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Correlations of a bound interface over a random substrate

Joël De Coninck⁽¹⁾, François Dunlop⁽²⁾, Thierry Huillet⁽²⁾

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.

PACS. 02.50.-r Probability theory, stochastic processes, and statistics — 02.50.Ng Distribution theory and Monte Carlo studies — 05.70.Np Interface and surface thermodynamics.

1. Introduction

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 [AS1, AS2] 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

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

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

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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 on Fig. 1.

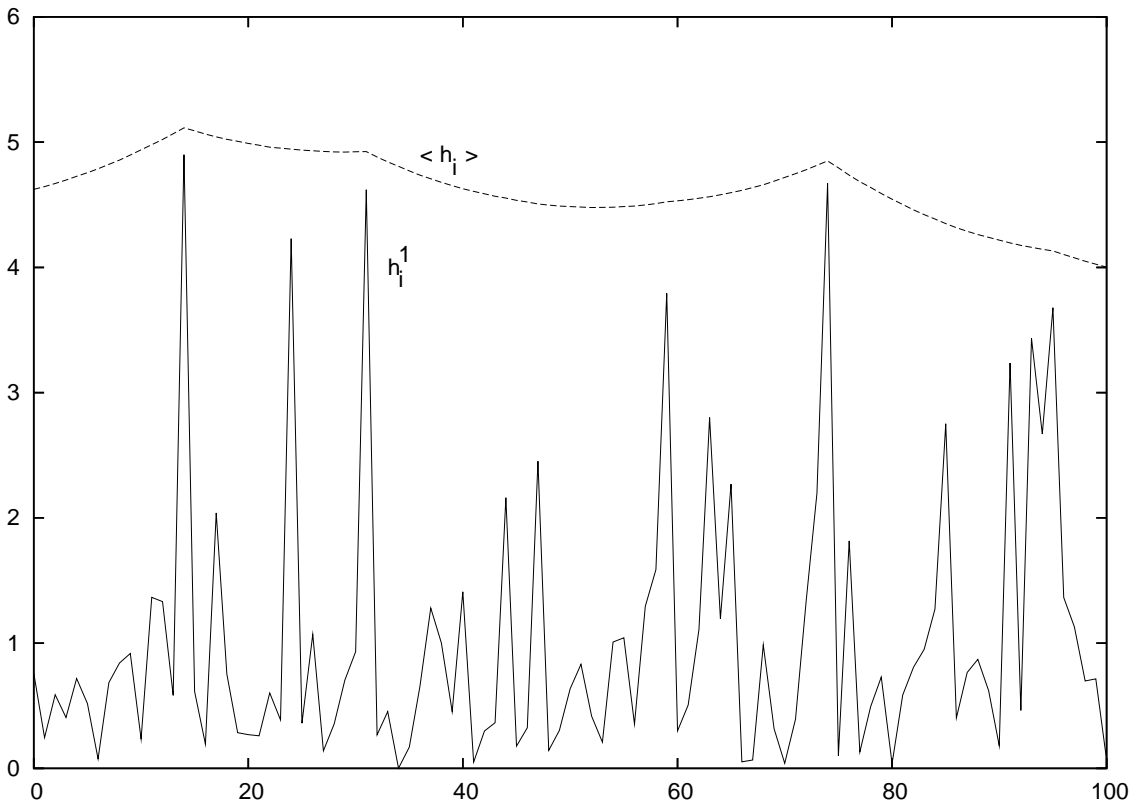


Fig. 1: Substrate h_i^1 and film $\langle h_i \rangle$ for $K = 0.1$ and $J = 10$.

As may be guessed from Fig. 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 [DDH]. In the present paper, we investigate the

correlation function averaged over the disorder,

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

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 $h_i = h_i^1 + K^{-1} \quad \forall i$.

2. 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.

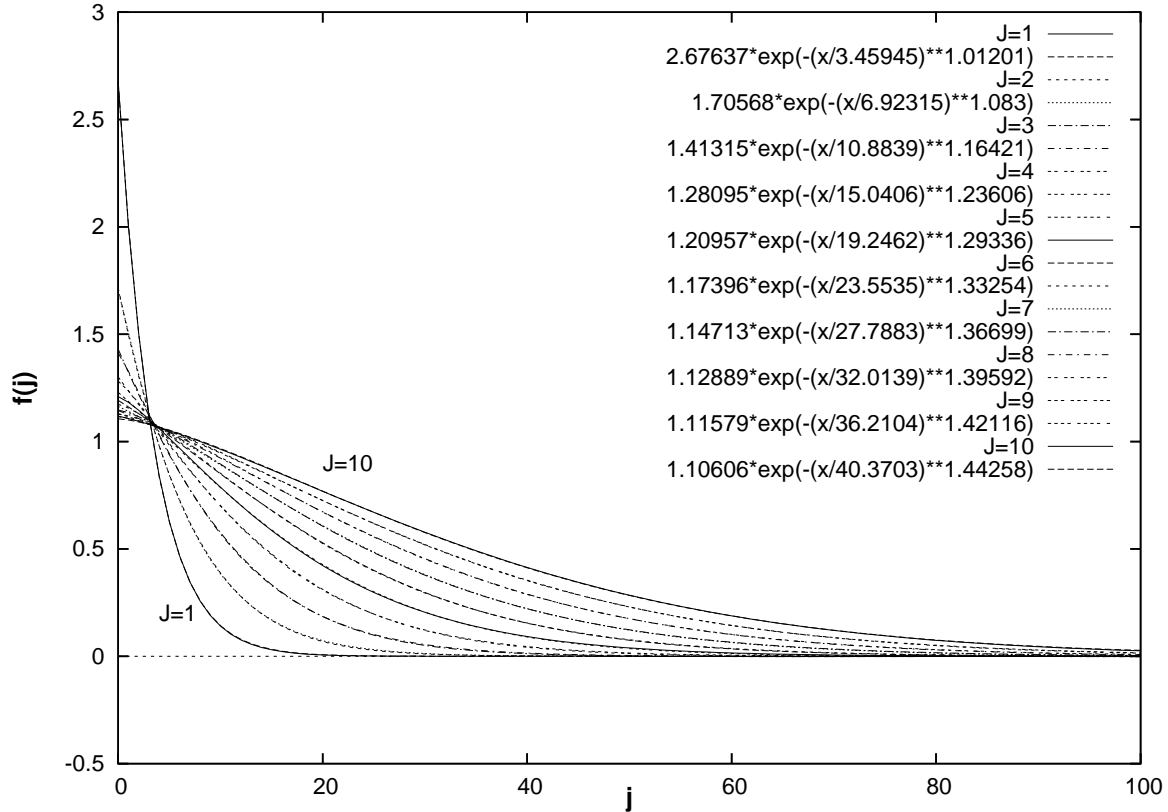


Fig. 2: Film correlation function $f(j)$ and fit $a e^{-(j/b)^c}$ for $K = 0.1$ and $J = 1, \dots, 10$.

At the precision of the graphs in Fig. 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 redundant three parameters a, b, c of the fit depend upon the two parameters J, K of the model. Fig. 3 shows how the fixed point changes with K .

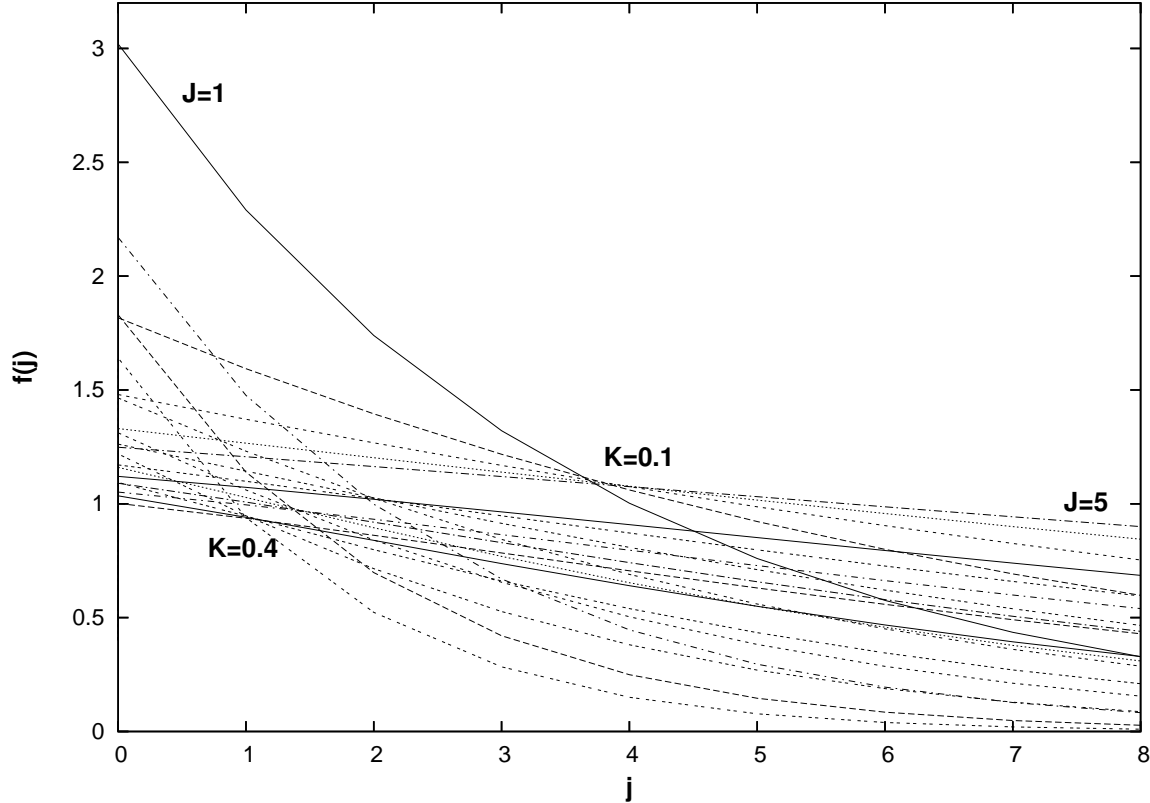


Fig. 3: Film correlation function $f(j)$ for $K = 0.1, 0.2, 0.3, 0.4$ and $J = 1, 2, 3, 4, 5$

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.

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 on Fig. 4. The top and bottom of the error bars in Fig. 4 correspond to a fit of the correlation function in ranges $0 \leq j \leq b$ and $j > b$ respectively.

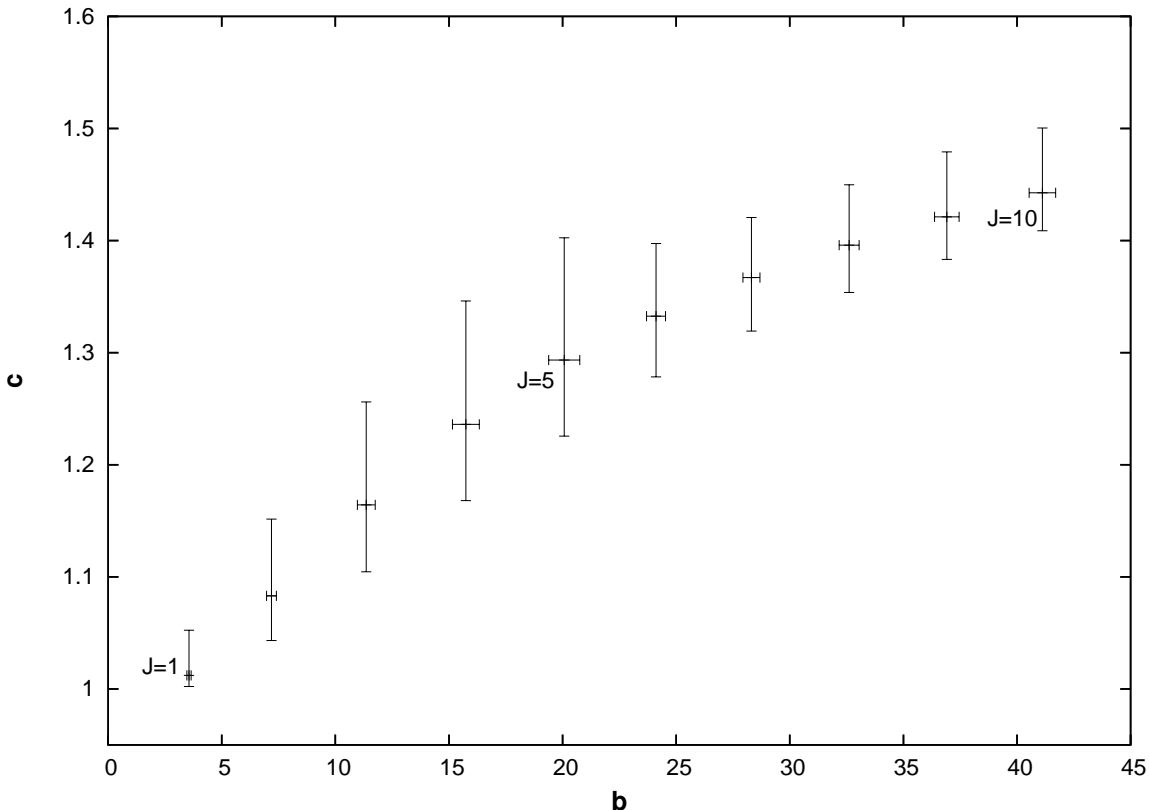


Fig. 4: Film exponent c versus correlation length b for $K = 0.1$, at $J = 1, \dots, 10$.

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 [AS1, AS2]. 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 Fig. 5.

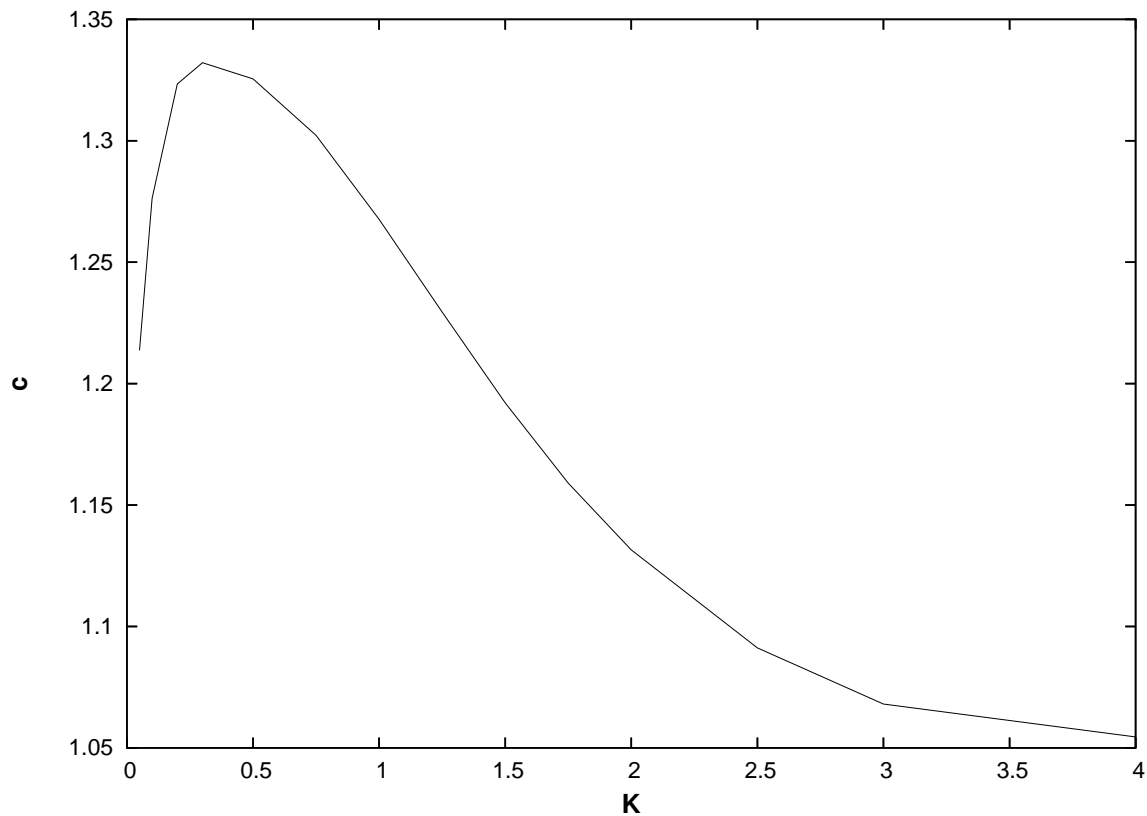


Fig. 5: Film exponent c versus pressure K for $J = 5$.

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