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High precision measurement of the SOS surface thickness in the rough phase

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Abstract. — Using a cluster algorithm without critical slowing down for the discrete Gaussian SOS model, we verify to high precision the linear dependence of the surface thickness on the logarithm of the lattice size.

Solid-on-solid (SOS) models are of great interest both theoretically and in the study of crystal interfaces [1]. We recently developed a cluster algorithm for SOS models [2], which allows us to obtain very accurate results from simulations. Here we present a numerical study of the logarithmic dependence of the surface thickness on the lattice size in the rough phase. Although for very high temperatures T this behavior was proven in [3], doubts were repeatedly raised in the literature as to its validity for moderately high temperatures [4].

We chose to work with the discrete Gaussian model (see e.g. [5] for an introduction to this model), which is defined as follows. To each point x of a two-dimensional $L \times L$ square lattice with periodic boundary conditions an integer valued spin h_x is assigned, which can be viewed as the height of a surface without overhangs. The interaction Hamiltonian is a sum over nearest neighbors $< x, y >$,

$$H(h) = \sum_{<x,y>} \frac{1}{2}(h_x - h_y)^2 \,, \tag{1}$$

and the partition function Z is defined by

$$Z = \sum_h e^{-\frac{1}{T}H(h)} \tag{2}$$

From standard convergent expansion techniques it follows that at low temperatures the SOS surface is smooth, i.e. the surface thickness σ,

$$\sigma^2 := \lim_{|x-y|\to\infty} < (h_x - h_y)^2 > = \; 2 < (h_x - \overline{h})^2 > , \tag{3}$$

is finite. Here $\overline{h}$ is the average over the lattice of the h_x ($\overline{h}$ is not an expectation value). The second equality in (3) holds in the thermodynamic limit, and for finite lattice measurements we use the last term in the expression (3) for σ^2, averaged over lattice translations.

As the temperature T is increased, the surface fluctuates more and more. At high temperatures the discreteness of the spins is hardly felt. The surface thickness is infinite in the thermodynamic limit, i.e. the surface becomes rough. The large distance behavior is that of the massless free field theory (i.e. the model (1) with real instead of integer spins) [6, 3, 1]. In particular, we have the prediction

$$\sigma^2 = \frac{T_{\rm eff}}{\pi} \; (\ln L + c_1) \; , \tag{4}$$

with the constant $T_{\rm eff}$ ("effective temperature") defined such that in the free field theory $T = T_{\rm eff}$.

The phase transition, which is of the Kosterlitz-Thouless type [6], is located at $T_{\rm KT} = 0.752(2)$ [7] (in a recent preprint [8], the value $T_{\rm KT} = 0.752(5)$ is quoted from a Villain model simulation). We chose to perform our simulations at $T = 1$, which is not a very high temperature, but already far enough from $T_{\rm KT}$ to expect only small deviations from (4) (if the theoretical prediction is correct).

Let us give some technical details of these simulations. We considered lattice sizes $L = 8$, 16, 32, 64, 128, and 256. For each lattice size we performed a total of between 3.5 and 4 million cluster updates. Each cluster was grown around a randomly chosen seed, according to the procedure which was found in [2] to have no critical slowing down at all. The average cluster size was between 0.3 and 0.4 of the lattice volume. We used a new method for vectorizing the cluster update [9], which on a CRAY YMP resulted in a speed-up factor for the update of between three and four (the speed-up increases somewhat with the lattice size). With vectorization, even a lattice of $L = 512$ is accessible with a reasonable amount of computer time. However, the following analysis of the results for lattice sizes up to $L = 256$ is already very convincing.

Table I presents our values for the surface thickness. The main result is that (4) *fits all data*

Table I. — *The surface thickness for the DGSOS model at* $T = 1$.

L	8	16	32	64	128	256
σ^2	0.75471(36)	0.97523(36)	1.19415(34)	1.41442(32)	1.63364(39)	1.85396(42)

perfectly. Furthermore, the least square fit results are compatible with one another for different ranges $L_0 \le L \le 256$ and $L_0 \le L \le 128$, with $L_0 = 8, 16, 32, 64$. We shall argue below that, in order to be on the safe side, we should only use the values of σ^2 for $L \ge 32$. The fit for $32 \le L \le 256$ yields

$$T_{\text{eff}} = 0.9965(8) \text{ for } T = 1 \,. \tag{5}$$

Notice that $T_{\text{eff}} < T$, as predicted by the flow equations of the Kosterlitz-Thouless theory [6]. For the constant in (4) we obtained $c_1 = 0.302(2)$. The data and the fit are plotted in figure 1. The solid line is the fit with (4) for $L \geq 32$, the dashed line is its continuation to smaller L. In order to make the size of the errors more visible, we plotted in the inset the quantity $\sigma^2 - \frac{1}{\pi} \ln L$.

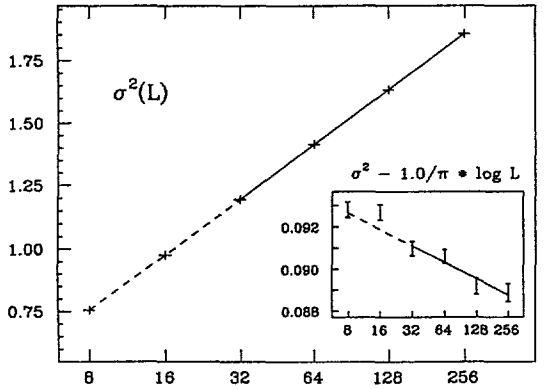

Fig. 1. — Surface thickness for the DGSOS model at $T = 1$. The x-axis is logarithmic. The solid line is the fit with (4) for $L \geq 32$. The dashed line is its continuation towards small L.

Equation (4) is a finite volume continuum approximation for $\sigma^2 = 2 < (h_x - \overline{h})^2 >$. Our model is however defined on a finite volume lattice. In order to estimate the magnitude of the finite lattice spacing effects, we compared the values of σ^2 for the free field theory at $T = T_{\text{eff}}$ on the lattice and in the continuum. On the lattice, σ^2 is a sum over momenta that can be evaluated numerically with high precision. For $L = 8$ the difference between the lattice and continuum values is not insignificant compared to the errorbars of our DGSOS simulation. At $L \geq 16$ however, this effect disappears. Thus taking $L \geq 32$ as a basis for the result (5) seems very safe.

The data are very precise, so we hoped to exclude with a high degree of confidence certain types of behavior different from (4). And indeed, the various least square fits we are going to discuss all indicate that the data strongly favor the linear dependence on $\ln L$.

We first tried a power fit, since quite often a logarithmic dependence looks very similar to a power law with a small exponent. The fits with

$$\sigma^2 = c_1 L^a + c_2 \tag{6}$$

were not very stable with respect to changes in the subset of data used. The constants c_1 and c_2 had a tendency to be very large. However, a reasonably small value for the χ^2 per degree of freedom could only be obtained with very small values of a (≤ 0.001). Thus the power law (6) can be excluded.

An ansatz sometimes discussed in the literature [4] is the power-of-log form

$$\sigma^2 = \frac{c_1}{\pi} (\ln L)^{1+b} + c_2 \,. \tag{7}$$

Fits with this form go rather well through all data. For $L \geq 32$ the fit results in $|b| < 0.01$, with a statistical error larger than $|b|$, and in $c_1 = 1.00(2)$, which is consistent with the value we determined for T_{eff} using (4). Thus a linear dependence on $\ln L$ is favored.

Next we tried to see if log-log corrections may play a role. We fitted the data with

$$\sigma^2 = \frac{c_1}{\pi} \ln L + c_2 \ln \ln L + c_3 , \tag{8}$$

and the fits were good for all L-ranges. For $L \geq 32$ we got $c_2 = 0.01(5)$, which shows that the absence of log-log corrections is favored. We also got $c_1 = 0.994(11)$, which is consistent with the previously determined value for T_{eff}.

Finally we fitted the data with

$$\sigma^2 = \frac{T_{\text{eff}}}{\pi} \ln L + \frac{1}{\pi^2} \ln(c_1 - L^{4-2\pi T_{\text{eff}}}) + c_2 . \tag{9}$$

This is the renormalization group improvement of (4) [6,7]. For large enough L the difference between (9) and (4) is negligible. Close to but still above T_{KT} we found this form to fit simulation results over a much wider L-range than (4) does [7]. Here, at $T = 1$, there was practically no difference between the fits with (9) and with (4). In particular, the fitted values for T_{eff} were almost identical in the two cases. Thus we have established that at $T = 1$ the asymptotic regime (large L) is reached very quickly.

We conclude that we have confirmed the validity of (4) with a high degree of accuracy.

Currently we are using our new cluster algorithm for a high precision study of the Kosterlitz-Thouless transition in various SOS models [7]. This includes the interface of the three-dimensional Ising model, which can be simulated with the cluster algorithm of [10].

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