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LETTER TO THE EDITOR

Kinetics of interface growth with next-nearest-neighbour interactions

Pierre Devillard

HLRZ, c/o KFA Jülich, Postfach 1913, D-5170 Jülich 1, Federal Republic of Germany

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Abstract. We study interface growth for SOS models with next-nearest-neighbour interactions and especially the relaxation to equilibrium via evaporation and deposition dynamics when the initial state is an ideally flat surface and the equilibrium state is a disordered flat phase. The width of the interface first increases logarithmically with time before decreasing towards its finite equilibrium value and the behaviour of the order parameter measuring the long-range up-down order of the steps is compatible with Lifshitz theory. When a finite driving force is applied, it is found that the disordered flat phase becomes rough, even for temperatures well below the equilibrium roughening temperature between rough and disordered flat phases.

There has been recent interest in understanding how the classical roughening of surfaces [1] is modified in non-equilibrium situations, for example, when a finite driving force is applied. Studies have used linear response [2], or have focused on simple solid-on-solid (SOS) models where some preference for growth over evaporation was imposed [3, 4]. Some work has also been done on the Kardar-Parisi-Zhang (KPZ) equation [5] in three dimensions, and modifications of it to try to include a periodic potential [4]. When next-nearest-neighbour (NNN) interactions between atoms are present, it has been shown [6] that a new type of phase can appear; disordered flat phases (DOF). Equilibrium phase diagrams and static properties of SOS models with NNN interactions have been studied in [6]. It is the purpose of this letter to examine the influence of NNN interactions on some problems already studied in the context of the dynamics of normal SOS models. In particular, DOF phases are intriguing because there is no nucleation barrier and the surface is still flat. We will focus on the relaxation to equilibrium when one starts from a flat surface and the equilibrium phase is a DOF phase. The analogous problem for normal SOS-type models at infinite temperature was studied in [7]. We shall also discuss the influence of a finite driving force. (See [2] for the case where NNN interactions are absent.)

We first want to study the case of zero driving force. Let us consider the following Hamiltonian [6]:

$$H = J \sum_{\mathrm{NN}} \delta(|h_i - h_j| - 1) + J' \sum_{\mathrm{NNN}} \delta(|h_i - h_j| - 1) + K \sum_{\mathrm{NNN}} \delta(|h_i - h_j| - 2). \tag{1}$$

h_i is an integer representing the height of site i, where the sites i lie on the square lattice. The first sum runs over all pairs (i, j) where j is a nearest-neighbour site of i and the last two sums are on all pairs of next-nearest-neighbour sites (i, j). The difference $h_i - h_j$ between nearest neighbours can only take the values -1, 1, or 0 (the model is

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a restricted solid-on-solid (RSOS) model). From now on, we restrict ourselves to the case $J = J' = 0$ and $K/kT > \ln 2$. For such a case, the equilibrium state is a DOF phase [6]. We want to understand how, starting from a flat phase, the system relaxes to equilibrium toward a DOF phase, using evaporation and deposition dynamics. This study is in the same spirit as former studies [7] on the same problem but without NNN interactions. It is known that, at infinite temperatures, the surface evolves according to the Edwards-Wilkinson theory [8].

We now describe our method of simulation. We use $(4n+2)\times 4n$ lattices with helical boundary conditions in the horizontal direction and periodic boundary conditions in the vertical direction. By convention, we set $L = 4n+1$. In order to get vectorization, four sublattices were used and all sites of each sublattice were updated simultaneously. We reached 2.6 MC steps per microsecond for systems of size $L = 17$ and up to 3.18 MC steps per microsecond for $L = 181$, on cone Cray YMP processor. The height on each site has a probability $\frac{1}{2}$ of increasing and $\frac{1}{2}$ of decreasing by one unit. If the final configuration still maintains the restricted SOS condition, the move is accepted with probability $\exp(-\Delta E/kT)$ where ΔE is the change in energy between the new and the old configuration. If the move leads to height differences between nearest neighbours larger than 1, it is rejected in any case and the old configuration remains.

The width w of the interface is defined as usual as

$$w \equiv \langle (h_r - \langle h_r \rangle)^2 \rangle^{1/2}$$

where the brackets mean the average on the sites r of the lattice. Another quantity of interest is the terrace order parameter

$$\langle \psi \rangle \equiv \langle \exp(i\pi h_r)(h_r - h'_r) \rangle \tag{2}$$

where $r' = (x-1, y)$ is the left neighbour of site $r = (x, y)$. x and y are respectively the abscissa and ordinate of site r. $\langle \psi \rangle$ is non-zero only in the DOF and body-centred SOS (BCSOS) flat phases [6]. In order to distinguish between DOF and BCSOS flat phases, we also looked at the staggered magnetization

$$\rho = \langle \exp(i\pi(x + y + h_r)) \rangle. \tag{3}$$

In the thermodynamic limit, ρ is non-zero only in the BCSOS flat phase. In the range of parameters where we were working, the steady state value of ρ went to zero as $1/L^2$. This ensured that we were not dealing with BCSOS flat phases.

Figure 1 shows w^2, the square of the width, plotted against $\ln t$, where t is the number of Monte Carlo (MC) attempts per lattice site, for samples of sizes $L = 17$ to $L = 121$. We work at $K/kT = \frac{10}{7}$, so that T is well below the roughening transition $K/kT = \ln 2$ between a rough phase and a DOF phase. One can see that w first increases and then decreases. After a time $t_1(L)$, it saturates to a constant value W, which we refer to as the saturation width.

We then want to study $\langle \psi \rangle$. Actually we calculate the quantity

$$\Psi \equiv [\langle \psi \rangle^2]^{1/2} \tag{4}$$

where the outer straight brackets mean the average over different samples, (the inner brackets mean the average over the different sites of a particular sample). Because of the indetermination on the sign of $\langle \psi \rangle$, averaging $\langle \psi \rangle$ over many samples would eventually give zero. Figure 2 shows $\ln \Psi$ against $\ln t$ for the same samples. One sees that Ψ first behaves as a power law and then, after a time $t^*(L)$ saturates to its

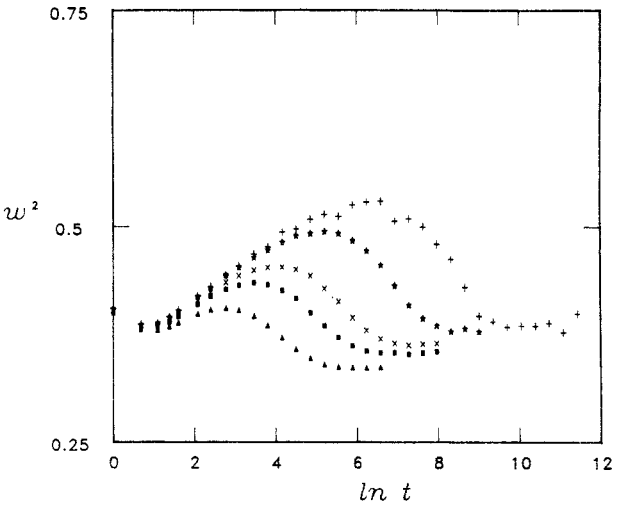

Figure 1. Squared width w^2 against ln t where t is the number of Monte Carlo steps per site, at zero driving force, for $K/kT = \frac{10}{7} \simeq 1.429$, for lattices of size $L = 17$ to $L = 121$ as explained in text. Symbols are: for $L = 17$ (▲), $L = 25$ (■), $L = 33$ (×), $L = 61$ (★) and $L = 121$ (+). Averages have been taken over 20 samples for $L = 121$, and up to 10 000 samples for $L = 17$.

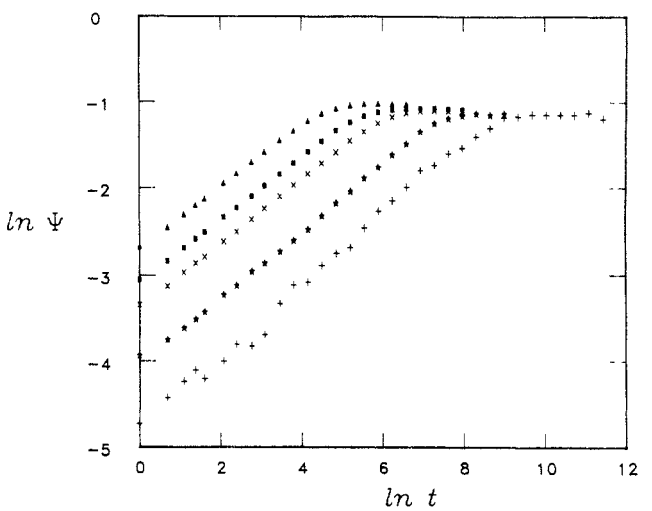

Figure 2. Time dependence of the order parameter Ψ. ln Ψ against ln t for the same samples as in figure 1.

equilibrium value. It is seen by comparing figure 1 and figure 2 that $t_1(L)$ and $t^*(L)$ coincide approximately. We would like to show that

$$t^*(L) \sim L^z \tag{5}$$

where z is some exponent. Figure 3 shows ln $t^*(L)$ against ln L. A least-squares fit gives $z = 2.07 \pm 0.13$.

Our interpretation of the simulation results is as follows. Starting from a flat interface, in the regime of parameters we are in, it is very easy to create steps, so that

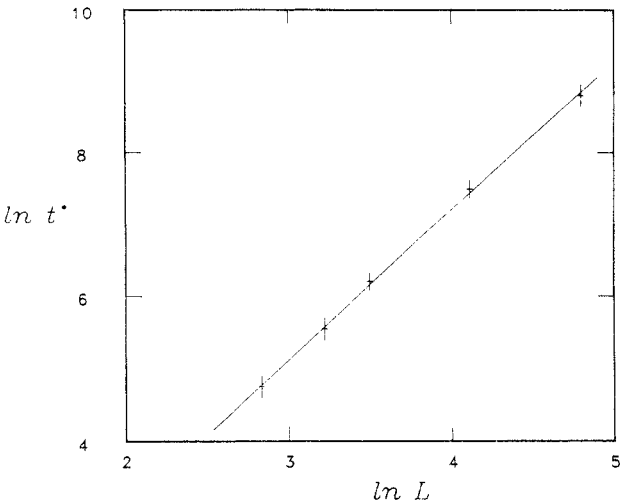

Figure 3. Finite-size scaling of the crossover time t^*. $\ln t^*(L)$ against $\ln L$ for the same samples as in figure 1. The full line is a least-squares fit to the data and has a slope 2.07.

after a few Monte Carlo steps per spin, there is a finite density of steps. The order parameter $\langle\psi\rangle$ is still low. Then the system begins to order in domains where ψ is 1 or -1. According to Lifshitz theory [9], the typical size of domains, l, grows as $\sqrt{t}$. When l becomes of order L, one domain with a certain sign will win and one comes into equilibrium. Thus, we should have $t_1(L) \simeq t^*(L) \sim L^2$. When $\langle\psi\rangle$ is not too far from its equilibrium value, so that there are few domains, one can very roughly say that, as the number of domains decreases, the number of successions of parallel steps decreases and therefore the roughness decreases. For early times (t larger than a few MC steps but much smaller than L^2), $\langle\psi\rangle$ is still small. In figure 1, one sees that in this regime (at least for $L=61$ and $L=121$), one has

$$w^2 \sim \kappa \ln t. \tag{6}$$

This behaviour is reminiscent of roughening for the hyperstacking model [6, 7], and for the usual RSOS model at infinite temperature. (The usual RSOS model is just the same as the model we are considering in this letter but without the NNN interactions.) At infinite temperature, the form of the Hamiltonian is not important, only the fact that nearest-neighbour heights are not allowed to differ by more than one unit count. The model we have considered so far reduces to the usual RSOS model at infinite temperature. We also simulated the usual RSOS model at infinite temperature and obtained for times $t \ll L^2$ a behaviour of the type (6) but with a larger value of κ than for the RSOS model with NNN interactions at finite temperature. What may happen is that the potential between NNN renormalizes κ but the long range order of terraces (controlled by $\langle\psi\rangle$) is still not strong enough to diminish the roughness.

We now examine the influence of a finite driving force. It is introduced via a term

$$H_D = -\Delta\mu \sum_i h_i \tag{7}$$

where $\Delta\mu$ is a chemical potential difference. If we start from an equilibrium configuration, and switch on $\Delta\mu$, the velocity of the interface should be for infinitesimal $\Delta\mu$ proportional to $\Delta\mu$, since even for $\exp K/kT > 2$, the step free energy is zero. After a

few MC steps, this should also hold for our case. We carried out simulations with small system size ($L=25$) and varied $\Delta\mu$.

For small $\Delta\mu$, ($\Delta\mu/kT=\frac{1}{7}$ and $\frac{2}{7}$), with $K/kT=\frac{10}{7}$, we observed that w^2 against ln t ceases to have a maximum. The width then saturates to a value W which increases with $\Delta\mu$ and simultaneously, the steady state value of Ψ decreases.

For moderate $\Delta\mu$, ($\Delta\mu/kT$ equal to $\frac{5}{7}$-$\frac{10}{7}$), we have $w^2\sim\ln t$ for short times and then w saturates at a constant value. It is however probable that, strictly speaking, as soon as $\Delta\mu$ is non-zero, the behaviour of the width is in fact governed by the strong coupling fixed point of the KPZ equation so that, for sufficiently large systems [7, 10], w behaves as a power law of time for short times before going to saturation for large times. However, the asymptotic regime may be attained only for huge systems if $\Delta\mu$ is sufficiently small.

For large $\Delta\mu$, ($\Delta\mu/kT=2$ for exampe), we have $w^2\sim t^{\beta}$ with β around 0.39, just as in the RSOS model of Kim and Kosterlitz [10]. When $\Delta\mu/kT$ is much larger than K/kT, the system forgets about the Hamiltonian (equation (1)). Numerous numerical studies of such types of models are in the literature [11]. We want to focus on the case of small $\Delta\mu$. Figure 4 shows the saturation width w^2 against ln L for $\Delta\mu=0$ and $\Delta\mu/kT=\frac{1}{7}$, with $K/kT=\frac{10}{7}$. For $\Delta\mu=0$, one sees that the curve W^2 against ln L becomes flat for large L. This confirms the fact that the equilibrium phase is a flat phase [12]. For $\Delta\mu/kT=\frac{1}{7}$, in contrast, the curve W^2 against ln L straightens up for large L, indicating a rough interface.

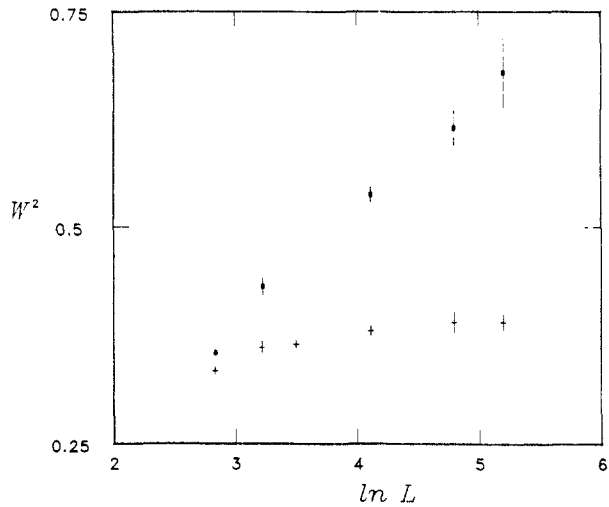

Figure 4. Size dependence of the saturation width W. W^2 against ln L for $K/kT=\frac{10}{7}\simeq 1.429$, $\Delta\mu=0$ (+) and $\Delta\mu/kT=\frac{1}{7}\simeq 0.142$ (■).

In normal SOS models, a mechanism for obtaining a rough surface below the equilibrium roughening temperature T_R by applying a driving force has been proposed in [2]. The basic idea is that the finite velocity v of the interface introduces some new length L^*, L^* is proportional to $\nu^{-1}a/v$ where a is the lattice constant, and ν has the dimension of a surface relaxation coefficient. When L^* gets below the correlation length ξ for the height-height correlation function, the surface becomes rough. Our numerical data are for $T\ll T_R$. Since the step-free energy in the DOF phase is zero, v

is proportional to $\Delta\mu/kT$ (for small $\Delta\mu/kT$). L^* decreases as $kT/\Delta\mu$ and easily becomes smaller than ξ, even with $T \ll T_R$, (whereas in the case of a roughening transition between a rough and an ordered flat phase, v falls very quickly below T_R). Our data prove that the value of $\Delta\mu/kT$ necessary to roughen a DOF phase is small with respect to K/kT, even for temperatures much below T_R. More detailed studies (involving the measurement of ξ and ν) would be needed to see if this mechanism also applies to our case.

Our results can be summarized as follows. We have performed numerical simulations of SOS models with NNN interactions and focused on the case where the equilibrium phase is a disordered flat phase. We find that, starting from a flat interface and letting it evolve via evaporation deposition dynamics, the squared width first increases logarithmically with time and then decreases. This non-monotonic behaviour can be understood within the Lifshitz theory, because the sign of the terrace order parameter $\langle\psi\rangle$ is not determined. We checked that the measured time necessary for both the width and the terrace order parameter to come to their equilibrium values are compatible with an L^2 dependence (L being the size of the system). When a finite driving force is applied, even for $\Delta\mu/kT = \frac{1}{7}$ and $T/T_R = 0.7 \ln 2$, we observe that the interface in the steady state regime has become rough.

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