Slow dynamics in a 2D Ising model with competing interactions

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The far–from–equilibrium low–temperature dynamics of ultra-thin magnetic films is analyzed by using Monte Carlo numerical simulations on a two dimensional Ising model with competing exchange (J_0) and dipolar (J_d) interactions. In particular, we focus our attention on the low temperature region of the (δ, T) phase diagram (where $\delta = J_0/J_d$) for the range of values of δ where striped phases with widths $h = 1$ ($h1$) and $h = 2$ ($h2$) are present. The presence of metastable states of the phase $h2$ in the region where the phase $h1$ is the thermodynamically stable one and viceversa was established recently. In this work we show that the presence of these metastable states appears as a blocking mechanism that slows the dynamics of magnetic domains growth when the system is quenched from a high temperature state to a low temperature state in the region of metastability.

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I. INTRODUCTION

In the last years a strong effort has been devoted to understand both the equilibrium and out-of equilibrium properties of ultrathin magnetic films[1]. These materials have attracted much attention mainly due to their potential applications, such as information storage[2]. Ultrathin films find also many important applications both in biotechnology and pharmacology. It is today a well established experimental fact that the magnetization processes in ultra-thin magnetic films are ruled by the microscopic competition between short range ferromagnetic couplings and long-range frustrated antiferromagnetic dipolar interactions, which give place to very novel dynamical and static behaviors[1].

It is worth mentioning that both the theoretical and the experimental interest in studying systems with competition between short-range ordering interactions and long–range frustrating interactions widely exceeds the field of ultra–thin films. Actually, many different experimental systems can be modeled by this kind of microscopic interactions, which give place to very rich dynamical and static properties. In soft–matter physics for instance, we can mention diblock copolymer melt and cross–linked polymer mixtures, among others. Type I superconductors and rare–earth layers that occur in the perovskite structure of $\mathrm{REBa_2Cu_3O_7} - \delta$ (where RE represents a rare earth from the lanthanide series) can be very well modeled with these interactions[3].

It has also been frequently suggested that competing interactions can explain many of the phenomenological features observed in the glass formation process and in supercooled liquids[4]. Summarizing, many of the conclusions drawn from this work can be surely be applied to a large variety of physical systems.

For sufficiently thin films the magnetic moments align perpendicular to the plane of the film, indicating that the surface anisotropy is sufficient to overcome the anisotropy of the dipolar interaction which favors in-plane ordering.

Works in two dimensional uniaxial spin systems, where the spins are oriented perpendicular to the lattice and coupled with these kind of interactions, have shown a very rich phenomenological scenario concerning both its equilibrium statistical mechanics[3,5] and non-equilibrium dynamical properties[2,6,7]. In particular, some of these results[2,6] showed the existence of different types of slow relaxation dynamics when the system is quenched from a disordered high temperature configuration to a subcritical temperature, depending on the relative strengths of the dipolar and exchange interactions.

Under these circumstance one can use a uniaxial Ising representation for describing the magnetic moments[8,9]. The ultra–thin film is then described by the Hamiltonian

$$H = -\delta \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \sum_{(i,j)} \frac{\sigma_i \sigma_j}{r_{ij}^3} \qquad (1)$$

where the spin variable $\sigma_i = \pm 1$ is located at site i of a square lattice, the sum $\sum_{\langle i,j \rangle}$ runs over all pairs of nearest neighbor sites and $\sum_{(i,j)}$ runs over all distinct pair of sites of the lattice; r_{ij} is the distance (in crystal units) between sites i and j, δ represents the quotient between the exchange J_0 and dipolar J_d coupling parameters ($\delta = J_0/J_d$). The energy is measured in units of J_d, which is always assumed to be antiferromagnetic ($J_d > 0$). Hence $\delta > 0$ means ferromagnetic exchange coupling.

We have recently studied in detail[10] the low temperature phase diagram of this system in the region where the change in the relaxation properties has been observed. We showed that for very low temperatures metastable states appear. In this work we investigate the effects of the presence of these metastable states on the far-from equilibrium dynamical properties of the system. In section II we present a review of the equilibrium phase diagram and metastability properties in the region of interest. In section III we analyze the magnetic domain growth or coarsening dynamics of the system when it is quenched from a disordered state (which corresponds to infinite temperature) to a temperature below the ordering transition for different values of δ. Using Monte Carlo simulations we study the statistics of domains of the striped phases h1 and h2. We then analyze the temporal behavior of the average linear size of the domains L. We show that the coarsening dynamics is strongly affected by the presence of metastable states, which generate blocking clusters of the metastable phase where the domain walls of the stable phase become pinned. Such blocking clusters generate free–energy barriers to the domain growth dynamics that are independent of the linear domain size. Some conclusions and remarks are summarized in section IV.

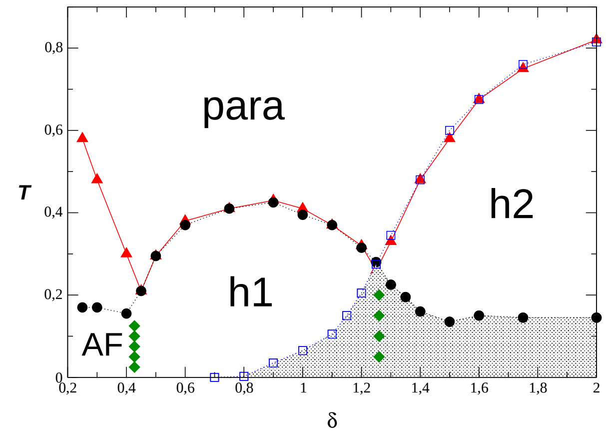

FIG. 1: Phase diagram (δ, T) in the region of parameters under study. Filled triangles correspond to the critical temperatures $T_c(\delta)$ obtained by specific heat calculations for the phase transition between the ordered antiferromagnetic (AF) and striped phases $h1$ and $h2$ and the paramagnetic (**para**) one. Filled circles (open squares) correspond to the stability line of the $h1$ ($h2$) phase, obtained by analyzing the staggered magnetization M_{h1} (M_{h2}). Filled diamonds correspond to the first order transition lines between the $h1$ and $h2$ phases and also between the $h1$ and AF phases, obtained by the free energy numerical calculations. The shaded region indicates the presence of metastable states.

II. EQUILIBRIUM PHASE DIAGRAM AND METASTABLE STATES

The overall features of the finite temperature phase diagram associated with Hamiltonian (1) were described by MacIsaac and coauthors[3] by means of Monte Carlo simulations on 16×16 lattices and analytic calculations of the ground state[1]. They found that the ground state of Hamiltonian (1) is the antiferromagnetic state for $\delta < 0.425$[11]. For $\delta > 0.425$ the antiferromagnetic state becomes unstable with respect to the formation of striped domains structures, that is, to state configurations with spins aligned along a particular axis forming ferromagnetic stripes of constant width h, so that spins in adjacent stripes are anti-aligned, forming a super lattice in the direction perpendicular to the stripes. At high temperatures, of course, the system always becomes paramagnetic. Specific heat calculations showed that the transition between the paramagnetic and the striped phases is a second order one[3].

We have recently[10] performed Monte Carlo simulations of Hamiltonian (1) on square lattices up to 48×48 sites using periodic boundary conditions and heat bath dynamics. Our calculations focused on the low temperature region of the (δ, T) phase diagram for values of δ between 0.2 and 2, which includes the transition line between the AF and the striped phase with width $h = 1$ ($h1$) and also the transition line between the $h1$ phase and the striped phase with width $h = 2$ ($h2$). First we calculated, through the energy fluctuations, the specific heat C as a function of temperature for different values of δ and different system sizes up to 48×48 sites. By considering the peaks in the specific heat we obtained the second order critical line between the paramagnetic and the low temperature ordered phases $h1$ and $h2$. These results (see Fig. 1) slightly improved those obtained by MacIsaac and coauthors[3] for 16×16 lattices, thus showing a fast convergence of the critical temperature for increasing system sizes, at least for small values of δ.

Next, through a numerical study of the free energy, we analyzed the transition between the $h1$ and $h2$ phases. The free energy of the phase $h1$ ($h2$) was calculated for increasing (decreasing) values of δ. We observed a continuous change of the minimal free energy from one phase to the other, with a discontinuous change in the slope for $\delta = 1.26(1)$ indicating the presence of a first order phase transition[10]. This transition is indicated by means of diamonds in Fig. 1. We have also repeated these calculations for the transition line between the $h1$ and AF phase, finding similar results.

Close to $\delta = 1.26(1)$ the free energy displays a multivalued behavior characteristic of a first order phase transition. This behavior signals the metastable nature of these phases in some parts of the phase diagram. To characterize the presence of metastable states observed in the transition between the $h1$ and $h2$ phases we introduced the staggered magnetizations M_{h1} and M_{h2}, and also their associated susceptibilities χ_{h1} and χ_{h2} for the $h1$ and $h2$ phases[10]. These quantities permitted us to analyze the stability of both phases in the different parts of the phase diagram. In Fig. 1 the shaded region indicates the presence of metastable states. It is important to stress that in the shaded region inside phase $h1$ the only phase observed to be metastable was $h2$. For $\delta > 1.26$ metastables states of phases of higher width were observed, leading to a much more complicated metastable region. In this work we will focus only on the dynamical behavior of the system in the $h1$ region. As we will show in the next section, for a fixed value of δ inside this region different dynamical regimes are observed as the temperature is lowered and one enters the region of metastability.

III. SLOW DYNAMICS

When a system is quenched from a high temperature disordered phase into a low temperature ordered phase domains form and grow, a process that is known as coarsening. The coarsening process has been extensively studied both experimentally and theoretically over the past decade[12].

Perhaps the most thoroughly studied system, and also the most common example is the Ising model. When this system is quenched from a high temperature to one below its critical temperature ($T < T_c$) ferromagnetic domains of up and down spins form and coarsen. The system presents curvature driven growth and the characteristic domain size L grows with time as $L(t) \sim t^{1/2}$. If the system is cooled to zero temperature the domain walls can be easily determined as bonds between oppositely oriented spins, but if the system is cooled to a temperature different from zero it becomes difficult to define domains and domain walls since small islands generated by thermal fluctuations arise. To overcome this problem, Derrida[13] proposed a new method to measure properties related to coarsening in the presence of thermal fluctuations. This method was extended by Hinrichsen and Antoni[14] to determine domain walls for nonzero temperatures. The method compares the state of a system with replicas in the different ground state configurations when they are all submitted to the same thermal noise, that is, when the same sequence of random numbers is used to update all systems. In this way, if one starts from a replica in the ordered state a spin flip will be a consequence of the thermal noise. When a spin flip occurs simultaneously in all the replicas it can be considered as a thermal fluctuation, otherwise the fluctuation will be due to the coarsening process. We used this technique to study the dynamics of domain walls, and characterize the coarsening process, when the system described by Hamiltonian (1) is quenched from a high temperature disordered state into the region where it orders. In particular we focus our interest on the growth of domains of the striped phase $h1$ when the metastability line is crossed for values of $0.8 < \delta < 1.26$ (See Fig.1).

To characterize the growth of the domains we determined first the domain areas $A(t)$, by counting the

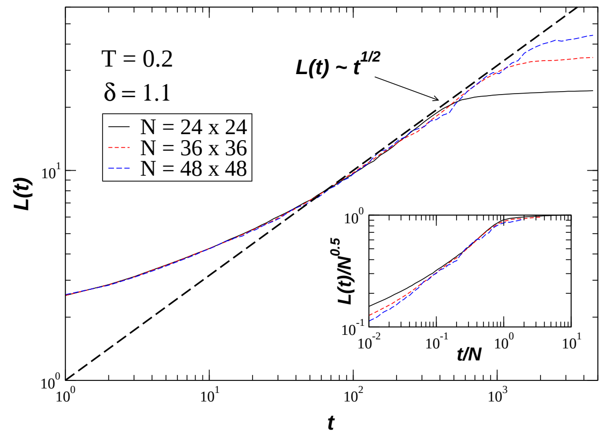

FIG. 2: Characteristic domain size $L(t)$ vs. t when $\delta = 1.1$ and $T = 0.2$ for three different system sizes $N = 24 \times 24$, $N = 36 \times 36$ and $N = 48 \times 48$. The dashed line indicates $L(t) \sim t^{1/2}$. The inset shows the data collapse obtained using finite size scaling analysis.

number of spins inside each domain. The characteristic (linear) domain size was calculated as $L(t) = \sqrt{\langle A(t) \rangle}$, where $\langle A(t) \rangle$ is the mean domain area of the system at time t.

In Fig. 2 we present the behavior of the characteristic domain size $L(t)$ when $\delta = 1.1$ and $T = 0.2$ for three different system sizes $N = 24 \times 24$, $N = 36 \times 36$ and $N = 48 \times 48$. After a short transient in which the characteristic length presents a slow growth the system enters into a coarsening regime where $L(t) \sim t^{1/2}$, as expected for a system with non–conserved order parameter[12]. For large times $L(t)$ presents a crossover to a saturation value. This saturation behavior is clearly a finite size effect, since a domain cannot grow beyond the system size N so that as the system size increase, the behavior $L(t) \sim t^{1/2}$ remains for larger periods of time.

In section II we observed and characterized the presence of metastable states in the low temperature region of the phase diagram. We will study now how the behavior of $L(t)$ changes as we lower the temperature and cross the metastability line for a fixed value of δ. In Fig. 3 we present the time evolution of $L(t)$ when $\delta = 1.1$ for eight decreasing temperatures. For low temperatures a regime of slow growth develops at intermediate time scales before the system crosses over to the $t^{1/2}$ coarsening regime. As we lower the temperature the intermediate regime extends to larger time scales, but all the curves eventually cross over to the $L(t) \sim t^{1/2}$ regime. Note that for short times there seems to be a change in the concavity of $L(t)$ when it crosses $T = 0.1$, which coincides with the boundary of the metastable phase for $\delta = 1.1$.

To characterize the behavior of $L(t)$ as we lower the temperature we studied the crossover time τ from the power law to the saturation regime. Note that the crossover time to the power law regime presents a similar

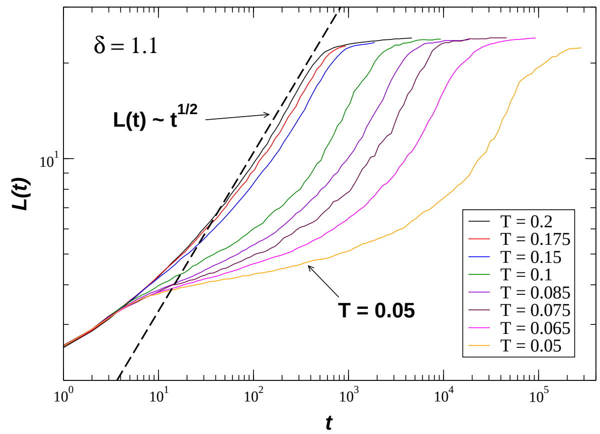

FIG. 3: Characteristic domain size $L(t)$ vs. t when $\delta = 1.1$ ($N = 24 \times 24$) for eight different temperatures, starting form the left curve $T = 2.0$, 0.175, 0.15, 0.1, 0.085, 0.075, 0.065 and $T = 0.05$. Note that all the curves eventually cross-over to the $L(t) \sim t^{1/2}$ regime indicated with a dashed line.

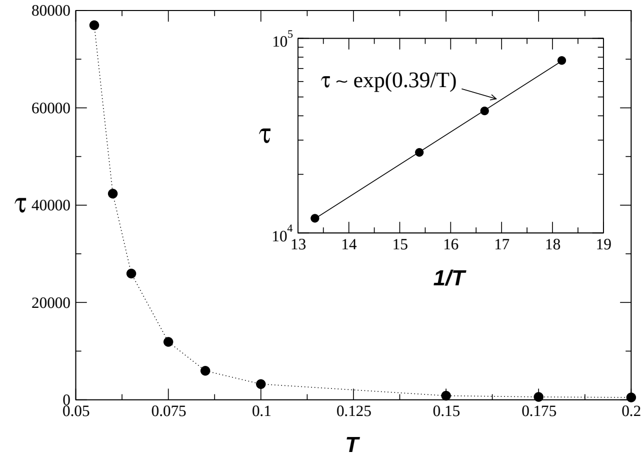

FIG. 4: Crossover time τ vs T for $\delta = 1.1$ and $N = 24 \times 24$. On the inset an Arrhenius plot τ vs $1/T$ for the four lower temperatures is presented. The straight line indicates the best fit.

behavior. However the study of the intersection of the power law branch of the curve and the horizontal saturation branch allows for a sistematic approach. This is so since the saturation value always correspond to the linear size of the system. In figure 4 we present how τ grows as the temperature is lowered. For temperatures greater than $T = 0.1$ the crossover time presents a linear dependency with $1/T$, while for temperatures lower than $T = 0.1$ it presents an exponential increase with $1/T$ as can be observed in the Arrhenius plot presented in the inset of Fig. 4.

The straight line indicates the best fit, given by a function of the form

$$\tau = \tau_0 \exp(\tau_1/T) \tag{2}$$

where $\tau_0 = 62.5(5)$ and $\tau_1 = 0.39(5)$. Using this expression we present in Fig. 5 a data collapse plot of $L(t)$ in the low temperature regime.

In the high temperature regime the crossover time decreases linearly as the temperature increases, and $L(t)$ collapses simply by scaling with T as can be seen in figure 6.

Summarizing, for $\delta = 1.1$ two different dynamical regimes were observed above and below the metastability line ($T = 0.1$). When the system is quenched to the ordered phase to a temperature $T > 0.1$, the characteristic domain size $L(t)$ grows as $t^{1/2}$ after a short transient. If, on the other hand, the system is quenched to a temperature $T < 0.1$, an intermediate regime with a slow growth appears. For long times the system always crosses over to the $t^{1/2}$ regime. That is, for every temperature we observe the same behavior presented in Fig.3, where $L(t)$ always reaches the asymptotic behavior $t^{1/2}$ as we increase the system size. However, as we lower the temperature the crossover time to this regime increases. We repeated these analysis for different values of δ, inside the $h = 1$ region, obtaining the same qualitative behaviors.

These dynamical behaviors present a strong resemblance with the ones observed in the two dimensional Shore model[15]. This model is a ferromagnetic Ising model on a square lattice with frustration added by introducing weak next-nearest-neighbor antiferromagnetic bonds, that is

$$H = -J_1 \sum_{NN} s_i s_j + \sum_{NNN} s_i s_j \tag{3}$$

The presence of NNN antiferromagnetic bonds in this model introduce free–energy barriers to domain coarsening that are independent of the domain size L[15]. Such barriers in this model are a consequence of a corner rounding process which generates structures that block the coarsening dynamics[15]. Hence, the system is stuck and coarsens little on time scales $t \ll \tau_B(T) = exp(F_B/T)$ (F_B being the height of the barrier), while on time scales $t \gg \tau_B(T)$ the free–energy barrier can be crossed and the $t^{1/2}$ behavior emerges.

Thus, it is interesting to see if structures that block the coarsening process are present in our system. In fact the presence of metastable states for low temperatures gives a strong hint of what to look for.

Figure 7 presents a series of snapshots of the coarsening process when a system of size $N = 48 \times 48$ and $\delta = 1.1$ is quenched to $T = 0.05$. For these values of δ and T the system evolves in the metastability region. Two different kind of domain walls can be clearly distinguished. When domains of phase $h1$ with different orientation meet, the

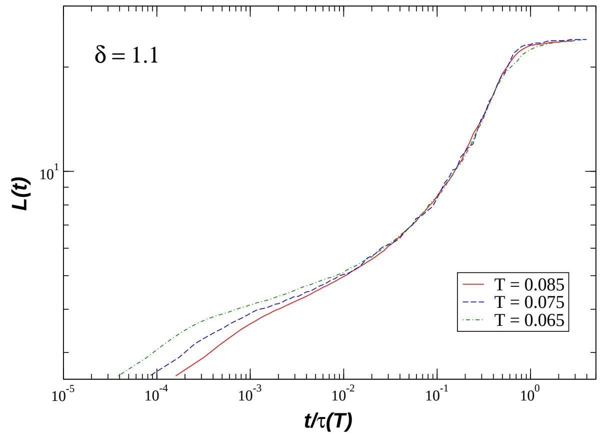

FIG. 5: Data collapse plot of $L(t)$ in the low temperature regime for three different temperatures ($\delta = 1.1$ and $N = 24 \times 24$). The crossover time τ corresponds to the best fit presented in Eq. (2).

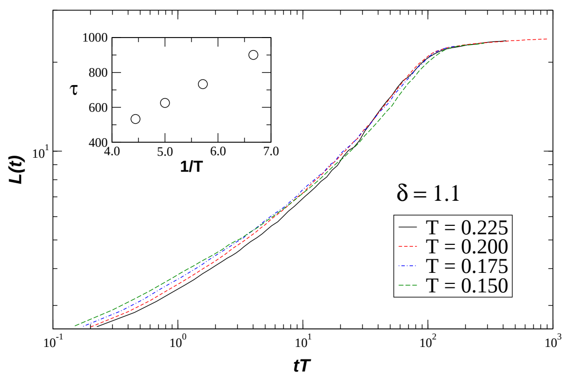

FIG. 6: Data collapse plot of $L(t)$ in the high temperature regime for three different temperatures $\delta = 1.1$ and $N = 24 \times 24$.

walls detected by the method are thin. The thicker walls correspond to bands of two spins, that is stripes of phase h2. We should stress that phase h2 is the only metastable phase in phase h1[10]. Notice how these small blocks of the h2 phase seem to slow the domain growth by pinning the domain walls. These small blocks were also observed at short times when the system was quenched to a temperature above the metastability line, however they are highly unstable and did not seem to block the domain growth. In order to quantify this effect, we studied the time for completely shrinking squares in phase h2 immersed in a system in phase h1 with fixed boundary conditions. A square was considered to be completely shrunk when the length of the sorrounding domain walls became zero. Fig.8 presents a series of snapshots of this process. In the first time steps the square quickly deforms. However, further advance seems to be blocked by small blocks of spins in the $h2$ phase. This coarsening behavior presents a strong resemblance to the one observed in the snapshots presented in Fig. 7.

Figure 9 shows the time τ_{h2} to shrink a 4×4 square in phase $h2$ immersed in a system with $N = 48 \times 48$ spins in phase $h1$ with fixed boundary conditions. As the temperature is lowered the shrinking time diverges as $\tau_{h2} \sim exp(0.41/T)$. This divergence agrees well with the divergence observed in the crossover time from the slow growth to the $t^{1/2}$ regime. We have also studied the shrinking time of blocks in different phases, such as combinations of vertical and horizontal $h1$ phases and also a ferromagnetic block immersed in the $h1$ phase. In all these cases a similar behavior was observed. The system quickly reached a configuration where small blocks of the $h2$ phase were present, with a slowing down of the domain growth similar to the one described above.

IV. CONCLUSIONS

In this paper we have studied some dynamical properties of a two-dimensional Ising Hamiltonian with competing interactions. We analyzed the coarsening process when the system is quenched from a high temperature disordered phase into the ordered phase $h1$. To characterize the growth of domains we considered the time evolution of the characteristic domain size $L(t)$. We found that for a fixed value of δ the system presents two different dynamical behaviors associated with the presence or absence of $h2$ metastable states. When the system is quenched into the ordered phase for temperatures above the metastability region, the characteristic domain length presents a power law $t^{1/2}$ growth. If, on the other hand, the system is quenched to temperature in the metastability region, the behavior of $L(t)$ presents a slow growth intermediate regime before crossing over to the $t^{1/2}$ power law growth. Through a direct examination of snapshots of the system during the coarsening process we found that the presence of small domains in the $h2$ phase slowed the coarsening when the system was quenched to the metastable region. These results are consistent with the presence of free–energy barriers independent of the domain size L, associated with blocking clusters of the metastable phase, which generates a crossover in the coarsening behavior as we cross the spinodal line. Since the cross over time diverges as the temperature is lowered, the very slow behavior at intermediate times may be indistinguishable from a logarithmic law. This could explain the apparently logarithmic scaling observed in the aging behavior of this model[6].

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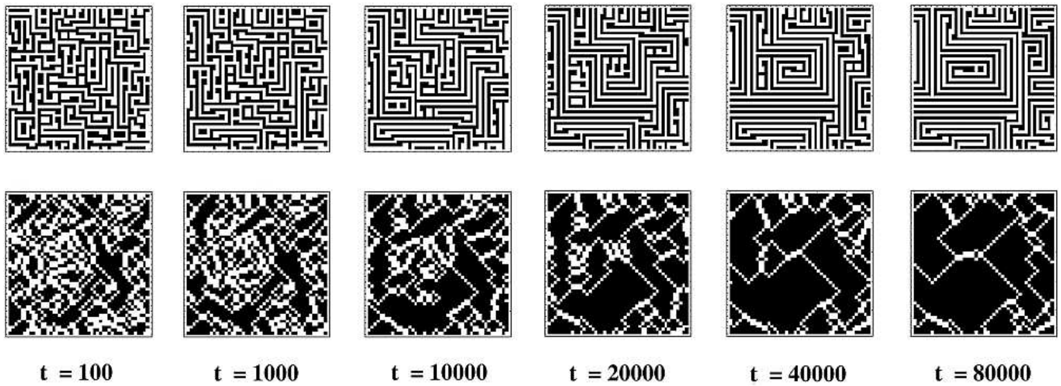

FIG. 7: Snapshots of the coarsening process for $\delta = 1.1$, $N = 48 \times 48$ and $T = 0.05$. The squares at the top correspond to spin configurations at different times of the coarsening (black points: up spins; white points: down spins). The black areas in the figures at the bottom are the corresponding domains of the $h1$ phase at every time, while the white lines correspond to the domain walls.

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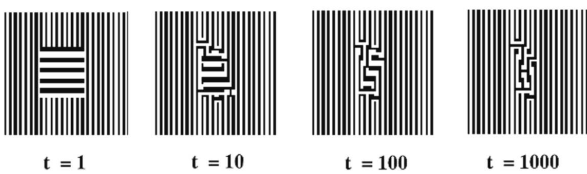

FIG. 8: Snapshots of the coarsening process for a 4×4 shrinking square in phase $h2$ immersed in a system in phase $h1$ with fixed boundary conditions.

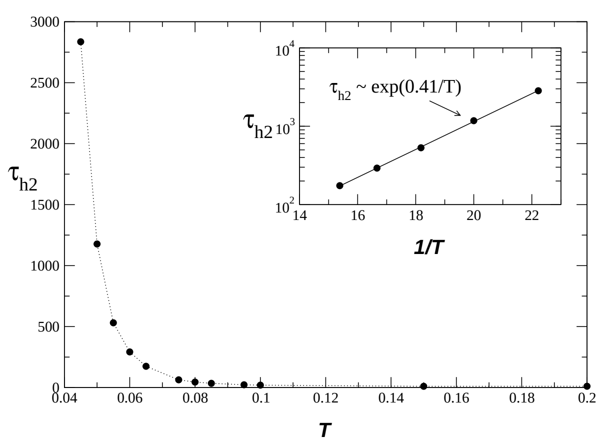

FIG. 9: Shrinking time of a 4×4 square in phase $h2$ immersed in a system in phase $h1$.

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[11] It is worth noting that MacIsaac and coauthors[3] definition of the Hamiltonian (Eq. (5) in that reference) is slightly different from ours (Eq(1)). While in that paper the dipolar term contains a sum over all pairs of spins, in Hamiltonian (1) we consider the sum over every pair of spins just once. This leads to the equivalence $\delta = J/2$, J being the exchange parameter in the above reference. Since the dipolar parameter also fixes the energy units in our work, there is also a factor 1/2 between the critical temperatures obtained in both works.
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