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The solid-on-solid surface width around the roughening transition

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We investigate the surface width W of solid-on-solid surfaces in the vicinity of the roughening temperature T_r. Above T_r, W^2 is expected to diverge with the system size L like $\ln L$. However, close to T_r a clean $\ln L$ behavior can only be seen on extremely large lattices. Starting from the Kosterlitz–Thouless renormalization group, we derive an improved formula that describes the small L behavior on both sides of T_r. For the discrete Gaussian model, we used the valleys-to-mountains-reflections cluster algorithm in order to simulate the fluctuating solid-on-solid surface. The base plane above which the surface is defined is an $L \times L$ square lattice. In the simulation we took $8 \leq L \leq 256$. The improved formula fits the numerical results very well. From the analysis, we estimate the roughening temperature to be $T_r = 0.755(3)$.

1. Introduction

Solid-on-solid (SOS) models are useful as interface models (for reviews on SOS models, see e.g. [1]). They belong to a large class of models that are believed to be in the Kosterlitz–Thouless (KT) universality class [2]. For SOS models, the KT transition is the roughening transition. It is still a challenge to devise methods for the accurate study of this transition and for unambiguous tests of the KT theory.

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As a prototype of an SOS model we consider the discrete Gaussian (DGSOS) model, defined by the partition function

$$Z = \sum_h \exp\left(-\frac{1}{2T} \sum_{\langle i,j \rangle} (h_i - h_j)^2\right), \tag{1}$$

where h_i are integer "height" variables defined on the sites i of an $L \times L$ square lattice with periodic boundary conditions. A configuration h can be viewed as a surface without overhangs, embedded in three dimensions; its energy is obtained by summing over all nearest neighbor pairs $\langle i, j \rangle$; T is the temperature (Boltzmann's constant is set to one). The square of the average surface width W is defined by

$$W^2 = \frac{1}{L^2} \sum_i \langle (h_i - h_j)^2 \rangle . \tag{2}$$

The model has two phases. At low temperatures the surface is smooth, and W stays finite as $L \to \infty$. When T is increased, we encounter the roughening transition at $T = T_r$. The KT theory predicts [1,2] that in the thermodynamic limit

$$W^2 \sim (T_r - T)^{-1/2} \sim \ln \xi , \tag{3}$$

as T approaches T_r from below (ξ is the correlation length). For $T \geqslant T_r$, W diverges as $L \to \infty$. The prediction for asymptotically large L is the "free field" behavior (i.e., continuous Gaussian – h_i is real instead of integer)

$$W^2 = \frac{T_{\text{eff}}}{\pi} \ln L + \text{const.} \tag{4}$$

T_{eff} is called "effective temperature" and

$$T_{\text{eff}} = \frac{2}{\pi} \qquad \text{for } T = T_r . \tag{5}$$

Furthermore, as T approaches T_r from above,

$$T_{\text{eff}} - \frac{2}{\pi} \sim (T - T_r)^{1/2} . \tag{6}$$

In principle, these formulas could be used in a numerical study in order to verify or disprove the KT theory. In practice, however, this is problematic. In the smooth phase, we would need unrealistically large lattices in order to test the power law (3). This problem is related to the difficulties encountered in the

study of the dual (Villain, XY) spin models, where it is hard to cleanly distinguish an essential singularity in the correlation length ξ (as predicted by KT) from a power law singularity [3,4]. In the rough phase, for large enough temperatures, the behavior (4) could be unambiguously verified numerically [5]. However, it turns out that close to T_r a clean logarithm is only seen on very large lattices, and in order to extract the values of T_{eff} in practice we need to know the corrections to eq. (4). Otherwise we cannot determine T_r by checking eq. (5). Furthermore, for the largest lattice sizes accessible with present day computers and algorithms, it turns out that eq. (6) is not yet fulfilled for the region where eq. (4) holds. Actually, the status of eq. (6) is even worse, as will be argued later.

In order to overcome these problems, we developed a renormalization group (RG) improved formula for the dependence of W^2 on L. This is our main theoretical result. The numerical part of our work shows that the improved formula can be used for extracting T_{eff} as close as desired to T_r, from numerical simulations on reasonably sized lattices. We mention that very high accuracy simulations were possible because we have a cluster algorithm that is free of critical slowing down (the valleys-to-mountains-reflections algorithm [6]). Vectorization [7] also helped. From our analysis, the best estimate for the roughening temperature is $T_r = 0.755(3)$.

In what follows, we first derive our improved formula, then present the analysis of the numerical results, and finally make some additional remarks and present our conclusions.

2. RG improved finite L formula for the surface width

The RG flow of the DGSOS model can be described in an x–y diagram [2]. The trajectories are parametrized by t, the logarithm of the changing length scale. $x(t)$ is related to the scale dependent ("running") temperature $T(t)$, $x(t) = \pi T(t) - 2$, while $y(t)$ is a constant times the fugacity [2]. The KT flow equations are [2]

$$\dot{y}(t) = -x(t)\, y(t)\,, \qquad \dot{x}(t) = -y(t)^2\,. \tag{7}$$

The trajectories are hyperbolas, characterized by the constant E which depends on the temperature T of the model (not on the running $T(t)$!),

$$y(t)^2 - x(t)^2 = E\,. \tag{8}$$

Denoting $\epsilon = \text{sgn}(E)\sqrt{|E|}$, and $x_0 = x(0)$, the full solution of eq. (7) is

$$E<0: \quad x(t)=\epsilon\left(1+\frac{2(x_0-\epsilon)}{(x_0+\epsilon)\exp(2\epsilon t)-(x_0-\epsilon)}\right),$$

$$E=0: \quad x(t)=\frac{x_0}{1+x_0 t}, \tag{9}$$

$$E>0: \quad x(t)=\epsilon\frac{x_0-\epsilon\tan(\epsilon t)}{\epsilon+x_0\tan(\epsilon t)}.$$

The trajectories in the rough phase reach the free field theory and have $\epsilon<0$; in the smooth phase they have $\epsilon>0$; at the KT transition the critical trajectory has $\epsilon=0$ [2]. Notice that in the rough phase $T_{\text{eff}}=T(t=\infty)=(2-\epsilon)/\pi$.

In order to use the RG for computing the surface width, we need to know the contributions corresponding to each length scale. Eq. (2) shows that W^2 is a sum of a two-point-function over all distances. When increasing the lattice size L, we get additional additive contributions from distances of order L. Let us choose

$$t=\ln\left(\frac{L}{L_0}\right), \tag{10}$$

with L_0 some reference length scale, and let us approximate the sum in eq. (2) by an integral. For the free field theory, the additional contributions to W^2 coming from an infinitesimal change in L are easily computed: since eq. (4) is always true, with T_{eff} replaced by the temperature T, we have $\mathrm{d}W^2/\mathrm{d}t=T/\pi$. In the case of the DGSOS model, the KT flow shows that for trajectories in the rough phase we are close to the free field theory if t is large enough. Moreover, we are close to the free field theory too for trajectories in the smooth phase, provided that L is much smaller than ξ but still large enough. Thus the main contribution to $\mathrm{d}W^2/\mathrm{d}t$ will be similar to the free field case, with the only (important) difference that we replace T by the running temperature $T(t)$,

$$\frac{\mathrm{d}W^2}{\mathrm{d}t}=\frac{T(t)}{\pi}. \tag{11}$$

Assuming that $T(t)$ behaves according to the KT flow for length scales larger than L_0, we can integrate eq. (11),

$$W^2=\frac{1}{\pi^2}\int_0^t [x(t)+2]\,\mathrm{d}t+C. \tag{12}$$

The constant C contains the contributions of distances smaller than L_0. Using

eq. (7) and eq. (8), we can express dt in terms of x and dx, after which eq. (12) reduces to an elementary integral. We thus obtain our final formula for W^2,

$$W^2 = \frac{2}{\pi^2} t + \frac{1}{2\pi^2} \ln\left(\frac{x_0^2 + E}{x^2 + E}\right) + C\,, \tag{13}$$

which has to be used in conjunction with eqs. (9) and (10).

The crucial point in the derivation of our improved formula was the replacement, at the appropriate stage, of the temperature T with the running temperature $T(t)$. While this is a commonly used procedure in field theoretical RG arguments, it is not completely rigorous. A more thorough argument, based on a block-spin calculation within the Wilson RG framework, will be presented elsewhere [8].

3. Simulation results

We performed simulations of the DGSOS model for ten different values of the temperature T. At each T we considered lattice sizes of $L = 8$, 16, 32, 64, 128 and 256. Typically, we generated about 2 000 000 to 2 500 000 clusters for each temperature and lattice size. The expectation value of the cluster size varied in the range $0.3L^2$ to $0.35L^2$. The whole project required about 400 hours on one CRAY-YMP processor. As will become clear from the analysis, we did not need more than half of our runs in order to obtain the best estimate for T_r. However, our aim was also to confirm our prediction for the L-dependence of W^2 and to determine the region in which the improved formula is really necessary. The simulation results for W^2 are given in table I.

Table I
Simulation results for W^2.

T	L					
	8	16	32	64	128	256
0.740	0.51429(34)	0.66739(33)	0.81589(32)	0.96185(33)	1.10558(34)	1.24908(39)
0.745	0.51984(37)	0.67560(34)	0.82571(32)	0.97408(33)	1.12248(33)	1.26710(40)
0.750	0.52537(37)	0.68222(35)	0.83542(35)	0.98661(34)	1.13615(35)	1.28461(36)
0.755	0.53137(30)	0.69052(34)	0.84475(33)	0.99877(33)	1.15066(34)	1.30165(38)
0.760	0.53733(37)	0.69725(34)	0.85444(33)	1.00956(29)	1.16440(28)	1.31721(39)
0.770	0.54900(35)	0.71185(32)	0.87292(33)	1.03164(36)	1.18993(34)	1.34726(37)
0.780	0.55902(36)	0.72606(34)	0.88941(33)	1.05190(38)	1.21432(36)	1.37515(40)
0.800	0.58006(38)	0.75240(34)	0.92271(35)	1.09176(40)	1.26032(37)	1.42846(40)
0.820	0.59963(37)	0.77776(34)	0.95355(34)	1.12807(36)	1.30248(38)	1.47770(42)
0.850	0.62762(37)	0.81304(37)	0.99679(36)	1.18076(38)	1.36315(40)	1.54571(43)

As a general rule, these data are extremely well fitted by eq. (13), with fit parameters ϵ, x_0 and C. Aside from the occasional statistical fluctuation, we did however notice that for $T \leq 0.755$ the quality of the fits deteriorated a little. The important results of such fits are the value of ϵ, which characterizes the trajectory, and the range of L for which the fits are good, which roughly tells us where the model enters the KT flow. Notice that we have to decide upon a value for L_0. The choice of L_0 only affects the values x_0 and C, as can be seen after a little algebra. Table II contains the fit results for ϵ, for all our values of T and for various fit ranges. Clearly, for $T \geq 0.76$ the various fit ranges give compatible results. In fact the data for $L = 256$ hardly improve things here. For $T \leq 0.755$, however, the fit results for ϵ sometimes change by more than two standard deviations if we remove the data for $L = 8$. It may be that for these temperatures the KT flow is well reached only above $L = 8$.

From table II our first main numerical result strikes the eye: since $\epsilon > 0$ for $T \leq 0.75$ and $\epsilon < 0$ for $T \geq 0.76$, T_r is between 0.75 and 0.76. This result relies solely on the fact that eq. (13) fits the data well, and on eq. (5).

In order to give a more precise determination of T_r, we plotted for each fit range ϵ versus T, with errorbars, and interpolated the two curves ϵ + error and ϵ − error. The intersection of the so-obtained band with the $\epsilon = 0$ line provides an estimate of T_r. In table III we collected these range dependent estimates. They are quite consistent with one another. Thus, taking into account the above observations about the quality of the fits for $T \leq 0.755$, it would not be

Table II
Fit results for the parameter ϵ.

T	L				
	8–256	16–256	32–256	8–128	16–128
0.740	0.204(06)	0.178(10)	0.151(23)	0.226(08)	0.206(16)
0.745	0.171(07)	0.139(14)	0.165(21)	0.168(11)	0.060(57)
0.750	0.126(09)	0.109(17)	0.103(35)	0.137(14)	0.117(30)
0.755	0.030(38)	−0.078(25)	0.059(60)	0.054(33)	−0.102(33)
0.760	−0.124(10)	−0.130(14)	−0.128(27)	−0.131(13)	−0.151(21)
0.770	−0.211(06)	−0.210(09)	−0.221(17)	−0.211(09)	−0.205(17)
0.780	−0.277(05)	−0.287(07)	−0.278(14)	−0.278(07)	−0.300(12)
0.800	−0.387(04)	−0.387(06)	−0.388(11)	−0.386(06)	−0.387(10)
0.820	−0.478(03)	−0.484(05)	−0.494(09)	−0.471(05)	−0.474(09)
0.850	−0.601(03)	−0.599(04)	−0.590(08)	−0.603(04)	−0.601(07)

Table III
T_r from the interpolated curves $\epsilon(T)$.

Fit range L	8–256	16–256	32–256	8–128	16–128
Estimated T_r	0.7555(25)	0.7535(15)	0.7550(30)	0.7555(25)	0.7515(55)

unreasonable to quote as our final result the value of T_r for the L-range 16–256.

For a more conservative estimate of T_r we plotted the values of ϵ from the ranges 8–256 and 16–256, together with their errorbars, on the same plot. We interpolated the upper and lower envelope of the errorbars. From the intersection of the so-obtained band with the $\epsilon = 0$ line we get the estimate $T_r = 0.755(3)$. Notice that the best estimate in the literature [11], $T_r = 0.7524(7)$, was obtained by a completely different method (matching with the critical block spin flow of the BCSOS model) that does not test directly any of the formulas derived from the KT theory. The best estimate by other authors [3], $T_r = 0.752(5)$ (from the analysis of the correlation length and susceptibility in the massive phase of the Villain model), is also consistent with the result presented here.

At the beginning of section 2 we explicitly wrote down the t dependence of the running temperature $T(t)$. With the numerically determined fit parameters ϵ and x_0, we can thus compute the flow of $T(t)$ numerically. If we use $x(t)$ instead of $T(t)$, we can neatly plot the points $(x(t), y(t))$ inside the standard KT flow diagram. We can now do the following consistency check. The differences $\pi\Delta W^2/\Delta t = (\pi/\ln 2)[W^2(2L) - W^2(L)]$, shown in table IV, should be discrete approximants of $T(t)$, by eqs. (10) and (11). Thus if we again plot the values of the points $(x(t), y(t))$, this time using the discrete approximation, we expect to obtain a similar diagram. We did this exercise and indeed the two diagrams were almost identical.

In the last column of table IV we show the values of $T_{\text{eff}} = (2 - \epsilon)/\pi$, obtained by again taking for each $T > T_r$ the envelope of the errorbars from the fits with L-ranges 8–256 and 16–256. Above T_r, if L is large enough for eq. (4) to hold, the running temperature stabilizes to the value T_{eff}. By looking at

Table IV
The differences $\pi\Delta W^2/\Delta t$ compared with T_{eff}.

T	L					T_{eff}
	8–16	16–32	32–64	64–128	128–256	
0.740	0.6939(21)	0.6731(21)	0.6615(21)	0.6514(22)	0.6504(24)	$T < T_r$
0.745	0.7059(23)	0.6804(21)	0.6724(21)	0.6726(21)	0.6555(23)	$T < T_r$
0.750	0.7109(23)	0.6944(22)	0.6852(22)	0.6778(22)	0.6729(23)	$T < T_r$
0.755	0.7213(21)	0.6990(22)	0.6981(21)	0.6884(21)	0.6843(23)	$T \approx T_r$
0.760	0.7248(23)	0.7124(21)	0.7031(20)	0.7018(18)	0.6926(22)	0.6777(48)
0.770	0.7381(21)	0.7300(21)	0.7194(22)	0.7174(22)	0.7131(23)	0.7035(29)
0.780	0.7571(22)	0.7404(22)	0.7365(23)	0.7361(24)	0.7290(24)	0.7267(35)
0.800	0.7811(23)	0.7719(22)	0.7662(24)	0.7640(25)	0.7620(25)	0.7598(19)
0.820	0.8074(23)	0.7967(22)	0.7910(22)	0.7905(24)	0.7942(26)	0.7900(22)
0.850	0.8404(24)	0.8328(23)	0.8338(24)	0.8267(25)	0.8274(27)	0.8273(16)

how the results in the rows of table IV stabilize, we see that our data for W^2 enter the asymptotic regime of eq. (4) for $0.8 \leq T \leq 0.85$ clearly, and for $T = 0.78$ just barely. For $T_r \leq 0.77$, however, this is far from being true, even at $L = 256$. Notice that in order to understand the validity region of eq. (4) we did need the values of W^2 for $L = 256$. More importantly, notice that our results show that the use of eqs. (4) and (5) for determining T_r (like e.g. in [9,10]) leads to a consistent underestimate.

In order to test eq. (6), we fitted the values for T_{eff} from table IV. The fit was not at all good. We then allowed for a free power instead of the power $\frac{1}{2}$. The fit was now good, but the power was 0.60(4). Disregarding the farthest away point from T_r, $T = 0.85$, the situation did not improve: the power changed to 0.62(7). The fitted value for T_r was 0.753(2) with the point $T = 0.85$ included, and 0.752(4) without it. While these values for T_r are reasonable, the fact remains that the power $\frac{1}{2}$ is not yet seen even as close to T_r as our data in the rough phase are. Notice that this conclusion implies in particular that we cannot use eq. (6) in order to fit results in a region where the simple behavior (4) applies on lattices of still manageable size.

As a last issue, let us remark that in the absence of a theory, one may be simply tempted to make some "reasonable" ansatz for the corrections to eq. (4). We tried to fit the data with a $\ln(\ln L)$ correction (the coefficient in front of $\ln(\ln L)$ is the third fit parameter besides T_{eff} and the constant). The fits were as good as those with eq. (13), if not better. However, the values of T_{eff} thus obtained were clearly wrong. It is not difficult to understand the numerics behind this phenomenon. The main point is however, to view this as another example of the danger of analyzing simulation results without a solid theoretical basis.

Along the same lines, let us remark that we found a different modification of eq. (4) to also fit the data very well: instead of taking $\ln L$ we took a power of $\ln L$ (this power is the third fit parameter). The power that allowed for good fits very close to T_r never deviated from the value 1 by more than 10%. Nevertheless, the fitted values for T_{eff} were again clearly wrong with this procedure.

4. Conclusions

We have derived a renormalization group improved formula for the finite size behavior of the SOS surface width in the vicinity of the roughening transition. The improved formula was tested in a high accuracy simulation of the DGSOS model, and found to describe the data excellently. As a result of our analysis, we

- verified an important aspect of the KT scenario,
- gave a precise determination of T_r,
- found the region in which eq. (4) cannot be used unless we consider much larger lattice sizes,
- found that the region of applicability of eq. (6) is much smaller than previously assumed.

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