Driven 3D Ising Interface:  
it’s fluctuation, Devil’s staircase, and effect of interface geometry

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Enchanting ripple pattern exist on interface, and manifest them self in it’s fluctuation profile as well. These ripples apparently flow as the interface struck with inhomogeneous externally driven field interface, moves fluctuating about it on a rectangular 3D Ising system. Ripple structure and flow have temporal periodicity, eventually with some modulation, and have signature of geometry of field interface. Dramatic transitions occur in fluctuation profile as a function of dynamics and geometry of the force field interface and is divided into two spatial regions : rippled and smooth. For the velocity we are concerned with, the interface is pinned with field interface, and for arbitrary orientations of the field profile local slope of the rippled part of the interface gets locked in to a combination of few rational values (Devil’s staircase) which most closely approximate the profile, thereby generating specular pattern of patches.

The study of interface and it’s properties is technologically a major concern for its prominent effects in many phase transitions and chemical reactions originating at surface, whose temporal characteristics are often synonymous with motion of resulting parent product interfaces[1]. In fabrication of magnetic materials for recording devices, where surface roughness[2] cause sharp deterioration in desired parameters, study of interface finds it’s application. Often interfaces undergo structural transitions like reconstruction and roughening, thereby being of prime concern for processes like catalysis and surface phase transition[3,4].

The dynamics and spatial structure of Ising interface driven by uniform externally driven field is rather well studied[5] subject. It’s velocity is function of field profile[9], interface is rough and coarsens with KPZ exponents[5,10]. For velocities when interface is pinned with field interface and moves with it, does it fluctuates about it? What are the spatial and temporal characteristics of fluctuation profile? Do these characteristics have signature of interface geometry? These are the questions we want to probe in this letter for a rectangular 3D Ising system. In our previous work we have shown the existence of Devil’s staircase structure for 2D Ising system[8]. Do these lock in regions exist in 3D Ising system as well and what impact velocity of interface have on this? By the end we would throw some light on this issue too.

Our system consists of \(N_x(=28) \times N_y(=28) \times N_z(=30)\) Ising spins arranged on a simple cubic lattice interacting ferromagnetically with their nearest neighbor only. The locus of all points over which force field changes sign is field interface \(Z(\mathbf{r},t)\). Few layers of spin close to \(Z\) have a non trivial dynamics, spins far away from it are frozen in direction of local field \(H(\mathbf{r},t)\) at that site. Periodic boundary conditions are used along \(x\) and \(y\) directions. In \(z\) direction we have open boundary condition the exact nature of which is irrelevant as the spins at the two extremities are, in any case, frozen to the values fixed by the sign of \(H\).

A typical run consists of equilibrating the spins in a given \(H(\mathbf{r},t)\), updating \(H(\mathbf{r},t)\) according to value of field velocity measured in units of lattice sites per Monte Carlo steps (MCS) and computing the magnetization. The value of magnetization is stored for each time step. This process is repeated 250 times taking independent initial condition each time. By averaging over the stored data average time dependent magnetization profile \(M(\mathbf{r},t)\) is obtained. To obtain the interface \(S(\mathbf{r},t)\) at any instant the averaged magnetization \(M(\mathbf{r},t)\) at any \((x,y)\) is fitted with \(\tanh(z-a)\), thereby the parameter \(a\) gives the value of interface at that \((x,y)\), this process is repeated for all \((x,y)\) and the complete interface at that instant is obtained. Then for each \((x,y)\) we obtain the fluctuation using \(F(x,y)=S(x,y)-Z(x,y)\). In this way the interface \(S(\mathbf{r},t)\)
and fluctuation profile $F(r,t)$ at that instant is obtained. Then this process is repeated for all time steps, thereby giving the interface $S(r,t)$ and corresponding fluctuation profile $F(r,t)$ for all time steps. We find the same with various geometries of $Z(r,t)$, like as in Fig 1, hemispherical and plane. To probe the distribution of the local slope we took a window of $5 \times 5$ spins, parametrize it’s orientation by $m_\theta$ and $m_\phi$ and scan the rippled part of the interface by moving this window on it at each time step and find the joint probability distribution for local slope of the interface. By varying the value of $\theta$ and $\phi$ we repeat this process for each set of $(\tan \theta, \tan \phi)$ in $\tan \theta - \tan \phi$ plane ranging from 0.2 to 0.4 along both axis, in steps of 0.01 and find the joint probability distribution for each set. We have simulated our system at temperature 1.0 in units of KT/J where K is Boltzmann constant, T is temperature in Kelvin and J is the coupling constant of spin-spin interaction. Metropolis update is used.

We start discussing our results with $Z(r,t)$ which has $\tan \theta = \tan \phi = 2/7$ and has geometry as shown in Fig 1. As it translates pinned with $Z(r,t)$, it fluctuates close to it. The spatial nature of fluctuation profile in pinned phase is considerably different from what is observed when $S(r,t)$ lags $Z(r,t)$ (see Fig 2). The central part of the interface has a unique feature which is microscopically smooth thereby separates it form the rest of the fluctuation profile which has rippled structure. Naively thinking one can contend that sharp pointed corner of profile shown in Fig 1 being entropically unfavorable, leads to this feature, but this feature is not limited to this profile only (see Fig 2). I don’t deny from entropy being one of the agents as by detail calculation with various geometries of the field interface like that in Fig 1, hemispherical and plane we observe that macroscopically interface attains geometrical shapes which are favored by entropy but in the central part it always has some strange feature. With profile that of Fig 1 and with hemispherical interface geometry central part is not only smooth microscopically but also flat macroscopically and is parallel to cross section of crystal perpendicular to direction of the field motion (see Fig 1). The interface fluctuates about the field interface in such a way that not only with profile shown overleaf or with hemispherical geometry of field interface, even with plane field interface the unique central feature of fluctuation profile has it’s signature, though relatively very weak in this case. Apart form the central region, interface (in case of plane geometry whole of it) has rippled structure (see Fig 1). These ripples apparently flow like waves as $S(r,t)$ translates pinned with $Z(r,t)$. Underlying physics is that in the pinned phase spatial profile of the field, forces magnetization to follow $H(r,t)$ as closely as possible. But the field interface is a continuous surface and the underlying lattice is discrete, thus $S(r,t)$ can never coincide with $Z(r,t)$, so settles up fluctuating about it, as the system equilibrates with particular $H(r,t)$ at any instant, with local slopes permitted by the discrete lattice. As $Z(r,t)$ translates environment of spins close to $Z(r,t)$ keeps changing, leading to specular changes in the spatial structure of $S(r,t)$, giving an illusion of waves flowing on the interface. With profile of Fig 1, these waves periodically converge and diverge, the period of which is slope($\theta, \phi$) dependent. With $\tan \theta = \tan \phi = 2/7$ we find waves to be diverging slowly and after some time all of a sudden converge. With $\tan(-\theta) = \tan(-\phi) = 2/7$ we find slow convergence and fast divergence. Sequence of convergence and divergence is repeated again and again with a period incommensurate with lattice constant as interface translates on the lattice. Qualitatively comparable behavior is obtained with hemispherical field geometry as well.

The central region of fluctuation profile is a rather interesting feature and needs some more focused attention. This feature undergoes various notable changes with time, step size and interface geometry in terms of the area covered by it on the interface and it’s position with respect to $Z(r,t)$. Moving along the line $y=x$, on the
fluctuation profile, the distance of first lattice site from the center whose vertical height is less than the previous one is defined as parameter radius, which reasonably parametrizes area covered by unrippled part on the interface, if not exactly. The value of this parameter is temporally periodic with a modulation of average increment whose rate is fast in the beginning and finally goes to saturation with time. Qualitative nature of radius vs time graph for various interface geometries is reasonably comparable (See Fig3).

We have also probed the variation of radius with θ and φ by varying them but keeping θ=φ, so that the symmetry of central feature is preserved. Ignoring fluctuation about the general trend we observe a continuous decrement in the radius with increase in value of θ and φ. But this trend breaks up after certain value of slope and interface undergoes a catastrophic transition. The exact numerical value of the slope at which transition occurs varies with step size. Simultaneous effect of entropy maximization and energy minimization along with the constrain of discrete nature of lattice can no longer go with a single interface and it breaks up. The central part of interface which was lagging the field interface up to this extent breaks from the rest of the interface and starts leading the field interface, thereby bringing a drastic change in the fluctuation profile of the interface. (see Fig4.)

For arbitrary orientations of the field profile, the local slope of the rippled part of the interface locks in to one of infinitely many rational values, which most closely approximates the local field at that point, which may be different form the average slope of the interface, thereby generating locked in regions in the tan(θ)-tan(φ) plane depicted as white and colored patches in Fig5. Careful observation of interface reveals that local slope of the rippled part of the interface continually fluctuates in space and time close to the field interface. The set of histograms of joint probability distribution reveal that at the velocity 0.01 lattice sites per MCS with step size of 0.1 lattice sites, instead of having a peak at (0.25,0.25) the joint probability distribution for tan(θ)=tan(φ)=1/4 has a set of peaks with almost equal probability, close to (2/9,2/9), (2/9,2/7), (2/7,2/7), (2/7,2/9) and few other fractions, with (2/7,2/7) being slightly more probable than others. In region close to (1/4,1/4) the most probable peaks of the locked in regions are either at one of these positions or a combination of these. Same is the case with tan(θ)=tan(φ)=1/3, where the dominant sets are close to (2/7,2/7), (3/7,3/7), (3/7,1/4), (1/4,3/7), (1/4,1/4) and few other fractions, with (2/7,2/7) being most probable. We expect more locked in regions to reveal there existence if we could increase our resolution, the most probable peaks of those would be a combination of these positions like one shown in Fig5. where both (2/9,2/7) and (2/7,2/7) are highly probable. In the whole central region, shown by three colors most probable peak is (2/7,2/7) but red region has a background corresponding to (1/4,1/4) i.e the joint probability distribution has a structure corresponding to (1/4,1/4) with (2/7,2/7) position being most probable. In the green region the background structure is of (1/3,1/3) with (2/7,2/7) being most probable. In the blue part there is transition from (1/4,1/4) background to (1/3,1/3) background, but in all the three regions (2/7,2/7) remains the most probable slope. The figure is expected to be symmetric about

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**FIG. 3**: Variation in radius with time and profile for velocity 0.01 site per MCS and step size 0.01 site (Pinned Phase). **Left**: Z(r,t) as in Fig1. with tanθ=tanφ=2/7. **Middle**: Z(r,t) having hemispherical geometry with radius of curvature=14 and center at x=14, y=14. **Right**: Z(r,t) as in Fig1. with tanθ=tanφ=slope varying in steps of 0.01.

**FIG. 4**: Fluctuation profile with tan(θ)=tan(φ)=1.0
y=x line which it is evidently. On increasing velocity to 0.05 lattice sites per MCS with step size of 0.1 lattice sites we find that histogram peaks get blurred on average. But as (1/4,1/4) structure breaks down at this velocity more prominent in area close to (1/4,1/4) as compared to that in vicinity of (1/3,1/3) which doesn’t breakup at this velocity. On increasing the velocity boundaries of patches shrink and expand thereby eventually revealing patches which were too small to be shown with previous velocity. On increasing velocity to 0.1 lattice sites per MCS lagging phase appears where there is no lock in region and most probable slope is always very close to global slope if not always exactly equal to, with a Gaussian distribution about it.

How sensitive are our results to the details of the dynamics? It is known that the intrinsic width of interfaces driven by uniform fields depends on such details [6]. The structure of pinned interface, on the other hand, is determined mainly by geometry and hence should be relatively unaffected. Nevertheless, we expect that our dynamical phase diagram and the location of the phase boundaries to be influenced by such details. In future we want to investigate this point in full three dimensional diagram in \( m_\theta, m_\phi \) and \( v_e \) space. Upto what extent our results are sensitive to exact nature of the update rule, this is also a point which we would like to probe in future. We hope our studies will be useful in understanding moving interfaces in more realistic systems [11] and the growth of colloidal crystals in using patterned substrates [7].

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