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COMMENT

A note on the kinetics of wetting transitions in two-dimensional lattice-gas systems

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Abstract. We present results of Monte Carlo simulations on the kinetics of wall-wall wetting transitions in the two-dimensional three-state chiral clock and anisotropic next-nearest-neighbour Ising models. We confirm the existence of an algebraic growth law for the width of the wetting layer $\langle W(t)\rangle \sim t^{1/4}$ in the limit of large systems and long enough times at non-zero temperatures. We also discuss finite-size and temperature dependence of the effective growth exponents in these two models.

1. Introduction

The kinetics of wetting transitions have recently been studied theoretically in various systems (Lipowsky 1985, Grant *et al* 1987, Mon *et al* 1987, Dietrich 1987, Grant 1988). Theoretical calculations of a continuum Langevin model with no conservation laws predict a universal algebraic growth law for the width of the wetting layer $\langle W(t)\rangle \sim t^x$, with $x = 1/4$ for short-range lattice-gas models in two dimensions above roughening temperature (Lipowsky 1985, Grant 1988). Recently, this prediction was qualitatively confirmed in the two-dimensional three-state chiral clock model (Grant *et al* 1987). In this study, however, a strong temperature dependence of x was observed, which made it difficult to verify universal behaviour at lower temperatures.

In this comment, we present a somewhat more detailed Monte Carlo study of the kinetics of wall-wall wetting transitions in two distinct lattice-gas models, namely in the two-dimensional three-state chiral clock (CC3) and the anisotropic next-nearest-neighbour Ising (ANNNI) models. We extend the previous results obtained for the CC3 model at various temperatures (Grant *et al* 1987) to include systems of different sizes, and confirm the existence of an asymptotic universal growth exponent $x = 1/4$ in the limit of large systems and long enough times. For the ANNNI model we present a similar but more limited study.

2. The chiral clock model

The three-state chiral clock model has been widely studied with different methods, and the equilibrium properties and details of its phase diagram are fairly well known (Ostlund 1981, Huse 1981, Selke and Pesch 1982, Selke and Yeomans 1982, Huse *et al* 1983, Houlrik *et al* 1983, Duxbury *et al* 1984, Armitstead *et al* 1986). This model has three equilibrium phases: a paramagnetic, a ferromagnetic (3×1) and a floating incommensurate phase.

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The Hamiltonian of the CC3 model is

$$H = -J \sum_{\langle ij \rangle}^{x} \cos\left(\frac{2\pi}{3}(n_i - n_j + \Delta)\right) - J \sum_{\langle ij \rangle}^{y} \cos\left(\frac{2\pi}{3}(n_i - n_j)\right) \tag{1}$$

where J is the interaction constant, $n_i = 0, 1, 2$ is the spin value at site i, and Δ is the chiral field which is applied in the anisotropic x direction. The summation is taken over nearest neighbours both in the x and y directions.

The wetting transition in this model occurs within the threefold degenerate ferromagnetic phase (with phases A, B and C) as a function of the chiral field Δ when an initially stable wall A‖C decomposes into two identical walls of the type A|B, namely A‖C → A|B|C. This wetting transition is of second order, and its properties have been studied in detail (Huse *et al* 1983, Huse and Fisher 1984, Fisher 1984, Armitstead *et al* 1986).

The kinetics of adsorption of the intruding layer B was studied by two of the present authors in an earlier letter (Grant *et al* 1987) by Monte Carlo (MC) methods using standard Glauber spin-flip dynamics. Various values of $k_B T/J$ were simulated for two large systems. After a non-universal early-time behaviour, it was found that the growth indeed reaches a universal dynamical behaviour, with $x \simeq 0.25$ at relatively high temperatures. However, a strong temperature dependence of x due to a crossover to a logarithmic growth law at $T = 0$, together with relatively short times studied, made it difficult to extract x below $k_B T/J \sim 0.3$.

In this comment we have extended the MC simulations to include a more systematic study of temperature and, in particular, finite-size dependence of x. First, to study temperature effects, systems of sizes 102×102 at $k_B T/J = 0.3$, 0.4 and 108×36 at $k_B T/J = 0.4$, 0.5, 0.6 were simulated (for details, see Grant *et al* (1987)). For these two sizes we expect the finite-size effect to be quite small. In table 1 we show the numerical results of least-squares fitting to simulated data of figure 1 at different temperatures. After one monolayer is completed, a fluctuation-driven growth is observed in the model and a universal dynamical exponent $x \simeq 0.25$ is extracted at all these temperatures. At lower T, relatively long times are needed to reach the asymptotic regime.

Finite-size effects in the CC3 model were studied by preparing lattices of sizes 16×16, 34×34, 64×64, 102×102 and 204×204 at $T = 0.6J$, where we expect to see the asymptotic growth law already at relatively early times (see table 2). In general, we expect the growth law at high temperatures (where crossover effects from $T = 0$

Table 1. Numerical least-squares fits to the CC3 data corresponding to figure 1. The exponent x is a result of fitting data to the expression $(W - W_0) = A(t - t_0)^x$ where t_0 is an initial time after which the fluctuation-driven growth was observed, and A is a constant. The other exponent $\tilde{x}$ was obtained by fitting a straight line to the logarithm of the raw data, i.e. $\ln(W - W_0) = B + \tilde{x} \ln(t - t_0)$, where B is a constant. Δ is the error bar estimated from the central-limit theorem and must be considered conservative.

$k_B T/J$	x	Δt/MCS	$\tilde{x}$	$\Delta \tilde{t}$/MCS	$\pm\Delta$
0.6	0.28	40–5000	0.28	100–5000	0.02
0.5	0.30	40–9500	0.29	240–9500	0.02
0.4	0.27	40–5000	0.25	940–5000	0.02
0.3	0.26	6000–10 000	0.26	7000–10 000	0.02

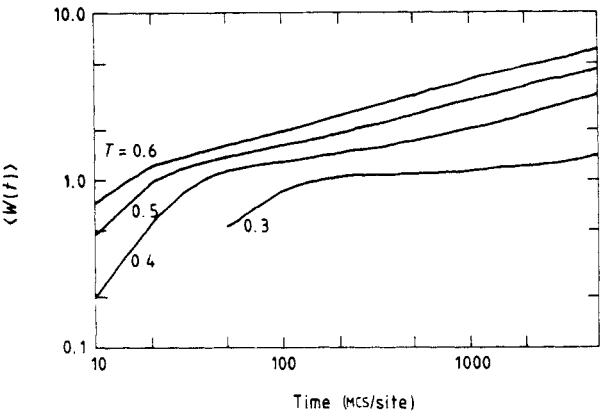

Figure 1. Time development of the net width $\langle W(t)\rangle$ of the wetting layer in the CC3 model at four different temperatures $k_B T/J = 0.3$, 0.4, 0.5 and 0.6. The lowest temperature data are for a 108×32 lattice, while the other results are for 102×102 lattices (at $k_B T/J = 0.4$ the simulations for a 108×32 lattice gave identical results to those for the larger lattice). Numerical fits to these data are given in table 1.

can be neglected) to have the finite-size scaling form† (Kroll and Gompper 1989)

$$\langle W(t)\rangle \sim t^{1/4} F(\xi_\parallel(t)/L) \tag{2}$$

where F is a scaling function with $F(0) = 1$, and $F(y) \sim y^{1/2}$ for $y > y_c$. Here L denotes

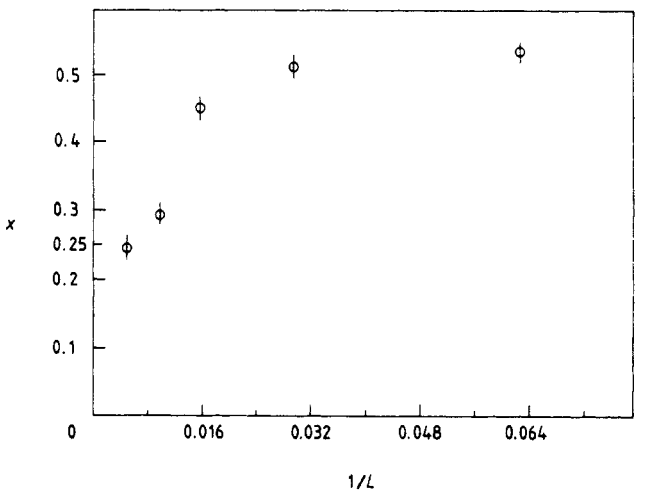

Figure 2. The effective dynamical exponent x as a function of $1/L$ for five different system sizes at $k_B T/J = 0.6$ (see the text). The data point for $L = 204$ was taken from an earlier study (Grant *et al* 1987). There is a crossover from a diffusive 1/2 exponent to the universal value $x = 1/4$ as the system size increases (see table 2).

† Here we consider only the effects of boundaries in the direction parallel to the walls, i.e. $L = L_\parallel$. In general, we expect the corresponding finite-size behaviour to be different from that in the direction perpendicular to the walls (where periodic boundary conditions are not used), since the behaviour of the two associated correlation lengths $\xi_\parallel(t)$ and $\xi_\perp(t)$ is different (Lipowsky (1985); see also Kroll and Gompper (1989)). A more general scaling function replacing $F(y)$ would be of the form $G(\xi_\perp(t)/L_\perp, \xi_\parallel(t)/L_\parallel)$, with $G(z, 0) \sim z^{-1}$ for $z > z_c$. This describes the final crossover to $\langle W(t)\rangle \sim L_\perp$.

Table 2. Numerical least-squares fits of the effective exponents x and $\tilde{x}$ for different system sizes for the CC3 model. Notation is the same as in table 1.

Size	x	Δt/MCS	$\tilde{x}$	$\Delta\tilde{t}$/MCS	$\pm\Delta$
16×16	0.54	30-500	0.56	244-500	0.02
34×34	0.51	30-800	0.51	218-500	0.02
64×64	0.46	15-800	0.45	110-800	0.03
102×102	0.28	40-5000	0.28	100-5000	0.02

the system size, and the diverging parallel interfacial correlation length $\xi_{\parallel}(t)\sim t^{1/2}$. Namely, for small systems as $y_c=\xi_{\parallel}(t_c)/L\sim1$, we expect to observe a crossover to a quasi-one-dimensional diffusive growth law $\sim t^{1/2}/\sqrt{L}$ (Mon *et al* 1987).

In figure 2 we plot the effective exponent x as a function of $1/L$ as obtained for the five different system sizes. For the smallest lattices, x is close to $1/2$ but crosses quite rapidly over to the asymptotic value $1/4$. As expected from a scaling law of the form (2), the effective *exponent* seems to follow no simple scaling form. This rather non-trivial finite-size behaviour clearly warrants further study.

3. The ANNNI model

The anisotropic next-nearest-neighbour Ising (ANNNI) model (Selke 1988) has a spin Hamiltonian of the form

$$H=-\sum_{\langle ij\rangle}[J_1 s_{i,j}s_{i+1,j}-J_2 s_{i,j}s_{i+2,j}+J_0 s_{i,j}s_{i,j+1}] \tag{3}$$

where $J_i>0$, $i=0,1,2$, and the summation goes over all sites of a square lattice with Ising spins $s_{ij}=\pm1$. Using the standard parametrisation $\alpha=J_2/J_0$ and $J_1=(1-\alpha)J_0$, for $\alpha>1/3$ (at $T=0$) the ANNNI model displays a uniaxial (4×1) phase with four degenerate ground states *A*, *B*, *C* and *D*. The wetting transition in the ANNNI model occurs when a soft superheavy/light A‖D wall decays into three heavy/light walls, i.e. A‖D→A|B|C|D. The properties of this wetting transition have been studied in detail, and the wetting line has been theoretically computed (Ala-Nissila *et al* 1986, Rujan *et al* 1985, 1986).

To study the dynamics of wetting in the ANNNI model, we have simulated systems of sizes 128×32 and 256×64, where the larger dimension is along the anisotropic x direction. The systems were made unstable by decreasing α instantaneously to a value within the wet region (typically values such as $\alpha=0.4$ and 0.47 were used for low and high temperatures, respectively). Consequently, the combined width of the adsorption layers B and C was monitored in time. A minimum of 1000 runs were performed for the smaller systems and time sampling of the data was done at 200 points. The results for the larger system are averages of 672 configurations.

In figure 3 we depict the net adsorption $\langle W(t)\rangle$ for 128×32 systems at four distinct temperatures, namely $k_BT/J_0=0.5$, 0.65, 0.75 and 1.0. A striking feature in these results is a clear change in the slope of these curves as a function of temperature. For $k_BT/J_0=0.5$ the slope is largest, and decreases monotonically for increasing temperature, as is evident in table 3. Nevertheless, there exists a reasonably well defined effective dynamical exponent x for all T. At $k_BT/J_0=0.5$ it is close to 0.5, and crosses over slowly to the expected value $x\simeq0.25$ as temperature increases.

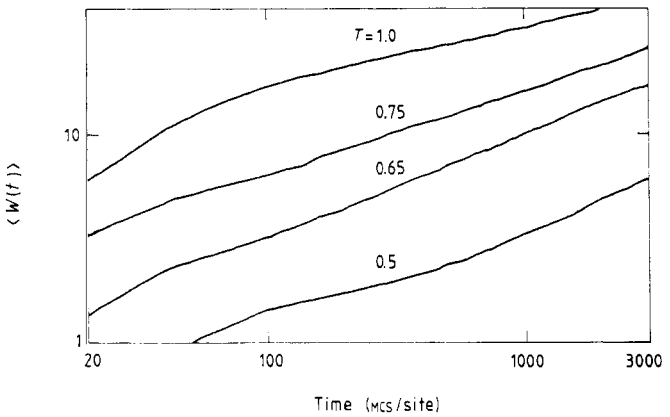

Figure 3. Time dependence of the net width $\langle W(t)\rangle$ of the wetting layer in the 2D ANNNI model at four temperatures $k_BT/J_0 = 0.5$, 0.65, 0.75 and 1.0. These simulations were performed for a 128×32 lattice. Numerical fits to this data are given in table 3.

Table 3. Numerical least-squares fits of the effective exponents x and $\tilde{x}$ to the kinetics of growth of the wetting layers B and C for ANNNI model for various temperatures and two lattice sizes. For notation, see table 1.

Size	k_BT/J_0	x	Δt/MCS	$\tilde{x}$	$\Delta\tilde{t}$/MCS	$\pm\Delta$
128×32	0.5	0.47	1000-5000	0.45	5000-10 000	0.02
128×32	0.65	0.42	500-2000	0.39	1000-3000	0.02
128×32	0.75	0.32	200-2000	0.34	1000-3000	0.02
128×32	1.0	0.23	100-2000	0.23	1000-2000	0.01
256×64	0.75	0.22	1050-5000	0.26	5000-10 000	0.02

As we can see from figure 3, the apparent temperature dependence of x is quite different from that of the CC3 model. To clarify this effect, we have also simulated a 256×64 system at $k_BT/J_0 = 0.75$. The last row in table 3 lists numerical fits to this data. Unlike the case for the smaller system, a dynamical exponent close to the value of 0.25 is readily obtained. Thus, we conclude that the finite-size effects are rather pronounced for the ANNNI model, but that the asymptotic exponent $x = 1/4$ still holds.

To summarise, in this comment we have verified the existence of an asymptotic growth exponent $x = 1/4$ for the kinetics of wetting transitions in the two-dimensional three-state chiral clock and anisotropic next-nearest-neighbour Ising models. We have studied in some detail the temperature and finite-size dependence of x for both models. Clearly, more theoretical work and more extensive simulations are needed to study these interesting and non-trivial effects in greater detail.

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