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Interface Motion in a Two-Dimensional Ising Model with a Field

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We determine by Monte Carlo simulations the width of an interface between the stable phase and the metastable phase in a two-dimensional Ising model with a magnetic field, in the case of nonconversed order parameter (Glauber dynamics). At zero temperature, the width increases as t^{β} with $\beta \simeq 1/3$, as predicted by earlier theories. As temperature increases, the value of the effective exponent β that we measure decreases toward the value 1/4, which is the value in the absence of magnetic field.

KEY WORDS: Ising model; interfaces; Monte Carlo simulation.

1. INTRODUCTION

In the two-dimensional Ising model, the dynamics of the interface between two phases has been the subject of recent interest.[1,2] In the case without magnetic field, if one starts with a sharp interface and lets it evolve via Glauber dynamics (nonconserved order parameter), the time-dependent behavior of the interface has already been studied.[1,2] It is the purpose of this paper to examine the case of nonzero magnetic field, for different temperature regimes.

We first describe the situation that we want to study and then give the details of the computational method. In a nonzero magnetic field, let us consider the metastable phase and the stable phase coexisting together, separated by a sharp straight interface. We want to let the system evolve via Glauber dynamics. Two processes will take place. First, the front between the stable phase and the metastable phase will advance. Second,

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there will be some nucleation of the stable phase within the metastable one. We want to have a sufficiently low nucleation rate of droplets, so that the concept of an interface between stable and metastable phases still makes sense after many Monte Carlo steps. Therefore, one should have

$$\beta \gg \frac{h}{\pi \gamma^2}, \tag{1}$$

where γ is the surface tension and h the magnetic field.

Another constraint is that the magnetic field be strong enough to overcome the nucleation barrier. To be specific, let us consider the case of zero temperature for an interface initially oriented along the (1, 0) direction. If the field h is lower than $2J$, where J is the coupling constant, nothing will happen. The situation is different if one considers an interface oriented along the (1, 1) direction. Any spin which is right at the interface has now two neighbors parallel to itself and two neighbors antiparallel. If a spin of the metastable phase which is right at the interface is flipped, it will still have two neighbors parallel to itself. Therefore, there is no nucleation barrier. We prefer to focus on this case of (1, 1) orientation because the field can be monitored from zero to any arbitrary value, provided that (1) still holds.

The case of zero temperature is exactly equivalent to the single-step model,[3–6] which is related to the Kardar–Parisi–Zhang (KPZ) equation.[7] The width w of an interface of size L is known to scale[8] as

$$w \sim L^{\chi} f(tL^{-z}) \tag{2}$$

where t is time (number of Monte Carlo steps per spin) and χ and z are a static and a dynamical exponent, respectively. In two dimensions, χ and z are known to be 1/2 and 3/2, respectively.[7] For nonzero temperature, the interface can no longer be described by simplified solid on solid (SOS) type models, because of holes and overhangs.

2. COMPUTATIONAL METHOD

We now discuss the details of the numerical computation. First, one has to prepare a stable phase. When the temperature is not close to the critical temperature T_c, relaxation times to equilibrium are of the order of a few MC steps per spin. It suffices to start from a state with all the spins parallel to the field and to let it evolve under Glauber dynamics for a few MC steps. The same holds for the metastable phase, except that one starts with spins antiparallel to the field. Two systems of length L and height H are prepared, one in the stable phase and one in the metastable phase.

Periodic boundary conditions are used in both the vertical and the horizontal direction. At time $t=0$, one glues the two systems together in the following way. For ordinates y such that $0 \leqslant y \leqslant H/4$, one has the stable phase, and for $H/4 < y \leqslant H$, one has the metastable phase. The simulation then continues. Spins are chosen randomly and successively updated.

At this stage, one might wonder why one does not divide the system into two sublattices in order to achieve vectorization and obtain a faster algorithm. The reason is that, if one does so, and updates all the spins of a sublattice in parallel, then at sufficiently low temperatures, the interface tends to have locally the shape of the sublattice. This introduces an extra contribution to the width,[9] which is due to short-length-scale undulations and has nothing to do with the long-wavelength fluctuations we are interested in. Though this extra width is unimportant, in principle, in the limit $L \to \infty$, it makes the numerical data more difficult to analyze and leads eventually to larger error bars.

We have to use random updating of the spins because otherwise, at zero temperature, we would obtain a front that propagates and after one MC step all the spins of the metastable phase would have been flipped. Suppose, for example, that the spins are numbered for height $H=1$, from the right to the left from 1 to L, and for $H=2$ from $L+1$ to L^2, and so on up to the last spin (number $H \times L$), which is at the right uppermost corner of our box at $H=L$. Then, if we update the spins sequentially, we will flip all layers one after the other, starting from the one immediately above the interface.

When $H \times L$ attempts have been made, we say that we have one MC step per spin (on average). From now on, the number of MC steps per spin will be referred to as time t. There are two interfaces, one initially located at $y=H/4$, the other at $y=0$ (because of the periodic BC in the vertical direction). The average position of the interface initially located at $y=H/4$ will move upward and the interface initially located at $y=0$ will move downward such that after some time, the metastable phase will have disappeared. We now explain the procedure that we adopted in order to avoid this disappearance. The average position of the interface initially located at $y=H/4$ reaches $3H/8$ at some time we denote by t_1. At time t_1, we take the part of our system contained between the planes $y=H/8$ and $y=H/2$. The interface of interest lies in that part. With this part, we make a new system of length L and height H, consisting of, (1) for $y \leqslant 3H/8$, the above-mentioned part of our old system which contains the interface, and (2) for $y > 3H/8$, a part of a metastable phase which has been evolving via Glauber dynamics for time t_1, and was at time $t=0$ with all spins antiparallel to the field.

We see that we need to run, in parallel with our system, another box of length L and height H containing a metastable phase (actually, a box of height $5H/8$ would be sufficient). The part of our old system for which $y \leqslant H/8$ is simply discarded. The correlations in the vicinity of the line $y = 3H/8$ will be somewhat perturbed by our gluing procedure, but after a few MC steps, correlations should have relaxed toward those of the steady state, provided one is not close to a critical point. Since this gluing occurs at a distance $H/8$ from the average position of the interface, if H is sufficiently large with respect to the width of the interface, it will not perturb the interface. This whole procedure is reminiscent of what is usually done for the Eden model, where only the active part of the cluster is stored.[10]

For the average position of the interface and its width, we used the standard definition.[11] For an interface located in a strip

$$H_{\min} \leqslant y \leqslant H_{\max}$$

the normalized gradient $g(y)$ is defined as

$$g(y) \equiv [M(y+1) - M(y)]/[M(H_{\max}) - M(H_{\min})] \tag{3}$$

where $M(y)$ is the magnetization of the layer at height y. The average position of the interface is defined as

$$\langle y \rangle \equiv \sum_{y=H_{\min}}^{H_{\max}} M(y)\, y \tag{4}$$

The squared width of the interface ω^2 is then

$$w^2 \equiv \langle y^2 \rangle - \langle y \rangle^2 \tag{5}$$

3. SIMULATIONS AND RESULTS

We first have to show that our two-dimensional Ising program correctly reproduces some of the properties of the single-step model at very low temperature. From (2), it follows that

$$w \sim t^{\beta} \tag{6}$$

with

$$\beta = \chi/z \tag{7}$$

if $t \ll L^z$. We measured the exponent β and therefore had to use large systems and times much smaller than L^z. Figure 1 shows $\ln w^2$ versus $\ln t$

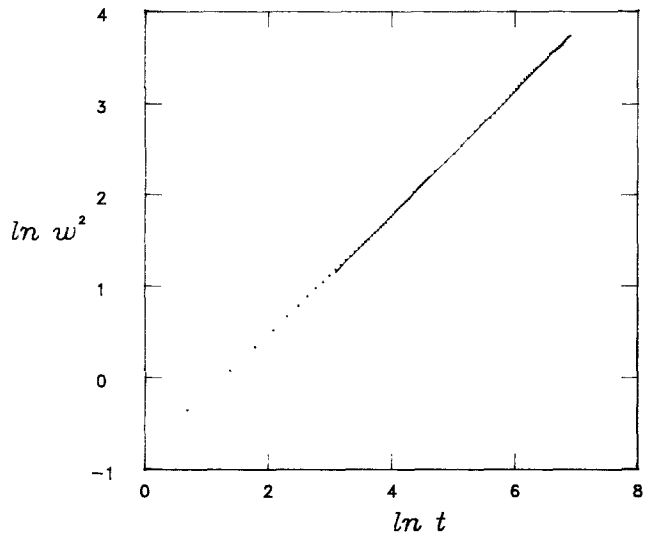


Fig. 1. Plot of $\ln w^2$, where w^2 is the squared width of the interface, versus $\ln t$, t being the number of Monte Carlo steps per spin, for a magnetic field $h = 0.1$ and inverse temperature $1/kT = 40$. Systems have length $L = 4000$ and height $H = 256$. Averages have been taken over eight samples. The solid line is a least square fit to the data in the range $20 \leqslant t \leqslant 990$, giving $\beta \simeq 0.34$.

for systems of length $L = 4000$ and height $H = 256$ at an inverse temperature $1/kT = 40$ and magnetic field $h = 0.1$, in units of J, the coupling constant. Results have been averaged over eight samples. To calculate the width [see Eqs. (3)–(5)], we used $H_{\min} = H/8$ and $H_{\max} = H/2$. Simulations were carried on SUN sparc workstations. A least square fit in the region $20 \leqslant t \leqslant 990$ gives $2\beta = 0.68 \pm 0.015$. This is compatible with the theoretical prediction $\beta = 1/3$, valid for zero temperature.[3,7] We also simulated smaller systems on a Cray YMP, up to lengths $L = 500$ and heights $H = 128$. We ran 64 samples at the same time and performed the vectorization on the number of samples. About 6.25 spins were treated per microsecond on one Cray YMP processor as opposed to 0.045 spins per microsecond on the SUN sparc workstations. No evidence of finite-size effects was found and the value of β was also compatible with $\beta = 1/3$.

Next, we turn to higher temperatures. Figure 2 shows $\ln w^2$ versus $\ln t$ for different inverse temperatures $1/kT$ between $1/kT = 1$ and $1/kT = 10$, at a field $h = 0.1$. Systems were of length $L = 500$ and height $H = 128$ and results have been averaged over 64 samples. Simulations were run on a Cray YMP because it turns out that one needs to average over more samples than for the low-temperature case ($1/kT = 40$). We see that the

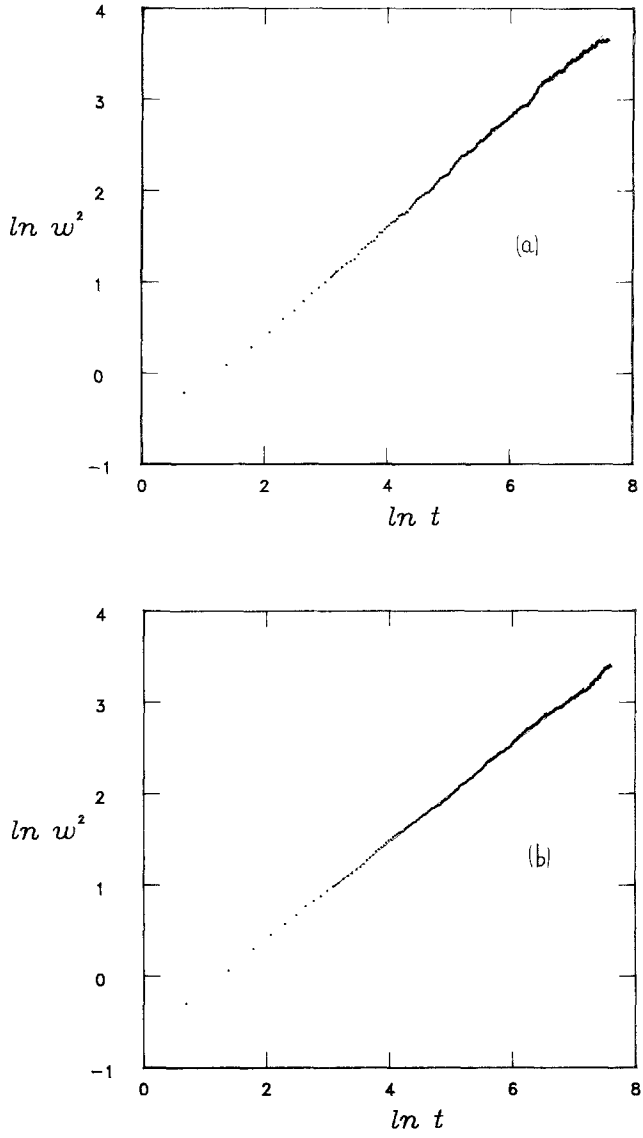
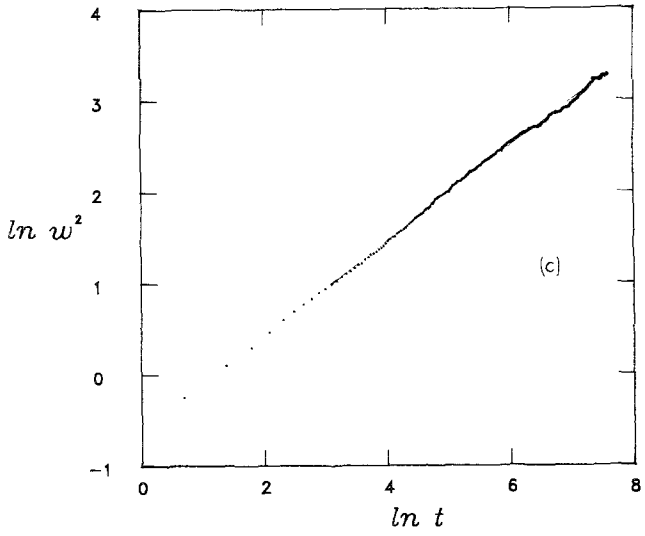


Fig. 2. Plot of $\ln w^2$ versus $\ln t$ for a field $h=0.1$ and various inverse temperatures, from $1/kT=10$ to $1/kT=1$: (a) $1/kT=10$, (b) $1/kT=4$, (c) $1/kT=3$, (d) $1/kT=2$, (e) $1/kT=1$. Averages have been taken over 64 samples of length $L=500$ and height $H=128$. We went up to $t=2000$. The solid lines are last square fits to the data in the range $20 \leqslant t \leqslant 1000$, except in (e), where the fit is in the range $20 \leqslant t \leqslant 500$, giving (a) $\beta=0.30$, (b) $\beta=0.268$, (c) $\beta=0.258$, (d) $\beta=0.249$, (e) $\beta=0.256$.



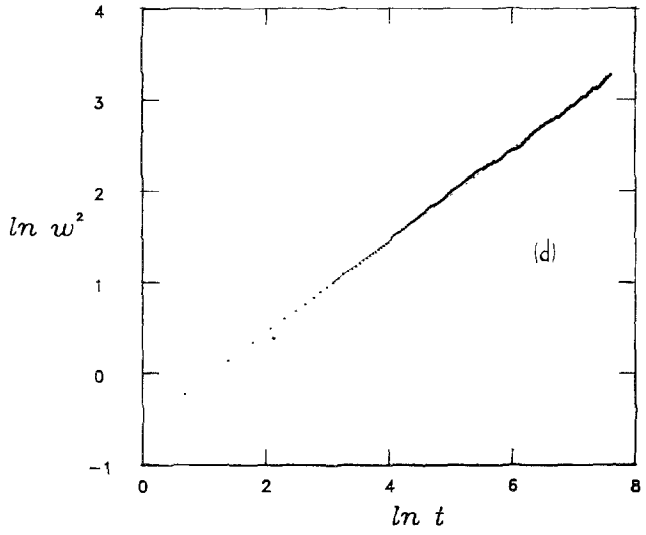


Fig. 2. (*Continued*)

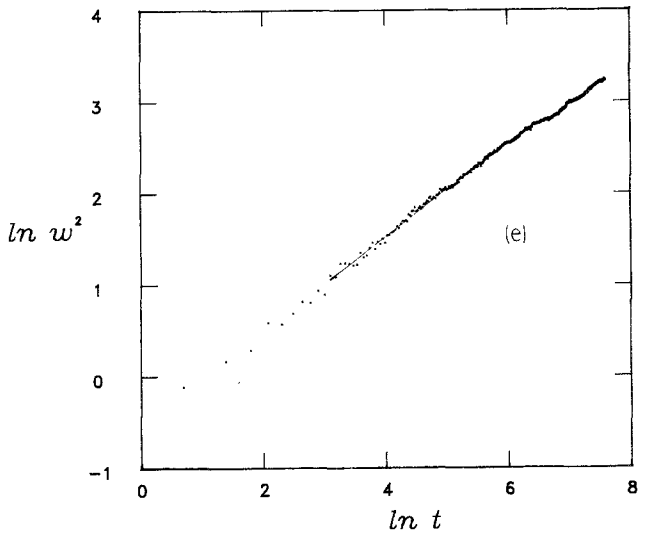


Fig. 2. (*Continued*)

effective exponent β is close to 1/4, which is the value in the absence of a field, already for $1/kT = 2$. For $1/kT = 2$, by a least square fit in the range $20 \leqslant t \leqslant 2000$, we obtain $2\beta = 0.50 \pm 0.02$. For $1/kT = 2$, we tried to increase the field, still satisfying (1). For h larger than 1, we started to have some problems with nucleation events. For $h = 1$, we obtained an effective exponent of $2\beta = 0.68 \pm 0.04$. This means that the value $\beta = 1/3$ may be retrieved for intermediate temperatures and sufficiently large fields.

4. CONCLUSION

In summary, we have performed Monte Carlo simulations of the interface between the stable and the metastable phases of the two-dimensional Ising model in a field evolving through Glauber dynamics. For small fields (of the order of 0.1 in units of the coupling constant), and reasonable temperatures (higher than $T = 1/3$), the effective value of the exponent β governing the short-time increase of the width was found to agree with the zero-field prediction $\beta = 1/4$ rather than with the large-field prediction $\beta = 1/3$, which is retrieved only at very low temperatures. This does not mean necessarily that there is phase transition, since the value of β we observe may cross over to 1/3 in the limit of infinite systems. For the sizes we used, no crossover is apparent from our simulations. At moderate temperatures but higher fields, the value $\beta = 1/3$ is retrieved.

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