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Late stage, non-equilibrium dynamics in the dipolar Ising model

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ABSTRACT

Magnetic domain structures are a fascinating area of study with interest deriving both from technological applications and fundamental scientific questions. The nature of the striped magnetic phases observed in ultra-thin films is one such intriguing system. The non-equilibrium dynamics of such systems as they evolve toward equilibrium has only recently become an area of interest and previous work on model systems showed evidence of complex, slow dynamics with glass-like properties as the stripes order mesoscopically. To aid in the characterization of the observed phases and the nature of the transitions observed in model systems we have developed an efficient method for identifying clusters or domains in the spin system, where the clusters are based on the stripe orientation. Thus we are able to track the growth and decay of such clusters of stripes in a Monte Carlo simulation and observe directly the nature of the slow dynamics. We have applied this method to consider the growth and decay of ordered domains after a quench from a saturated magnetic state to temperatures near and well below the critical temperature in the 2D dipolar Ising model. We discuss our method of identifying stripe domains or clusters of stripes within this model and present the results of our investigations.

1. Introduction

The properties of ultra-thin magnetic thin films have been the subject of study for sometime, but new experimental techniques to create and probe such systems has intensified the efforts of researchers to understand these systems in recent years [1–3]. Among the more interesting properties is the existence of stripe phases. These phases are the result of the competition between short-range exchange interactions and long-range, dipole–dipole interactions. Such pattern formation is of great interest as the foundations of future potential magnetic storage devices are based in part on the properties of such materials [4]. However, the phenomena is much more general and similar patterns have been observed in such diverse systems as Langmuir monolayers, diblock co-polymers, and type 1 superconductors [5]. More recently similar competition between long-range, dipole–dipole and short-range interactions has been seen in model systems as an essential control mechanism in the self-assembly process for nano-structures [6].

The static, equilibrium properties of ultra-thin magnetic films have been well studied experimentally [2] and the dipolar Ising model has been considered extensively in efforts to explain these properties [7]. However, a better understanding of the stability and dynamics of the domain structures in these materials is still needed and is highly desirable given that they determine many of the technologically important properties of these materials. It is widely known that the static and dynamic properties of a material can sometimes be determined by clusters or domains within the material. Such is the case the 2D Ising model with short-range interactions only [8], where the explicit connection between the geometric clusters of spins in the same state to the physical clusters which are characteristic of the critical phenomena in the system, has been formally established [9,10]. This connection has been exploited to gain a better understanding of the dynamics of the short range interaction Ising spin system, the nature of the phase transition, and also to develop acceleration algorithms for Monte Carlo simulations, which have greatly expanded the utility of the model [11,12]. A similar connection has yet to be established for the dipolar Ising model. Given the potential utility of the dipolar Ising model, and given the very slow dynamics that have observed in simulations to date, such a connection and the development of acceleration algorithms would be quite useful. The methods and results presented in this work are an initial step toward the development of such an algorithm and at the same time provide insight in to the dynamics of the dipolar Ising model itself.

1.1. The dipolar Ising model

The Hamiltonian for the dipolar Ising model in reduced units can be written as

$$\mathscr{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j + g\sum_{i,j}\sigma_i\Gamma_{ij}\sigma_j + H\sum_i\sigma_i, \qquad (1)$$

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where $\langle i,j\rangle$ in the first term indicates a sum over all pairs of nearest neighbor spins i,j, $\sigma_i = \pm 1$ is the magnetic moment at site i and J is the strength of the exchange interaction. The second term is a long-range dipole–dipole interaction of strength g and the sum is over all pairs of spins. The final term treats the interaction with an applied field, H, which we do not consider in this work. The system is assumed to be infinite, but restricted to states which are periodic. Periodic boundary conditions are therefore used to treat the exchange interaction and Ewald sums are used to account for the long-range nature of the dipolar interaction. The exact form of Γ_{ij} and other details related to the Ewald summation are as given by Ref. [13]. In this paper we assume the spins are perpendicular to the plane of the film.

1.2. Previous work

The equilibrium properties of dipolar Ising model have been studied extensively and a review of this work can be found in De'Bell et al. [7] and the works cited therein. In the work presented here the ratio of J to g has been fixed at $J/g = 8.9$, which has been shown previously to lead to an ordered ground state, in a monolayer, of stripes of width eight spins parallel to a lattice axis [14]. The nature of this transition is still the subject of some debate, much of which centers on the characteristics of the equilibrium phase just above the critical temperature and the comparison to experimental results.

In contrast the non-equilibrium dynamics of the dipolar Ising model have not been so extensively considered. The earliest work considered the relaxation of the magnetization from the saturated magnetic state, $(\{\sigma_i\} = 1)$, after a quench toward equilibrium at a temperature below T_c. Sampaio et al. [15] found that depending on the relative strengths of the dipolar and exchange interactions, one can have either exponential or power-law relaxation. The time frame considered was very short, typically on the order of 5000 Monte Carlo steps (MCS) at most, and the relative strength of the interactions was such that the stripe width in the ground state was limited to at most four spins. Rappoport et al. [16] reported similar results on larger lattices, but with a truncated dipolar interaction.

The phenomena of aging in the dipolar Ising model was considered in a number of articles, all of which considered small stripes of width one or two spins. By measuring the spin auto-correlation function,

$$C(t,t_w) = \frac{1}{N}\sum_i \langle \sigma_i(t+t_w)\sigma_i(t_w)\rangle, \tag{2}$$

Toloza et al. [17] were able to observe aging, the nature of which was dependent on the relative strength of the interactions. Stariolo and Cannas [18] expanded upon this earlier work to show how $C(t,t_w)$ crosses over from logarithmic decay to algebraic decay as the ground state stripe width increases. Gleiser et al. [19] and Gleiser and Montemurro [20] measured the time evolution of the domain size of stripes of width one and two spins and hypothesized that the differences in the nature of the dynamics was related to the existence of metastable states. All of these studies were concerned with short to intermediate time scales (up to $t = 10^6$) and only for the case of small stripe widths.

Bromley and his co-authors [21,22] considered the dynamics of systems with a larger stripe width (eight spins) during a quench from the saturated magnetic state toward equilibrium near the critical temperature. They were able to establish the existence and character of three relaxation regimes. They considered results from simulations on the order of at most 1,000,000 MCS, to develop a general understanding of the relaxation in their system in each of three regimes that they identified. At very early times they found that the dynamics of the system was characterized by the nucleation of small islands, where the spins are oriented in the direction opposite to the initial saturation direction. As these small islands grew the net magnetization approached zero. In the second regime there remained a small remnant magnetization. This remnant magnetization decays at a rate which is much slower than that in the first regime. In the final regime, at late times, they found that the islands become elongated and arranged into regions which manifest the stripe pattern of the expected equilibrium phase. However, these local regions did not yet share a common orientation and hence the system was not completely in the smectic phase. To support this conjecture, they provided three snapshots of an extended simulation that showed single spin configurations at times $t = 300{,}000$, $600{,}000$ and $900{,}000$, where by hand they determined the regions of local smectic ordering. Their results were consistent with those of Desai and Roland and Sagui and Desai who had conducted similar studies using Langevin dynamics for a model with a continuous uniaxial "spin" variable, with an additional significant difference being the use of open boundaries [23,24].

Mu and Ma [25] considered a dipolar model system under going a quench from a random state. They discussed qualitatively the early stages of the relaxation to equilibrium, and felt that the depth of the quench fundamentally changed the nature of the relation process. Their simulations were run for times on the order of 100,000 MCS for stripes of various width from approximately one to nine spins. For a deep quench they claimed that the labyrinth structure they observed became frozen due to the frustration induced by the competition between the short- and long-range interactions.

It is the late stage relaxation identified by Bromley and Mu and Ma, but which was not considered in depth due to computer time constraints, that we wish to address in this article. We also wish to consider ground state stripes of the size treated by Bromley and by Mu and Ma, rather than the very small stripes considered in the other works discussed above. We have extended the length of simulation by at least a factor of 10 compared to previous studies, and have recorded the spin configurations every 1000 MCS [26]. Our simulations have a run length of between 2 million and 14 million Monte Carlo time steps, depending on the temperature of the simulation. The longest of our simulations required over 30 days to run using a 4 way parallel code on 4 CPUs. Thus this single simulation required 120 days of CPU time. Because of this huge computational demand we have only considered a few temperatures and conducted two sets of simulations at each temperature. However, even this small number of simulations required over 4 years of CPU time.

While we will be drawing analogies between the standard 2D Ising model and the dipolar Ising model, one must remember that unlike the standard 2D Ising model, the ordering observed in the dipolar Ising model is a mesoscopic ordering of the stripes and not a microscopic ordering of the spins themselves. Therefore one must be cautious about characterizing the transition in terms of spin properties rather than in terms of properties of the stripes. For stripes of small width this can be a serious concern as the spins fluctuations and the stripe fluctuations can occur on similar length scales. For example, if one were to consider a system with stripes of width $h = 2$, a spin flip would be equivalent to half the width of a stripe and even in the ground state of the system 100% of the spins would lie on a stripe boundary. If instead one where to consider a system with a ground state of stripes of width $h = 8$ (or greater), then only 25% of spins lie on a boundary in the ground state and a single spin flip is no longer comparable to the excitation required to disorder the mesoscopic stripe order. This is also important as the smallest of ground state stripe widths seen experimentally is still quite large, typically on the order of