Growing Smooth Interfaces with Inhomogeneous Moving External Fields: Dynamical Transitions, Devil's Staircases, and Self-Assembled Ripples

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We study the steady state structure and dynamics of an interface in a pure Ising system on a square lattice placed in an *inhomogeneous* external field with a profile designed to stabilize a flat interface and translated with velocity v_e. For small v_e, the interface is stuck to the profile, is macroscopically smooth, and is rippled with a periodicity in general incommensurate with the lattice parameter. For arbitrary orientations of the profile, the local slope of the interface locks in to one of infinitely many rational values (devil's staircase) which most closely approximates the profile. These "lock-in" structures and ripples disappear as v_e increases. For still larger v_e the profile detaches from the interface.

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The ability to grow flat solid surfaces [1] is often of major technological concern, for example, in the fabrication of magnetic materials for recording devices where surface roughness [2] causes a sharp deterioration of magnetic properties. Most growing surfaces or interfaces, on the other hand, coarsen [3] with a width, σ, which diverges with system size as L^α and time as t^β, where α and β ($\alpha, \beta \geq 0$) are the *roughness* and *dynamical* exponents, respectively. Is it possible to drive such an interface with a predetermined velocity v_f and, at the same time, keep it flat (i.e., $\alpha = \beta = 0$)? In this Letter, we explore this possibility by studying growing interfaces in a nonuniform field with an appropriately shaped profile moving without change of shape at an externally controllable velocity v_e. We find that for v_e less than a limiting value v_∞, it is possible to produce a macroscopically flat, interface growing with average velocity $v_f = v_e$. Microscopically, however, the interface shows an infinity of *dynamical* ripple structures similar to self-assembled, commensurate-incommensurate (C-I) [4] domains produced by atomic mismatch [5]. The ripples vanish with increasing v_e through a *fluctuation induced* C-I transition.

Real solid-solid interfaces being complex [6], an understanding of the dynamics of such interfaces in a general time-dependent, inhomogeneous field may be achieved only by beginning with a relatively simple, but nontrivial, system, viz., an interface in the two-dimensional (2D) Ising model. Our results, therefore, concern mainly this model system, though towards the end we discuss possible modifications, if any, for solid interfaces.

The dynamics of an Ising interface in a (square) lattice driven by uniform external fields is a rather well studied [3] subject. The velocity v_∞ of the interface depends on the applied field h and the orientation θ measured with respect to the underlying lattice. The interface is rough and coarsens with Kardar-Parisi-Zhang (KPZ) [3] exponents $\alpha = 1/2$ and $\beta = 1/3$.

Consider an interface $Y(x, t)$ between phases with magnetization, $\phi(x, y, t) > 0$ and $\phi(x, y, t) < 0$, in a 2D square lattice [7] obeying single-spin flip Glauber dynamics [8] in the limit $h/J, T/J \to 0$. Here J is the Ising exchange coupling and T the temperature. An external nonuniform field with a profile $h(y, t) = h_{\max} f(y, t)$ where $f(y, t) = \tanh[(y - v_e t)/\chi]$ and χ is the width of the profile [see Fig. 1(a)] is applied such that $h = h_{\max}$ in the $\phi > 0$ and $h = -h_{\max}$ in the $\phi < 0$ ϕ regions separated by a sharp *edge*. The driving force depends on the relative *local* position of $Y(x, t)$ and the edge. In the low temperature limit the interface moves solely by random corner flips [3] [Fig. 1(b)], the fluctuations necessary for nucleating islands of the minority phase in any region being absent. We study the behavior of v_f and the structure of the interface as a function of v_e and orientation.

Naively, one expects fluctuations of the interfacial coordinate $Y(x, t)$ to be completely suppressed in the presence of $h(y, t)$. Indeed, as we show below, a mean field theory obtains the exact behavior of v_f as a function of v_e [Fig. 1(c)]. Using model A dynamics [9] for a coarse-grained Hamiltonian (which, for the moment, ignores the lattice) of an Ising system in a external nonuniform field together with the assumption that the magnetization ϕ is uniform everywhere except near the interface, one can derive [10] an equation of motion for the interface.

$$\frac{\partial Y}{\partial t} = \lambda_1 \frac{\partial^2 Y}{\partial x^2} - \lambda_2 \left(\frac{\partial Y}{\partial x}\right)^2 f(Y, t) - \lambda_3 f(Y, t) + \zeta(x, t), \quad (1)$$

where λ_1, λ_2, and λ_3 are parameters and ζ is a Gaussian white noise with zero mean. Note that Eq. (1) lacks Galilean invariance [11] $Y' \to Y + \epsilon x$, $x' \to x - \lambda_2 \epsilon t$, $t' \to t$. A mean field calculation amounts to taking $Y \equiv Y(t)$, i.e., neglecting spatial fluctuations of the interface and noise. For large times ($t \to \infty$), $Y \to v_f t$, where v_f is obtained by solving the self-consistency equation; $v_f = \lim_{t\to\infty} -\lambda_3 \tanh\{(v_f - v_e)t/\chi\} = -\lambda_3 \mathrm{sgn}(v_f - v_e)$. For

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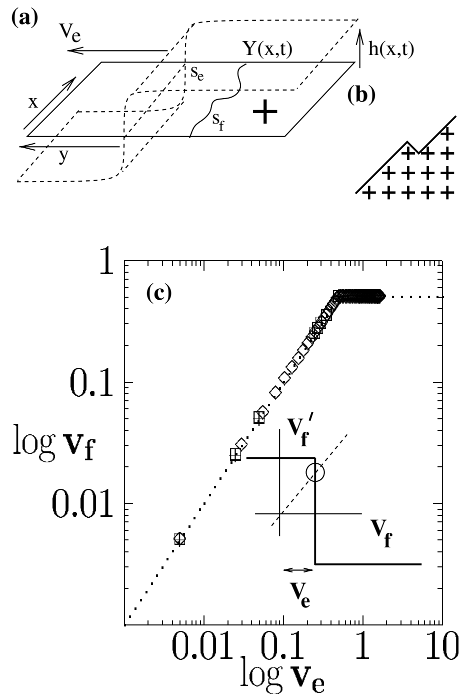

FIG. 1. (a) An Ising interface $Y(x, t)$ (bold curved line) between regions of positive (marked +) and negative (marked −) magnetization in an external, inhomogeneous field with a profile which is as shown (dashed line). The positions of the edge of the field profile and that of the interface are labeled S_e and S_f, respectively. (b) A portion of the interface in a square lattice showing a corner. (c) The interface velocity v_f as a function of the velocity of the dragging edge v_e for $N_s =$ 100(□), 1000(◇), 10 000(+), and $\rho = 0.5$. All the data (□, ◇, +) collapse on the mean field solution (dashed line). Inset shows the graphical solution (circled) of the self-consistency equation for v_f; dashed line represents $v_f = v_f$.

small v_e the only solution [Fig. 1(c), inset] is $v_f = v_e$, and for $v_e > v_\infty$, where $v_\infty = \lambda_3$, we get $v_f = \lambda_3 = v_\infty$. We thus have a sharp transition [Fig. 1(c)] from a region where the interface is stuck to the edge to one where it moves with a constant velocity. How is this result altered by including spatial fluctuations of Y? This question is best answered by mapping the interface problem to a 1D cellular automaton [3,12].

The interface coordinate $Y(x, t)$ in a square lattice is represented [12,13] by the set of integers $\{y_i\}$, $1 < i < N_p$ denoting positions of N_p hard-core ($y_{i+1} \geq y_i + 1$) particles in a 1D lattice of N_s sites. The particle density $\rho = N_p/N_s$ determines the mean slope of the interface $\tan\theta_f = 1/\rho$, and the motion of the interface by corner flips corresponds to the hopping of particles with right and left jump probabilities p and q ($p + q = 1$). Trial moves are attempted sequentially on randomly chosen particles [12] and N_p attempted hops constitute a single time step. In our case, p and q are position dependent such that $\Delta_i(v_e t) = p - q = \Delta\,\mathrm{sgn}(y_i - i/\rho - v_e t)$ with $\Delta = 1$. The bias $\Delta_i(v_e t)$ is appropriate for a step function ($\chi = 0$) profile with the slope of the profile edge equal to the average slope of the interface. We track the instantaneous particle velocity $v_f(t)$ defined as the number of particles moving right per unit time, the average position $\langle y(t)\rangle = N_p^{-1}\sum_{i=1,N_p} y_i(t)$, the width $\sigma^2(t) = N_p^{-1}\sum_{i=1,N_p}\langle(y_i(t) - \langle y_i(t)\rangle)^2\rangle$, and the local slope of the interface given by the local density of particles. Angular brackets denote an average over the realizations of the random noise. The usual particle hole symmetry for an exclusion process [3,12,13] is violated since exchanging particles and holes alters the relative position of the interface compared to the edge.

We perform numerical simulations [12] of the above model for N_s up to 10^4 to obtain v_f for the steady state interface as a function of v_e as shown in Fig. 1(c). A sharp dynamical transition from an initially stuck interface with $v_f = v_e$ to a free, detached interface with $v_f = v_\infty = \Delta(1 - \rho)$ is clearly evident as predicted by mean field theory. The detached interface coarsens with KPZ exponents [10]. Note that, even though the mean field solution for $v_f(v_e)$ neglects the fluctuations present in our simulation, it is exact. The detailed nature of the stuck phase ($v_f = v_e$ and σ bounded) is, on the other hand, considerably more complicated than the mean field assumption $Y(x, t) = Y(t)$.

The ground state of the interface in the presence of a stationary ($v_e = 0$) field profile is obtained by minimizing $E = 1/N_p\sum_i(y_i - i/\rho - c)^2$ with respect to the set $\{y_i\}$ and the constant, c, subject to the constraint that y_i are integers. The form of E leads to an additional nonlocal, repulsive, interaction between particles. The minimized energy may be calculated exactly, $E(\rho = m/n) = \frac{1}{6}(\frac{1}{2} - \frac{1}{m})(1 - \frac{1}{m}) + \frac{1}{4m} - \frac{1}{4m^2}$ for m *even* and $\frac{1}{12}(1 - \frac{1}{m^2})$ for m *odd,* where the density $\rho = m/n$ is a rational fraction. The energy satisfies the bounds $E(1/n) = 0 < E(m/n) < \lim_{m\to\infty} E(m/n) = 1/12$ where the upper bound is for an irrational density. For an arbitrary $0 < \rho < 1$ the system ($\{y_i\}$) prefers to distort, conforming within local regions, to the nearest low-lying rational slope $1/\tilde{\rho}$ interspersed with an *ordered* array of "discommensurations" of density $\rho_d = |\rho - \tilde{\rho}|$ which appear as long wavelength *ripples* [see Fig. 3(c), inset, below]. The $\tilde{\rho}$ as a function of ρ shows a "devil's staircase" structure (complete for $v_e \to 0$) with a multifractal [14] measure. We observe this in our simulation by analyzing the instantaneous distribution of the local density of particles to obtain weights for various simple rational fractions up to generation $g = 9$ in the Farey tree of rationals [15]. A time average of the density corresponding to the fraction with largest weight at any t, then give us the most probable density $\tilde{\rho}$—distinct from the average ρ which is constrained to be the inverse slope of the profile. For small v_e the interface is more or less locked in to a single $\tilde{\rho}$, shown as white regions in the phase diagram (Fig. 2) in the $v_e - \rho$ plane.

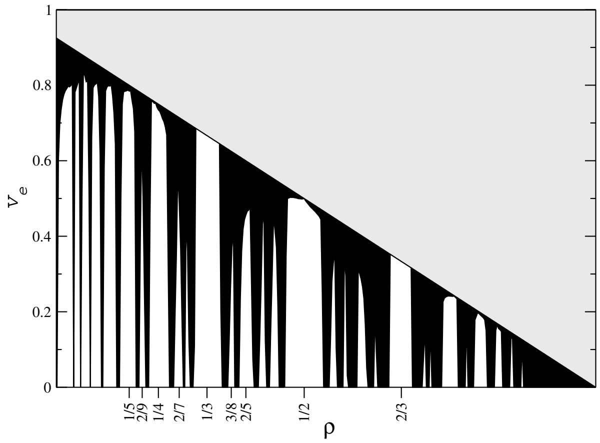

FIG. 2. The dynamical phase diagram in v_e and ρ plane. The numbers on the ρ axis mark the fractions $\tilde{\rho}$, which determine the orientation of the lock-in phase. The three regions—white, black, and grey—correspond to the rippled, the disordered, and the detached phases, respectively.

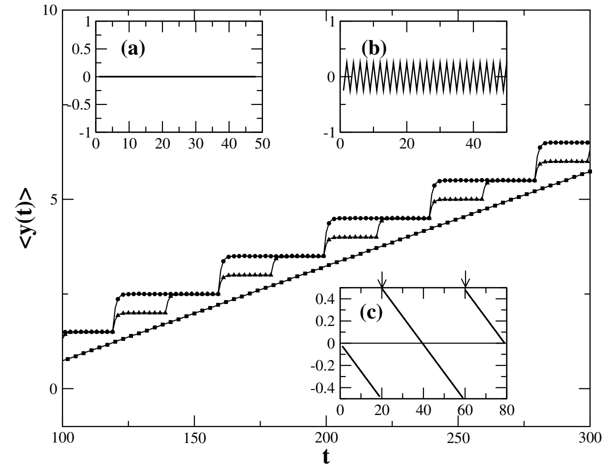

FIG. 3. Variation of $\langle y(t) \rangle$ with t for $v_e = 0.025$ and $p = 1.0$. Lines denote analytic results while points denote Monte Carlo data for $\rho = 1/5$ (uppermost curve), $2/5$, and an incommensurate ρ near $1/3$. Insets (a)–(c) show the corresponding ground-state interfaces ($y_i - i/\rho$). The arrows in (c) mark the positions of two discommensurations.

For low velocities and density where correlation effects due to the hard-core constraint are negligible, the dynamics of the interface may be obtained exactly [10]. Under these circumstances the N_p particle probability distribution for the y_i's, $P(y_1, y_2, \ldots, y_{N_p})$ factorizes into single particle terms $P(y_i)$. Knowing the time development of $P(y_i)$ and the ground-state structure, the motion of the interface at subsequent times may be trivially computed as a sum of single particle motions. A single particle (with, say, index i) moves with the bias $\Delta_i(v_e t)$ which, in general, may change sign at $y < i/\rho + v_e t < y + 1$. Solving the appropriate set of master equations [10] we obtain, for $v_e \ll 1$, the rather obvious steady state solution $P(y_i) = 1/2(\delta_{y_i,y} + \delta_{y_i,y+1})$, and the particle oscillates between y and $y+1$. Subsequently, when $i/\rho + v_e t \geq y + 1$, the particle jumps to the next position and $P(y_i)$ relaxes exponentially with a time constant $\tau = 1$ to its new value with $y \to y+1$. In general, for rational $\rho = m/n$, the motion of the interface is composed of the independent motions of m particles each separated by a time lag of $\tau_L = 1/m v_e$. The result of the analytic calculation for small v_e and ρ has been compared to those from simulations in Fig. 3 for $\rho = 1/5$ and $2/5$. For a general irrational $\rho < 1/2$, $m \to \infty$ and, consequently, $\tau_L \to 0$. The y_i's are distributed uniformly around the mean implying $\sigma^2 = 1/3$ independent of system size and time. For $\rho > 1/2$ the width $\sigma^2 = (1-\rho)/3\rho$ since the number of mobile particles decreases by a factor of $(1-\rho)/\rho$.

The forward motion of an irrational interface is accompanied by the motion of discommensurations along the interface with velocity v_e which constitutes a kinematic wave [3,13] parallel to the interface. As the velocity v_e is increased, the system finds it increasingly difficult to maintain its ground-state structure, and for $\tau \geq \tau_L$ the instantaneous value of $\tilde{\rho}$ begins to make excursions to other nearby low-lying fractions and eventually becomes free. Steps corresponding to $\tilde{\rho} = m/n$ disappear (i.e., $\tilde{\rho} \to \rho$) sequentially in order of decreasing m, and the interface loses the ripples. The interface is disordered though α and β continue to be zero (black region in Fig. 2). The locus of the discontinuities (within an accuracy of $1/N_p$) in the $\tilde{\rho}(\rho)$ curve for various velocities v_e gives the limit of stability of the lock-in rippled phases.

While the stability of mismatch domains [5] is decided, mainly, by competition between mechanical, long-ranged (elastic), and short-ranged (atomistic) interactions [4], dynamical ripples vanish with increasing v_e through increased fluctuations. We argue that it is sufficient to project the entire configuration space y_i of the stuck interface onto the single variable ρ. In Fig. 4 (inset) we have plotted the energy $E(\rho)$ for the ground-state configuration with density ρ. As is obvious from the figure, $E(\rho)$ has a structure similar to the free energy surface of a 1D "trap" model [16] often used to describe glassy dynamics. The distinction, of course, is the fact that the energies of the traps in this case are highly correlated. We may then describe the dynamics of the stuck interface as the Langevin dynamics [9] of a single particle with coordinate ρ' diffusing on a energy surface, given by $F(\rho') = E(\rho') + \kappa(\rho' - \rho)^2$, kicked by a Gaussian white noise of strength T. The second term, containing the modulus κ, ensures that $\rho' \to \rho$ for $t \to \infty$. At intermediate times, however, the system may get trapped indefinitely in some nearby low-lying minimum with $\rho' = \tilde{\rho}$ if T ($\propto v_e^2$ by symmetry) is not large enough. As T increases, the time spent in jumping between minima may exceed the residence time in the minimum, resulting in a noise induced C-I transition (Fig. 4) from $\tilde{\rho}$.

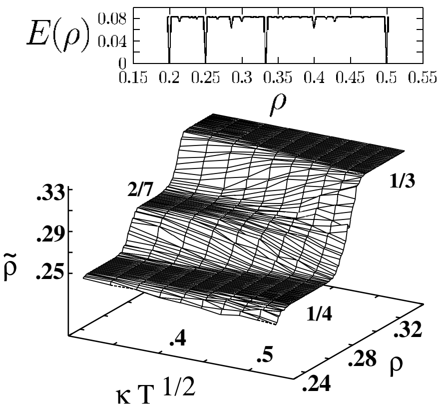

FIG. 4. A surface plot of $\tilde{\rho}$ vs ρ and $\sqrt{T}\kappa$ showing steps for the fractions 1/4, 2/7, and 1/3. Note that the step corresponding to 2/7 vanishes at $\sqrt{T}\kappa > 0.5$. Inset (top) shows a plot of $E(\rho)$ for a $N_s = 420$ site system.

In this Letter, we have studied the static and dynamic properties of an Ising interface in 2D subject to a nonuniform, time-dependent external magnetic field. The system has a rich dynamical phase diagram with infinitely many steady states. The nature of these steady states and their detailed dynamics depends on the orientation of the interface and the velocity of the external field profile. How are our results expected to change for real driven solid interfaces? First, real field profiles would have a finite width $\chi > 0$. However, as long as χ is comparable to atomic dimensions we find no appreciable change in the results. Second, elastic interaction between "particles" or steps in the interface [6] may smoothen the devil's staircase though we expect that for typical solids this will be minimal. Third, the structure of the underlying lattice may influence the stability of particular orientations. Finally, exciting new physics may come into play as new modes, e.g., point and line defects [17], as well as phonon degrees of freedom (leading to acoustic emissions [6]) are accessed as v_e increases.

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