r. \quad (5)$$

The critical temperature is expected to be $T_c = \frac{\kappa}{\pi}$ in both approaches.

The renormalization group approach finds that for $T < T_c$ one has a super-rough broken phase characterized by

$$C_{T<T_c}^{\text{RG}}(r, T) \simeq a \log r + b \log^2 r \quad b = \frac{2}{\pi^2} \left(\frac{T_c - T}{T_c} \right)^2 \quad (6)$$

where a is a non-universal coefficient.

On the other hand, the Gaussian ansatz of the variational approximation suggests no $\log^2 r$ contribution, and the broken phase turns out to be described by a one-step replica symmetry broken solution with

$$C_{T<T_c}^{\text{VAR}}(r, T) \simeq \frac{T_c}{k\pi} \log r \quad (7)$$

i.e. where the slope of the logarithmic term freezes at the critical point T_c .

Let us recall in a few lines some of the main numerical results relevant to the problem. The authors of [15] studied the continuous model without being able to detect any signature of the transition when measuring static quantities, probably [16] because of the small λ value they used. Indeed, for such small values of the coupling the difference from the pure case becomes sizeable only on very large-length scales. In [17] numerical estimates for the correlation function $C(r)$ of the discrete model were found to be compatible with the picture expected from the variational theory. Finally, evidence for the $(\log r)^2$ contribution to $C(r)$ in the broken phase has been obtained in the case of the discrete model [7] and in that of the continuous model for different λ values [19].

[†] We remind the reader again that here we are in the framework of a one-step replica broken solution, and that this kind of criticism [7] does not apply to the variational theory when describing a continuum breaking [5].

2. The binder parameter

In this note we will mainly discuss the distribution function of the height–height correlation functions at distance r . We define the probability distribution

$$\mathcal{P}[\Delta(r), T] \equiv \overline{\delta[\Delta(r) - (\phi(\mathbf{r}_0) - \phi(\mathbf{r}_0 + \mathbf{r}))]} \quad (8)$$

where $\langle \dots \rangle$ denotes the thermal average (and here also an average over different values of \mathbf{r}_0), and $\overline{\dots}$ denotes the average over disorder. For the sake of computational simplicity, in the following we will only consider displacements, \mathbf{r} , of the form $(r, 0)$ or $(0, r)$. The second moment of \mathcal{P} is the usual height–height correlation function $C(r)$, the focus of the investigation of [7, 19]. Here we will try to use the knowledge of the full probability distribution (8) in order to gather more information concerning the system.

To characterize the probability distribution we measure

$$D(r, T) \equiv 3(\overline{\langle \Delta^2(r) \rangle})^2 - \overline{\langle \Delta^4(r) \rangle} \quad (9)$$

and together with $C(r)$ it allows us to define the Binder cumulant of \mathcal{P} :

$$B(r, T) \equiv \frac{1}{2} \left(3 - \frac{\overline{\langle \Delta^4(r) \rangle}}{(\overline{\langle \Delta^2(r) \rangle})^2} \right). \quad (10)$$

In the thermodynamic limit a value $B = 0$ characterizes a Gaussian behaviour.

The work of [7] was based on the analysis of the Binder parameter for $r = 1$, that was providing evidence for a non-Gaussian behaviour in the low- T region. Here we will try to answer some questions that are still open after [7], looking at the long-distance behaviour of correlation functions: that will allow us to exhibit more evidence for a clear non-Gaussian behaviour. A purely Gaussian behaviour could indeed be hidden for small r by short-distance effects, and manifest itself only in the large r region. Analysing $B(r)$ in the large r region would make this effect clear.

In order to understand what to expect for B we will use the renormalization group (replica symmetric, to start with). We will mainly follow the approach described by Bernard in his Les Houches lecture notes [13]. In the field theoretical renormalization group approach we start from the continuum version of (2) by writing

$$S = \int \frac{d^2x}{4\pi} \left(\frac{\kappa}{2} (\partial_\mu \Phi(x))^2 - \lambda \cos(\Phi(x) - d(x)) \right) \quad (11)$$

where $\Phi(x)$ are the basic fields of the theory, and $d(x)$ are the quenched random fields which make the system disordered. Universality is used to argue that these different systems exhibit the same critical behaviour. Following Bernard renormalization calls for a generalization of this model: one introduces, in addition to the random phases, a random potential. If one did not do that at the start the random potential would in any case be generated by renormalization. So one writes

$$S = \int \frac{d^2x}{4\pi} \left(\frac{\kappa}{2} (\partial_\mu \Phi(x))^2 - A_\mu(x) \partial_\mu \Phi(x) - \xi(x) e^{i\Phi(x)} - \xi^*(x) e^{-i\Phi(x)} \right) \quad (12)$$

where the quenched fields, ξ , are distributed according to

$$P[\xi] = e^{-\frac{1}{2\sigma} \int \frac{d^2x}{4\pi} \xi \xi^*} \quad (13)$$

and the field A_μ can be written, by noticing that the rotational part decouples, as $A_\mu(x) \equiv \partial_\mu \Lambda(x)$, and it is distributed as

$$P[A_\mu] = e^{-\frac{1}{2g} \int \frac{d^2x}{4\pi} (\partial_\mu \Lambda)^2}. \quad (14)$$

A $U(1)$ symmetry guarantees that the model has some remarkable properties. For example the g -dependence of the correlation functions of the vertex operator $e^{i\alpha\Phi}$ can be factorized.

Now one has to play the usual replica trick (at this stage with exact replica symmetry by definition). One writes an effective action for n replica's of the system, and takes the $n \rightarrow 0$ limit. The β functions of the model (for the running of κ , g and σ) turn out to be

$$\begin{aligned}\beta_\sigma &= 2x\sigma - 2\sigma^2 + \dots \\ \beta_g &= \frac{\sigma^2}{2} + \dots \\ \beta_\kappa &= 0\end{aligned}\tag{15}$$

where we have defined $x \equiv \frac{\kappa - \kappa_c}{\kappa}$, and κ is not renormalized. So in the low T phase, for $\kappa > \kappa_c$, a non-trivial infrared fixed point exists at σ_* , with

$$\sigma_* = x + \dots \quad \text{for } x \ll 1.\tag{16}$$

At σ_* we have $\beta_g = \frac{x^2}{2}$, i.e. g still flows (see Bernard [13] for the characterization of such a *run-away fixed point*).

We are interested in renormalization group predictions for correlation functions. At the infrared fixed point one finds that

$$G(r) \equiv \overline{\langle e^{i\alpha(\phi(r) - \phi(0))} \rangle_*} = r^{-2\gamma_*} e^{-\frac{\alpha^2 \beta_{g*}}{2\kappa^2} (\log r)^2}\tag{17}$$

where γ_* is the anomalous dimension at the fixed point, $\gamma_* = \frac{\alpha^2}{\kappa} \rho_* + O(\alpha^4)$, and $\rho_* = 1 + O(x)$. We have already noticed that $\beta_{g*} = \frac{x^2}{2}$ (and it gives the large-distance $(\log r)^2$ behaviour of the correlation function).

By expanding G in powers of α one finds that at all orders in the perturbation theory (in the replica-symmetric renormalization group approach)

$$\overline{\langle (\Phi(r) - \Phi(0))^2 \rangle} = \frac{4\rho_*}{\kappa} \log r + \frac{\beta_{g*}}{\kappa^2} (\log r)^2\tag{18}$$

and for small x

$$\overline{\langle (\Phi(r) - \Phi(0))^2 \rangle} = \frac{4}{\kappa} \log r + \frac{x^2}{2\kappa^2} (\log r)^2.\tag{19}$$

In the same way for the four point correlation function we find that

$$\overline{\langle (\Phi(r) - \Phi(0))^4 \rangle} = 3 \left(\frac{4\rho_*}{\kappa} \log r + \frac{\beta_{g*}}{\kappa^2} (\log r)^2 \right)^2 - 48d_* \log r\tag{20}$$

where we have defined d_* , the unknown coefficient of the α^4 contribution, to the anomalous dimension γ_* , which we expect to depend on the temperature and could even be zero. That means that in the renormalization group approach we find that

$$D_{T < T_c}^{\text{RG}}(r, T) = 48d_* \log r\tag{21}$$

where $D_{T < T_c}^{\text{RG}}$ does not depend on β_g^* , and

$$B_{T < T_c}^{\text{RG}}(r, T) = \frac{24d_* \log r}{\left(\frac{4\rho_*}{\kappa} \log r + \frac{\beta_{g*}}{\kappa^2} (\log r)^2 \right)^2} \underset{r \gg 1}{\simeq} \frac{24d_* \kappa^2}{\beta_g^* \log^3 r}.\tag{22}$$

So, if $d_* \neq 0$, $D(r)$ grows logarithmically with r . On the other hand, according to the renormalization group picture $\lim_{r \rightarrow \infty} B(r) = 0 \simeq (\log r)^{-3}$. These are the theoretical predictions we use to interpret our numerical findings.

As a last remark, we want to notice that by studying a large N version of the random phase Sine–Gordon model, Bernard and Bauer [12] found β_{g^*} to be $O(\frac{1}{N^3})$. This means that there is no $(\log r)^2$ contribution to the height–height correlation function in the $N \rightarrow \infty$ limit in which the Gaussian ansatz of the variational approach, corresponding to the leading order in a $\frac{1}{N}$ expansion, is expected to be exact.

3. Numerical results

We have obtained our numerical data from simulations done on the Ape-100 computer [23]. We have used square lattices of linear size, $L = 64$ and $L = 128$, with periodic boundary conditions. We have fixed the surface tension, κ , to 2. We have chosen the quenched random variables $\{\eta_i\}$ uniformly in the range $(-\frac{1}{2}, +\frac{1}{2})$.

We have simulated in parallel a total of 256 different realizations of the quenched substrate, and two uncoupled replicas for each sample. We have used a simple Monte Carlo local dynamics, by proposing to update in turn the $\{d_i\}$ by an increment of ± 1 . We have used an annealing scheme, in which we have visited in turn decreasing values of the temperature T ($T = 1.0, 0.95, 0.90, \dots, 0.40$ for $L = 64$ and $T = 0.90, 0.80, 0.70, 0.65, 0.60, 0.45, 0.35$ for $L = 128$). At each of the T values the thermalization sweeps were 500 000 for $L = 64$ and 700 000 for $L = 128$ (for further details see [7]).

In figure 1 we show $B(r)$ as a function of T for different $r \geq 4$ values. We plot the data obtained on the smaller lattice, $L = 64$, since here we had a larger number of T values, but the behaviour at $L = 128$ is very similar. When comparing $L = 64$ with $L = 128$ in the statistical precision of our runs there is no size dependence for $r \leq 20$.

Deviations of $B(r)$ from the Gaussian behaviour at small distances become evident even for $T \leq 0.85$. The breakdown of the curves (for higher r values) in figure 1 is, in contrast,

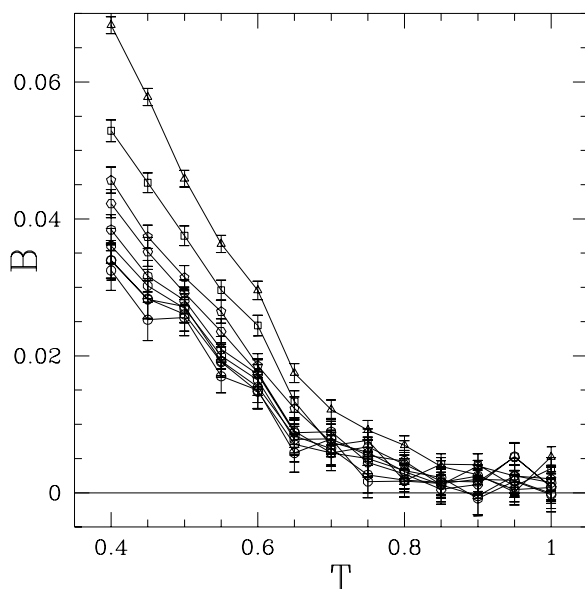


Figure 1. The Binder parameter as a function of T at different $r \geq 4$ values. $L = 64$. Lines are only meant to join neighbouring points. Triangles ($r = 4$), squares ($r = 5$), pentagons ($r = 6$), hexagons ($r = 7$), etc.

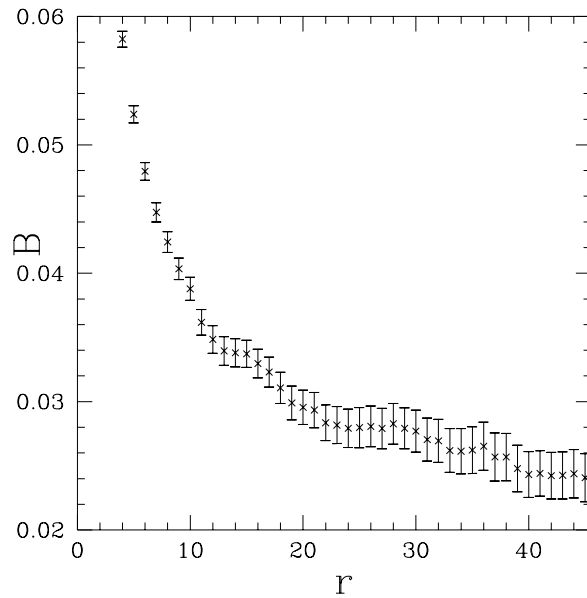


Figure 2. B as a function of r for $T = 0.45$ and $L = 128$.

compatible with the theoretical prediction $T_c = \frac{2}{\pi}$. When looking at finite distances one finds a crossover (that does not correspond to a true critical behaviour) for $T > T_c$ [19]. Only measuring on large lattices real long-distance properties does one recover the correct critical point, which turns out to coincide with good precision with the theoretical predictions.

So, at lower T values the Binder parameter remains non-zero on larger-length scales. What is even more important is the breaking of the slope of B versus T (see figure 1). From our data we can say that for $T < 0.65$ the system is surely in its broken phase.

In figure 2 we plot $B(r)$ as a function of r for $T = 0.45$ and $L = 128$. Here the fast decay at short distances and the slow decay for large r is very clear.

In figure 2 the data shown are qualitatively in a very good agreement with the prediction of (22), with a non-zero value of d_* .

In figure 3 we show $D(r)$ as a function of r for $L = 64$ at the highest temperature we have considered ($T = 1.0$) and at the lowest one ($T = 0.4$). That makes clear the difference between the high- T region, where $D(r)$ is extremely small even at short distances and when increasing r becomes soon compatible with zero, and the broken phase where it is definitely non-zero and shows an evident increasing behaviour.

The fact that in the broken phase D increases with r is clear from figure 4, where $D(r)$ is plotted as a function of r for $T = 0.45$, $L = 128$. That clearly shows that the non-Gaussian behaviour of the model in the broken phase is not a short-distance effect.

We have tried a quantitative analysis of the behaviour of $D(r)$, at a temperature well below the critical point. Following [7, 19], we use in the fit the lattice Gaussian propagator

$$P(r) \equiv \frac{1}{2L^2} \sum_{n_1=1}^{L-1} \sum_{n_2=0}^{L-1} \frac{1 - \cos\left(\frac{2\pi r n_1}{L}\right)}{2 - \cos\left(\frac{2\pi n_1}{L}\right) - \cos\left(\frac{2\pi n_2}{L}\right)} \simeq_{L \gg 1} \frac{1}{2\pi} [\log r + \gamma \log(2\sqrt{2})] \quad (23)$$

which enables us to keep finite-size effects under control. The data are very well fitted by the expected behaviour $D = c_1 P(r) + c_2$. Unfortunately errors grow quickly with r and data for $r \geq 40$ basically do not influence the fit.

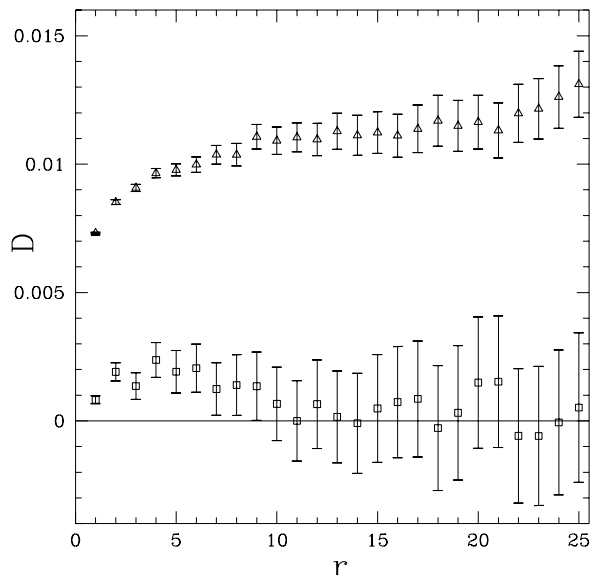


Figure 3. D as a function of r at $T = 0.40$ (triangles) and $T = 1.0$ (squares) for $L = 64$.

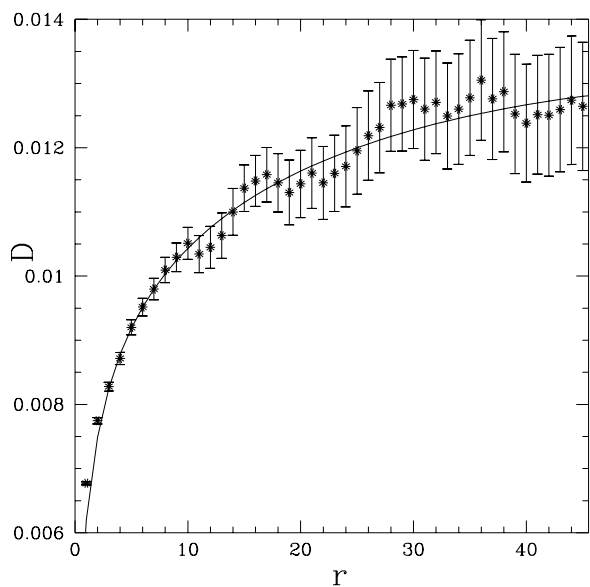


Figure 4. D as a function of r for $T = 0.45$, $L = 128$. The line is our best fit to the behaviour $D(r) = c_1 P(r) + c_2$ by using data with $3 \leq r \leq 45$.

In figure 4 we show our best fit obtained by using data with $3 \leq r \leq 45$ (disregarding 10 more points at short distances does not change the results):

$$10^4 D = (114 \pm 3)P(r) + (36 \pm 3) \tag{24}$$

where errors have been evaluated by using the jack-knife method. The value of the residual χ^2 (per degree of freedom) is very good, close to 0.2 (but since the data points are very

correlated, the number does not necessarily have a deep meaning). The agreement with the renormalization group prediction (see equation (21)) is very good. Our best numerical estimate for d_* is $\pi c_1/24$.

4. Conclusions

Our main conclusion is that the discrete Gaussian model for surfaces with a disordered substrate in the low- T region is non-Gaussian on large-length scales. Such evidence was needed to exclude the possibility of a short-distance effect that could disappear in the asymptotic long-distance regime.

The picture which emerges from our analysis is therefore incompatible with the Gaussian variational ansatz, calling for the broken phase to be super-rough. Finally, our data give numerical evidence for d_* to be non-zero, the behaviour of $D(r)$ at low temperatures resulting in a good agreement with the logarithmic growth expected from the renormalization group approach.

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