Growing smooth interfaces with inhomogeneous, moving external fields: dynamical transitions, devil’s staircases and self-assembled ripples

Abhishek Chaudhuri, P. A. Sreram and Surajit Sengupta
Satyendra Nath Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Calcutta - 700098.

(Dated: November 18, 2018)

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 dissipate as \( v_e \) increases. For still larger \( v_e \), the profile detaches from the interface.

PACS numbers: 05.10Gg,64.60.Ht,68.35.Rh

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, \( \sigma \), which diverges with system size as \( L^\alpha \) and time as \( t^\beta \), where \( \alpha \) and \( \beta \) \((\alpha, \beta \geq 0)\) are the roughness and dynamical exponents respectively. Is it possible to drive such an interface with a pre-determined 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 non-uniform 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 \( v_{\infty} \), 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 fluctuated 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 only be achieved by beginning with a relatively simple, but non-trivial, system viz. an interface in the two -dimensional (2-d) 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, \( v_{\infty} \) of the interface depends on the applied field, \( h \) and the orientation \( \theta \) measured with respect to the underlying lattice. The interface is rough and coarsens with 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 2-d 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 non-uniform field with a profile \( h(y,t) = h_{\text{max}} \phi(y,t) \) where \( \phi(y,t) = \tanh((y-v_f t)/\chi) \) and \( \chi \) is the width of the profile (see Fig.\(^1\)a) is applied such that \( h = h_{\text{max}} \) in the \( \phi > 0 \) and \(-h_{\text{max}} \) in the \( \phi < 0 \) 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\(^8\) (Fig.\(^1\)b)), the fluctuations necessary for nucleating islands of the minority phase in any region being absent. We study the behaviour 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 behaviour of \( v_f \) as a function of \( v_e \) (Fig.\(^1\)c)). Using model A dynamics\(^3\) for a coarse-grained Hamiltonian (which, for the moment, ignores the lattice) of an Ising system in a external non-uniform field together with the assumption that the magnetization \( \phi \) is uniform everywhere except near the interface, one can derive\(^1\) an equation of motion for the interface.

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

where \( \lambda_1, \lambda_2 \) and \( \lambda_3 \) are parameters and \( \zeta \) is a Gaussian white noise with zero mean. Note that Eq.\(^1\) lacks Galilean invariance\(^1\) \( Y' \to Y + \epsilon x, x' \to x - \lambda_2 \epsilon t, t' \to t \). 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; \( v_f = \lim_{t \to \infty} -\lambda_3 \tanh\left( (v_f-v_e) t / \chi \right) \equiv -\lambda_3 \text{sign}(v_f-v_e) \). For 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 \( v_f = \lambda_3 = v_{\infty} \).
such that, $\Delta i p$ time step. In our case, a cellular automaton$^{[3, 12]}$. The best answered by mapping the interface problem to a 1-d lattice of $N$ particles$^{[12]}$ and $N$ particles in a 1-d lattice of sites. The instantaneous particle density $\rho$ determines the mean slope of the interface $\sigma$ between regions of positive (marked +) and negative (marked −) 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 $v_f = v_f$.

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 1-d cellular automaton$^{[12]}$.

The interface coordinate $Y(x, t)$ in a square lattice is represented$^{[12]}$ 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 1-d 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, $\Delta i(v_e t) = p - q = \Delta \text{sign}(y_i - i/\rho - v_e t)$ 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 $<y(t)> = N_p^{-1} \sum_{i=1}^{N_p} y_i(t)$, the width $\sigma^2(t) = N_p^{-1} \sum_{i=1}^{N_p} <(y_i(t) - <y(t)>)^2>$ and the local slope of the interface given by the local density of particles. Angular brackets denotes an average over the realizations of the random noise. The usual particle hole symmetry for an exclusion process$^{[12]}$ 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 $v_f = v_e = \Delta(1 - \rho)$ is clearly evident as predicted by mean field theory. The detached interface coarsens with KPZ exponents$^{[11]}$. 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 $\sigma$ 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 $E = 1/N_p \sum (y_i - i/\rho - c)^2$ 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 non-local, repulsive, interaction between particles. The minimized energy may be calculated exactly, $E(\rho = m/n) = \frac{1}{12} (\frac{1}{\rho} - \frac{1}{n}) (1 - \frac{1}{\rho} - \frac{1}{m})$ for $m$ even and $\frac{1}{12} (1 - \frac{1}{\rho^2})$ 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 $1/\hat{\rho}$ interspersed with an ordered array of “discommensurations” of density $\rho_d = |\rho - \hat{\rho}|$ which appear as long wavelength ripples (see Fig. 3 inset (c)). The $\hat{\rho}$ as a function of $\rho$ shows a “devil’s staircase” structure (complete for $v_e \to 0$) with a multifractal$^{[13]}$ 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$^{[14]}$.

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 $\rho$ 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.

For low velocities and density where correlation effects

---

**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 labelled $S_e$ 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 $N_s = 100(\bigcirc), 1000(\bigcirc), 10000(+)\,$ and $\rho = 0.5$. All the data (\bigcirc, \bigcirc, +) 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 $v_f = v_f$. 
due to the hard core constraint are negligible, the dynamics of the interface may be obtained exactly \[11\]. 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 \[11\] we obtain, for \( v_e \ll 1 \) the rather obvious steady state solution \( P(y_i) = 1/2(\delta_{y_i,y_{i+1}} + \delta_{y_i,y_{i-1}}) \) 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 it’s 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 \( \rho \) has been compared to those from simulations in Fig. 3 for \( \rho = 1/5 \) and 2/5. For a general irrational \( \rho < 1/2 \), \( m \to \infty \) 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 \[15\] 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 \( \rho \) begins to make excursions to other nearby low-lying fractions and eventually becomes free. Steps corresponding to \( \rho = m/n \) disappear (i.e. \( \rho \to \rho \)) sequentially in order of decreasing \( m \) and the interface loses the ripples. The interface is disordered though \( \alpha \) and \( \beta \) continue to be zero (black region in Fig. 2). The locus of the discontinuities (within an accuracy of \( 1/N_p \)) in the \( \rho(\rho) \) curve for various velocities \( v_e \) gives the limit of stability of the lock-in rippled phases.

While the stability of mismatch domains \[8\] 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 \( \rho \). In Fig. 3 (inset) we have plotted the energy \( E(\rho) \) for the ground-state configuration with density \( \rho \). As is obvious from the figure, \( E(\rho) \) has a structure similar to the free energy surface of a 1-d “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 \[8\] of a single particle with coordinate \( \rho' \) 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 \( \kappa \), 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 \( \rho' = \hat{\rho} \) 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 $\dot{\rho}$.

In this Letter, we have studied the static and dynamic properties of an Ising interface in 2-d subject to a non-uniform, 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 depend 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? Firstly, real field profile. How are our results expected to change for real driven solid interfaces? Secondly, elastic interaction between “particles” or steps in the interface may come into play as new modes e.g. point and line defects [17], as well as phonon degrees of freedom (leading to acoustic emmissions [6]) are accessed as $v_e$ increases.

**Acknowledgement:** The authors thank M. Barma, J.K. Bhattacharya, J. Krug, S. N. Majumdar, A. Mukherjee and M. Rao for useful discussions; A. C. thanks C.S.I.R., Govt. of India for a fellowship.

---

[1] R. Kern et. al., Current Topics in Materials Science, Vol. 3, E. Kaldia, Eds. (North-Holland, 1997); D. Kandel and E. Kaxiras, cond-mat/9901177

[2] D. Zhao et. al., Phys. Rev. B 62, 11316, (2000).

[3] M.Kardar, G.Parisi, and Y.C.Zhang Phys.Rev.Lett. 56 889 (1986); A.L.Barabasi and H.E.Stanley Fractal Concepts in Crystal Growth (Cambridge University Press, 1995); M. Barma, in Non Linear Phenomenona in Materials Science III, G. Ananthakrishna et. al., Eds. (Trans Tech Publications Ltd. Switzerland, 1995), Solid Sate Phenomena, Vol. 42-43, 1995 (pp 19-26); see also S. N. Majumdar and P. L. Krapivsky, Phys. Rev. E 63, 45101(R), (2001) for an example of a flat interface in economics.

[4] Y.I. Frenkel and T. Kontorowa, Zh. Eksp. Teor. Fiz. 8, 1340 (1938); S.Aubry, Physica D 7, 240 (1983); P. Bak, Rep. Prog. Phys. 45, 587 (1981); W. Selke, in Phase Transitions and Critical Phenomena, Vol. 15, Eds. C. Domb and J. L. Lebowitz (Academic Press, New York, 1993); Weiren Chou and R. B. Griffiths, Phys. Rev. B, 34, 6219 (1986).

[5] P. Bak et. al., Phys. Rev. B , 19, 1610 (1979); D. V. Klyachko et. al., Phys. Rev. B 60, 9026, (1999); R. Plass et. al., Nature (London) 412,875 (2001); E. D. Tober et. al., Phys. Rev. Lett. 81, 1897 (1998).

[6] A. P. Sutton and R. W. Balluffi, Interfaces in crystalline materials (Oxford Science Pub., Oxford, 1995)