Suppression of Interface Roughness in Driven Nonequilibrium Systems

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The interface of an Ising lattice-gas model of ions, driven by an external electric field *parallel* to the interface, is studied in two bulk dimensions with extensive Monte Carlo simulations. Even for weak field, numerical results indicate strong suppression of interfacial capillary-wave excitations. This is qualitatively similar to the effects of gravity on fluid interfaces, but some differences are observed in the structure factors. We argue that the physical picture may apply in general to driven systems in steady state, and in higher dimensions.

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The physics of surface and interface roughness is an important and broad subject, relevant to a wide range of physical phenomena, ranging through roughening transitions,[1] wetting problems,[2] crystal growth,[3] and to spinodal decomposition.[4] In particular, a roughening transition is believed to occur generally in three-dimensional ($d=3$) systems,[1] where the interface separating the two coexisting phases becomes rough as the temperature (T) approaches the roughening transition temperature T_R from below. In contrast, for $d=2$ the interface is rough at all $T>0$, i.e., $T_R=0$. Associated with the divergent interface width (in the thermodynamic limit) is an infinite correlation length related to the algebraic decay of the height-height correlation function. Both the width and the correlation length become finite when a pinning field is applied, resulting in a smooth interface.[5] Common examples of pinning fields are the gravitational field in fluids and a magnetic field gradient in magnetic systems. In most experimental situations, the interface is influenced to some extent by an external field.

Most of the known results apply only to systems in thermodynamic equilibrium. However, many interesting systems are driven by an external field away from equilibrium. Their properties can be very different. Therefore the study of the relevance of the external field in the interface roughening is physically interesting. From conceptual as well as practical considerations, the simplest system which models such a situation is probably the Ising lattice-gas model of charged particles driven into a steady state by an uniform external electric field (E) *parallel* to the interface.[6] For some properties of this model, progress has emerged mainly from computer simulations. This is due to the inherent difficulties of formulating statistical mechanical treatments for nonequilibrium systems. In both $d=2$ and $d=3$, phase separations were shown to occur below a certain critical temperature.[6] Such separations are very anisotropic, with the interface parallel to the field direction, for systems with periodic boundary conditions. According to these simulations, the transition is believed to be of second order (at critical density), and the critical properties in $d=2$ seem to belong neither to the Onsager-Ising universality class nor the mean-field one. Qualitatively similar, though less conclusive results were also obtained in $d=3$.[7] The nature of the critical behavior is still controversial, as theories predict mean-field behavior,[8] disagreeing with simulation results. Below criticality, there are studies of linear stabilities of the interface based on a phenomenological theory.[9]

In this Letter we report the first exploratory study, by Monte Carlo (MC) simulation, of roughening in such a model. We present numerical evidence of the suppression of the interface roughness (in $d=2$) by E, for a wide range of values of E. We conjecture possible crossover phenomena as the system size L varies; and a possible phase diagram in the (E,T) plane for the roughness, based on simulation results and physical arguments. In the case of $E=0$, the width squared (w^2) in the steady state is found to scale as L, confirming well-accepted statics results,[10-12] and is consistent with the common belief that the *static* bulk and interfacial properties in equilibrium are independent of the detailed dynamics (e.g., whether the order parameter is conserved or not).

We use the standard MC method[13] to simulate the driven Ising model on a $L_x \times L_y$ two-dimensional square lattice, using spin-exchange dynamics[14] (locally con-

served order parameter). [We will use spin or particle language interchangibly: + (−), spin corresponding to a particle (hole).] E is chosen to be along the $+x$ direction (with unit vector $\hat{\mathbf{x}}$). The spins interact via the usual Ising Hamiltonian $H=-J\sum_{nn}\sigma_i\sigma_j$, where $J>0$, $\sigma=\pm 1$, and the sum is over nearest neighbors. As an open system, this model is defined, not by a Hamiltonian,[6] but by the jump rate W: Particle jumps along (opposite to) E are enhanced (suppressed) by a factor $\exp(E\hat{\mathbf{x}}\cdot\hat{\mathbf{a}}/k_BT)$, with $\hat{\mathbf{a}}$ a unit vector along the jump direction, and k_B the Boltzmann constant. In our units, the zero-field bulk critical temperature is $T_c(0)\approx 2.269$.[15] We fix all spins on the top (bottom) row as down (up), and we use periodic boundary conditions (PBC) along E. Under these boundary conditions, an interface parallel to E is obtained below $T_c(E)$.

There are two length scales associated with the interface[16]; the intrinsic width, and the "wandering" width due to long-wavelength capillary-wave fluctuations. They can be comparable and are not easily separated near T_c, because there, the intrinsic width is of the order of the bulk correlation length ξ_B. For this reason, T must be low enough for the interface to be well defined; but if T is too low, the dynamics would be so slow that the simulation would not be practical. Thus, our simulation for the interface is restricted to a limited range of T.

An interface configuration denoted by $\{h(x)\}$, with $h(x)$ the local height, is defined as follows: After every certain number (typically 25 or 50) of updates in units of Monte Carlo steps per site (MCS), we coarse grain a copy of the spin configuration, in order to average out small-distance (or order ξ_B) fluctuations to remove bubbles in the bulk and overhangs near the interface. Hence a single-valued function $h(x)$ can be defined simply as the total number of up spins in the column x. Our simulation is thus in the same spirit as the capillary-wave theory, which treats a fluctuating interface with an intrinsic width.[10] This enables us to compute the local height-height correlation function $C(a)\equiv\langle[h(y)-h(y+a)]^2\rangle$ and the average width squared $w^2\equiv\langle(h-\langle h\rangle)^2\rangle$ whose dependence on L_x is of primary interest. Here $\langle\ \rangle$ denotes the ensemble average in steady states. All systems studied here are half-filled, $\langle h\rangle=L_y/2$. Note that when $E=0$, $w^2\sim L_x$ in $d=2$, L_y must be large enough to avoid interactions of the interface with the boundaries. This is checked by some large-L_y test runs. L_y is typically 30 for L_x in the range of 30 to 60.

We have performed large-scale MC simulations for $E=0$, 0.5, 2, and 50 (effectively infinite and denoted by ∞ below). Because of the limited accessible range of T as mentioned above, simulations were done only at $T=0.75T_c(0)$ for $E=0$ and 0.5, and $T=0.9T_c(0)$ for $E=2$ and 50. To overcome very long interface relaxation times, long runs (by usual MC standards) are needed to generate meaningful samplings. This restricts the sizes studied: L_x ranges from 10 to 60. Typically a run lasts from 0.5 to 2×10^6 MCS (longer for smaller E). Each data point in Fig. 1 is an average over three or four independent runs.

Since small-E runs are extremely time consuming, for practical reasons we leave the case of $0<E<0.5$ for future studies. The following results therefore do not include the case of very small E. Since E is measured in units of bond strength, $E=0.5$ can already be regarded as small.

There are several possibilities for the behavior of the width squared $w^2(L_x,E)$: (1) $w^2\approx A_wL_x$, with an E-dependent amplitude A_w; (2) nonuniversal behavior of the form $w^2\sim L_x^{p(E)}$, with an E-dependent exponent[17]; and (3) w^2 saturates to a finite value as L_x increases, resulting in a smooth interface. We have plotted w^2 vs L_x in Fig. 1. We have also plotted w^2 vs L_x^p for various trial p's. This is more reliable than log-log plots. For all the finite E's studied, the best straight-line fits apparently occur at $p<1$. This rules out possibility (1). For large field, the curvature of such plots persists even for very small p (see, e.g., the inset of Fig. 1). This implies, should (2) be true, that $p(E)$ would be very small for strong field. Naturally we cannot completely rule out possibility (2), since errors are finite and sample sizes are limited. However, the data are fitted better (more so for larger E), statistically, by a functional form for the case (3). Furthermore, additional numerical evidence from spatial and temporal correlation functions (to be presented elsewhere) and an analogy with gravity on fluid interfaces support the last possibility. Because of great

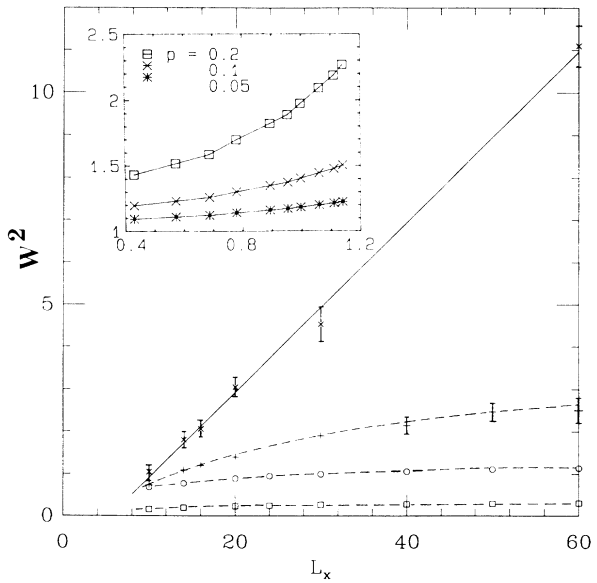

FIG. 1. MC results, w^2 vs L_x for different E ($\times=0$, $+=0.5$, $\circ=2$, and $\square=50$). The straight line is a linear fit for $E=0$, which confirms the well-known scaling of w on L_x. Dashed lines are guides for the eyes. Error bars larger than the size of symbols are shown. Inset: An example of a plot of L_x^p vs w^2 for various trial p's. These plots provide bounds on the effective p.

demand on computational effort, we cannot study with precisions the behavior of $w^2(L_x, E<0.5)$. Such low-E results would be needed to probe the finite-size scaling[18] properties near the possible rough-smooth transition at $E=0$. Analysis of our results indicates that even for $E=0.5$, the data are outside the finite-size scaling regime. However, should w^2 diverge, a reasonable upper bound on p for the smallest E ($=0.5$) studied would be 0.2 (in contrast to $p=1$ for $E=0$).

The numerical evidence that strong E suppresses long-wavelength, large-amplitude interface modulations appears to be compelling. One possible physical picture of this suppression is for E to introduce an effective crossover length, denoted by λ_E, so that w^2 is finite as $L_x \to \infty$, in a way controlled by L_x/λ_E. To get some feelings of λ_E, we fitted w^2 by an exponential form: $A - B\exp(-L_x/\lambda_E)$. We find $\lambda_E \approx 17$, $A \approx 0.31$ for $E=\infty$; $\lambda_E \approx 19$, $A \approx 1.2$ for $E=2$; and $\lambda_E \approx 30$, $A \approx 3.0$ for $E=0.5$. As expected, λ_E and $w^2(\infty, E)$ both increase with decreasing E. To be consistent with known results,[10-12] they must both diverge as $E \to 0$. We get similar results when the data are fitted with an arctan functional form as predicted by capillary-wave theory for an interface stabilized by gravity.

For $E=0$, the long relaxation time poses the most serious problem. Errors are large, in spite of very long runs (2×10^6 MCS). Fitting the data as above gives $p=1.0\pm0.1$.[19] This confirms the $d=2$ results obtained by various other means.[10-12] Besides computing w^2 using $h(x)$, we have also used other independent measurements: one is $C_{\max}=C(L_x/2)$; another is the second moment of the gradient of the density profile $m(y) \equiv (1/L_x)\sum_x \sigma(x,y)$. Both give similar results and support our interpretation.

The structure factor $G(q,E)$ is defined as the Fourier transform of the two-point correlation function $\langle h(x)h(0)\rangle - \langle h\rangle^2$. Figure 2 exhibits the divergence of $G(q\to 0, E=0)$, representing long-range correlations (equivalently Goldstone modes) along the interface.[20] Numerically, the data give a $1/q^2$ dependence of $G(q,E=0)$. Results for $E\neq0$ clearly display deviations from pure $1/q^2$ dependence as $q\to 0$. The limitation in system size prevents us from probing this limit further. Even with $q^2_{\min} \approx 0.01$, the data cannot unambiguously determine whether there is a gap at $q=0$ (as for gravity alone),[5] or just a weaker divergence than $1/q^2$. This question deserves further studies.

It is by no means obvious, though physically reasonable, that E suppresses capillary-wave excitations to produce a smooth interface. Gravitylike external fields produce a similar effect,[5] with the capillary length playing the role of λ_E. Although both are symmetry-breaking fields (with respect to Ising and rotational symmetries), pulling particles one way and holes the other, the directions in which they act on the interface are orthogonal.

Although we have not formulated a complete theory

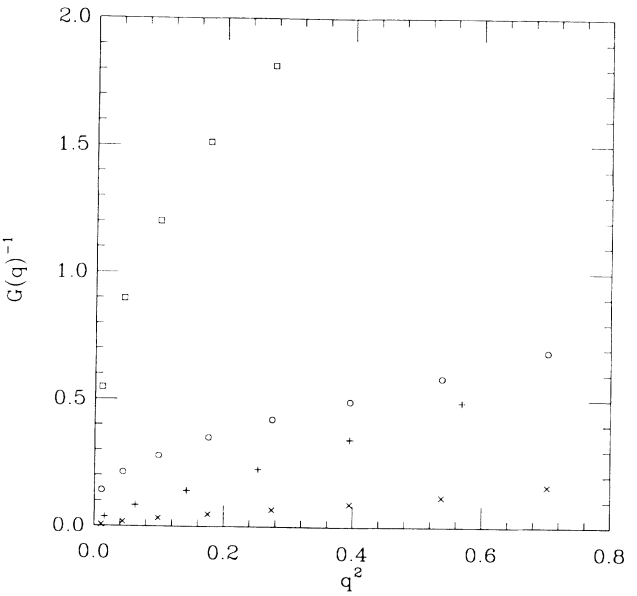

FIG. 2. MC results for the inverse of the structure factor, G^{-1}, vs q^2. Note the linear approach to $q^2=0$ for $E=0$, and the differences for $E\neq0$. Meaning of symbols are the same as in Fig. 1.

for the effects of E on interface roughness, we can nevertheless give some heuristic arguments. The time scale for the decay of a long-wavelength ($q^{-1} \equiv \lambda \gg \xi_B$) fluctuation away from planar interface is of the form[9]

$$\tau(\lambda,E)^{-2} \approx D^2 q^6 \xi_B^2 + D^2 q^5 \xi_B^2 (q^2 + \lambda_E^{-2})^{1/2},$$

where $\lambda_E \propto 1/E$, and D is the diffusion coefficient. Thus, $\tau_0 \approx \lambda^3$ for $E=0$ and $\tau_E \approx (\lambda^5 \lambda_E)^{1/2}$ for large $E\neq0$. Comparing these, we get $\tau_0/\tau_E \sim (\lambda E)^{1/2}$. Our *interpretation* is that E destroys large fluctuations quickly, resulting in an essentially smooth interface beyond the crossover wavelength λ_E, at which $\tau_0/\tau(\lambda \approx \lambda_E, E) \sim 1$. This essentially expresses the fact, as observed from the evolution of the interface in simulations, that large-amplitude modulations are very difficult to create, since particles near the interface are constantly driven along the field, effectively suppressing such formations. On the basis of these arguments, we *speculate* that the interface is smooth for any $E\neq0$, probably for all $T<T_c(E)$, analogous to the effects of gravity.

We end with two remarks. First, the above description is likely to apply to a wide range of nonequilibrium systems, driven into a steady state by an external field. Second, the results can easily be generalized to $d>2$. It is especially interesting in $d=3$ where $0<T_R<T_c$.[1] Since that transition is very delicate (being of infinite order), one would expect the effects of E to be more profound. We hope that this exploratory study will stimulate further experimental and theoretical investigations.

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