

# Correlations of a bound interface over a random substrate

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**Abstract.** The correlation function of a one-dimensional interface over a random substrate, bound to the substrate by a pressure term, is studied by Monte-Carlo simulation. It is found that the height correlation  $\langle h_i; h_{i+j} \rangle$ , averaged over the substrate disorder, fits a form  $ae^{-(j/b)^c}$  to a surprising precision in the full range of  $j$  where the correlation is non-negligible. The exponent  $c$  increases from 1.0 to 1.5 when the interface tension is taken larger and larger.

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## 1 Introduction

Surfaces play a very important role in many processes such as painting, coating, oil recovery... The study of a surface is usually based on its topography  $h(x, y)$  and its chemical constituents. Different tools exist to get this information, each working at a different scale. The measured topography is thus a function of the scale at which the measurements are performed. For instance, the topography obtained with an optical profilometer is not the same as obtained with an Atomic Force Microscope.

The topography is also known to play a crucial role in wetting. It is well established that roughness will enhance hydrophobicity or hydrophilicity [1,2]. Suppose that you are considering a hydrophilic polymer surface  $h^1$ , on top of which you deposit a hydrophobic polymer, the surface of which is denoted  $h$ . For a given surface  $h^1$ , in practice, one is often willing to modify the surface properties of  $h$  by varying the amount  $h - h^1$  of hydrophobic polymer. The natural question is thus to study the link between  $h^1$  and  $h$ .

For simplicity, let us assume that the topography can be characterized by a one-dimensional function  $h_n$ . Let

$\hat{h}(k)$  denote its Fourier transform,

$$\hat{h}(k) = \frac{a}{L} \sum_{n=1}^N h_n \exp(2i\pi n a k)$$

where  $a$  is the sampling distance,  $h_n$  is the height profile at the  $n$ th position, and  $Na = L$ . The power spectrum density (PSD) is defined by  $PSD(k) = |\hat{h}(k)|^2$ . Practical tools in optical scattering [3] measure directly this spectrum. On the other hand, it is also possible to get information about surfaces by studying the autocovariance function

$$f(j) = \frac{a}{L} \sum_{n=1}^N h_n h_{n+j} - \left( \frac{a}{L} \sum_{n=1}^N h_n \right)^2.$$

Of course, whenever the measurements of the heights  $h_i$  are not precise enough, this will lead to a very bad estimate of  $f(\cdot)$ , this is why it is often better to determine directly the PSD. But in model systems or numerical simulations, it may be interesting to study  $f(\cdot)$ . This is the motivation of this work. For an SOS model over a quenched random substrate, we will study the link between the autocovariance  $f(\cdot)$  of  $h$  and some characteristics of both the substrate and the film (roughness, surface tension, volume).

Background and references to the mathematical literature about SOS interfaces, including cases with disordered

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substrates, can be found in review articles by Velenik [4] or Giacomin [5]. Our present work differs from previous work with disordered substrates by the pressure term in (1) below which controls the film thickness and leads to different issues.

## 2 Model

A quenched one-dimensional random substrate is modelled by a sequence of independent, exponentially distributed random variables of mean one, the heights  $h_i^1$ ,  $i \in \mathbb{Z}$ . A film is then deposited and thermalized according to the Gibbs measure with the Abraham-Smith [6, 7] Hamiltonian

$$\mathcal{H} = J \sum_{|i-j|=1} |h_i - h_j| + K \sum h_i \quad (1)$$

at temperature  $kT = 1$ . The film height  $h_i \in \mathbb{R}_+$  at point  $i$  obeys  $h_i \geq h_i^1$ . For a precise definition, one may start from a Markov chain with state space  $\mathbb{R}_+$ , indexed by  $i = -N/2, \dots, N/2$ , with initial condition  $h_{-N/2}$  fixed to a constant independent of  $N$ , and transition probabilities

$$\mathbb{P}(dh_{i+1}|h_i) = dh_{i+1} e^{-J|h_{i+1}-h_i|-Kh_{i+1}} \mathbf{1}_{h_{i+1} \geq h_{i+1}^1} / \text{normalization}. \quad (2)$$

No phase transition is expected in this one dimensional model with short range correlations, so that equivalence of suitable ensembles will hold, for almost every realization of the substrate  $h^1$ .

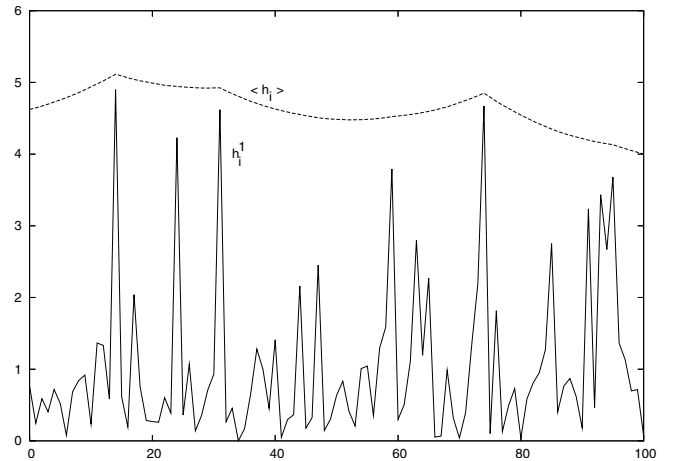
In the language of statistical mechanics, the Gibbs measure with Hamiltonian (1) over  $[-N/2, N/2]$  is an isobaric ensemble where the film volume  $\sum(h_i - h_i^1)$  is controlled by the pressure  $K$  while being allowed to fluctuate. In the thermodynamic limit, local functions of the film height will follow the same law as if obtained from a fixed volume ensemble where  $\sum(h_i - h_i^1)$  is fixed.

We keep the isobaric ensemble, but replace the fixed initial condition and free final condition of the Markov chain by periodic boundary conditions. The resulting model of a film on a quenched substrate is studied by Monte-Carlo simulation with sub-lattice parallel dynamics, and a heat bath algorithm. Simulations were performed for system size up to  $N = 10^7$  and time up to  $10^5$  MCS/S. A typical window of the thermal or empirical time average

$$\langle h_i \rangle = \lim_{T \nearrow \infty} \frac{1}{T} \sum_t h_i(t) \quad (3)$$

versus  $i$ , for one substrate sample  $h^1$ , is shown in Figure 1.

As may be guessed from Figure 1, this thermal averaged profile  $\langle h_i \rangle$  is very close, for large  $J$ , to a sequence of Wulff shapes pinned at the peaks of the substrate. This point of view was investigated by the authors in [8]. In



**Fig. 1.** Substrate  $h_i^1$  and film  $\langle h_i \rangle$  for  $K = 0.1$  and  $J = 10$ .

the present paper, we investigate the correlation function averaged over the disorder,

$$\begin{aligned} f(j) &= \lim_{N \nearrow \infty} \frac{1}{N} \sum_{i=-N/2}^{N/2} \left( \mathbb{E} h_i h_{i+j} - \mathbb{E} h_i \mathbb{E} h_{i+j} \right) \\ &= \lim_{N \nearrow \infty} \frac{1}{N} \sum_i \langle h_i; h_{i+j} \rangle \\ &= \lim_{T \nearrow \infty} \lim_{N \nearrow \infty} \frac{1}{T} \sum_t \left[ \frac{1}{N} \sum_i h_i h_{i+j} - \left( \frac{1}{N} \sum_i h_i \right)^2 \right] \end{aligned} \quad (4)$$

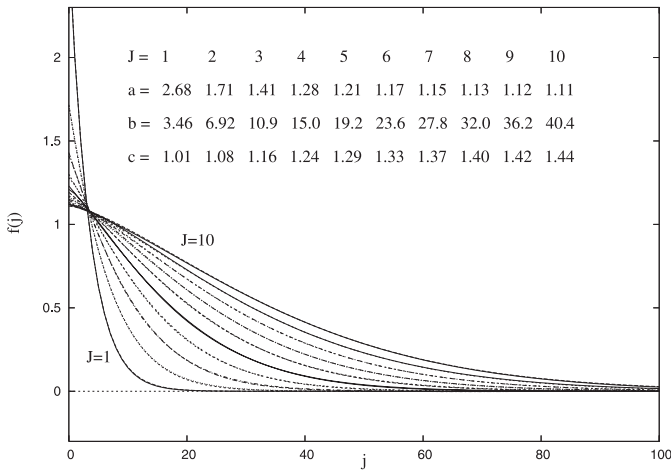
where the first line is for the Markov chain (2), the second line for one of the Gibbs measures, and the third line for our Monte-Carlo Markov chain, which we start from  $h_i = h_i^1 + K^{-1} \quad \forall i$ . The second line, for the Gibbs measure in the isobaric ensemble, is positive by the FKG inequality [9].

## 3 Numerical results

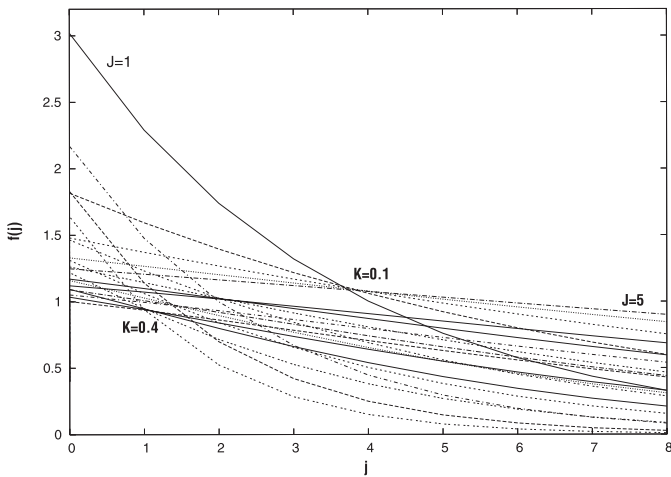
Time averages here and below were taken after  $10^4$  MCS/S for thermalization, during the remaining time, once in every 10 MCS/S, altogether  $T$  measurements. In the ranges of  $j$  shown and discussed below, the limits  $T \nearrow \infty$  and  $N \nearrow \infty$  were clearly attained. Because of disorder effects together with thermalization time of order  $L^2$  for wavelength  $L$ , larger  $j$ 's were not accessible within reasonable computing time.

At the precision of the graphs in Figure 2, the correlation  $f(j)$  and the fitted  $a e^{-(j/b)^c}$  are undistinguishable, over the whole range  $0 \leq j \leq 100$ , for each value of  $J = 1, \dots, 10$ . The parameter  $b$  may be considered as a correlation length. The exponent  $c$ , varying between 1 and 1.5 in our range of parameters, shows that  $f(j)$  is concave for small  $j$  and convex for large  $j$ , with an inflexion point at  $j = b(\frac{c-1}{c})^{1/c}$ .

For a given  $K$ , the curves for different  $J$ 's go through a common point, which gives an indication of how the



**Fig. 2.** Film correlation function  $f(j)$  and fit  $ae^{-(j/b)^c}$  for  $K = 0.1$  and  $J = 1, \dots, 10$ .

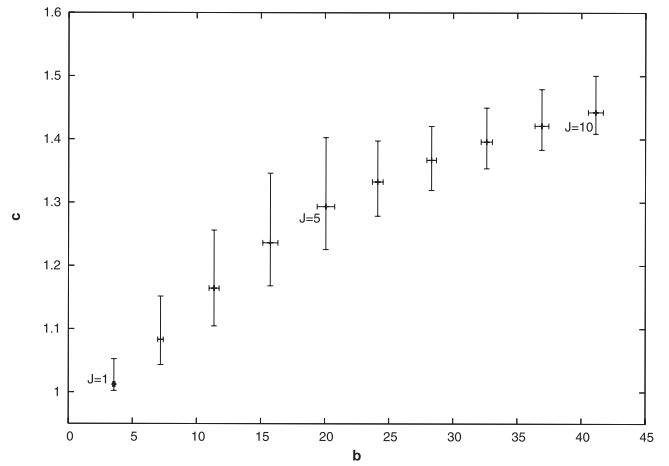


**Fig. 3.** Film correlation function  $f(j)$  for  $K = 0.1, 0.2, 0.3, 0.4$  and  $J = 1, 2, 3, 4, 5$ .

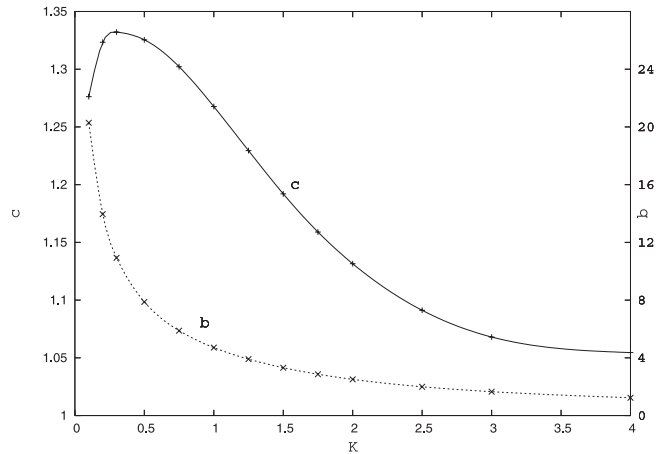
redundant three parameters  $a, b, c$  of the fit depend upon the two parameters  $J, K$  of the model. Figure 3 shows how the fixed point changes with  $K$ .

The super-exponential decay of the correlation function would need to be confirmed for larger values of  $j$ . The fact that the disorder makes the long-distance correlation smaller can be understood as follows. The interval between  $i$  and  $i + j$  contains a family of substrate peaks, whose number and heights go to infinity as  $j \nearrow \infty$ . Such peaks tend to decouple the interface, because the interface can hardly fluctuate above a peak, so that the two sides of a peak tend to become independent. The largest peak between  $i$  and  $i + j$  only makes, with large probability, a power law correction to the flat substrate exponential decay, but the collective effect of a density of peaks might yield super-exponential decay.

It may be, on the contrary, that exponential decay is recovered when  $j$  becomes much larger than  $b$ , when the correlation is too tiny to be measured within our Monte-Carlo simulation, out of the disorder and thermal noises.



**Fig. 4.** Film exponent  $c$  versus correlation length  $b$  for  $K = 0.1$ , at  $J = 1, \dots, 10$ .



**Fig. 5.** Film exponent  $c$  and correlation length  $b$  versus pressure  $K$  for  $J = 5$ .

As  $J$  increases, the film tension increases, and the correlation length  $b$  increases too. But the correlation function at distance  $j > b$  decreases because of the decorrelation effect of large peaks, whose mechanism is more effective when the surface tension is bigger: the interface tends to be pinned at the large peaks. This results in more “super”-exponential decay, larger exponent  $c$ , as appears in Figure 4. The top and bottom of the error bars in Figure 4 correspond to a fit of the correlation bars in ranges  $0 \leq j \leq b$  and  $j > b$  respectively.

As  $K$  decreases, the film volume increases. For large  $K$ , the film is thin and follows closely the substrate profile, so that exponential decay is expected. For small  $K$ , the film is thick, far from the substrate, and exponential decay is also expected. More precisely, one may assume that the film thickness scales when  $K \searrow 0$  as  $K^{-1/3}$  and the correlation length  $b$  as  $K^{-2/3}$ , like for a flat substrate [6,7].

For our random substrate, i.i.d.  $\exp(1)$ , a peak of height  $K^{-1/3}$  is likely to appear after a distance of order  $\exp(K^{-1/3})$ , which is so much larger than the correlation length  $b$  that it should affect only very weakly the exponential decay. This is consistent with Figure 5.

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