Temperature-Induced Domain Shrinking in Ising Ferromagnets Frustrated by a Long-Range Interaction

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Abstract. We investigate a spin model in which a ferromagnetic short-range interaction competes with a long-range antiferromagnetic interaction decaying spatially as $\frac{1}{r^{d+\sigma}}$, d being the dimensionality of the lattice. For σ smaller than a certain threshold $\hat{\sigma}$ (with $\hat{\sigma} > 1$), the long-range interaction is able to prevent global phase separation, the uniformly magnetized state favored by the exchange interaction for spin systems. The ground state then consists of a mono-dimensional modulation of the order parameter resulting in a superlattice of domains with positive and negative magnetization. We find that the period of modulation shrinks with increasing temperature T and suggest that this is a universal property of the considered model. For $d = 2$ and $\sigma = 1$ (dipolar interaction) Mean-Field (MF) calculations find a striking agreement with experiments performed on atomically-thin Fe/Cu(001) films. Monte Carlo (MC) results for $d = 1$ also support the generality of our arguments beyond the MF approach.

Keywords: frustrated systems, modulated systems, long-range interactions, competing interactions, Ising model.

The competition between a short-ranged interaction favoring a uniformly *charged* state and a long-range interaction preventing its realization on larger spatial scales is often assumed to be the mechanism underlying pattern formation in chemistry, biology and physics as well as opinion cluster emergence in social networks. A minimal spin model in which the ferromagnetic nearest-neighbor exchange interaction, J, competes with a long-range antiferromagnetic interaction of strength g may hopefully contain enough complexity to be paradigmatic for a variety of realistic systems. For $\sigma \leq \hat{\sigma}$ (see next Sect.), the lowest energy configuration – which is indeed realized at $T = 0$ – is given by a succession of domains with saturated positive and negative magnetization, which alternate in a sharp mono-dimensional modulation of period $2h_{gs}$. At finite T, the spins located at the interface between two oppositely magnetized domains are significantly more susceptible to thermal fluctuations than spins in the interior of the domains. As a result, the balance between the ferromagnetic exchange and the antiferromagnetic long-range interaction is biased in favor of the latter, which finally makes the modulation period shrink as T is increased.

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Ground-State Properties. The spin Hamiltonian we consider is

$$\mathcal{H} = -J \sum_{\langle \underline{i},\underline{j} \rangle} \sigma_{\underline{i}} \sigma_{\underline{j}} + \frac{g}{2} \sum_{\{\underline{i} \neq \underline{j}\}} \frac{\sigma_{\underline{i}} \sigma_{\underline{j}}}{|\underline{r}_{ij}|^{d+\sigma}}, \tag{1}$$

where $\sigma_{\underline{i}} = \pm 1$ (Ising variables), J and g are positive constants, $\langle \underline{i}, \underline{j} \rangle$ and $\{\underline{i} \neq \underline{j}\}$ indicate that the sum is extended either to nearest neighbors only or to all the couples respectively. The site indices have to be thought of as integer coordinates locating a spin in a lattice of any dimension, e.g. $\underline{i} \equiv (i_x, i_y, i_z)$ if $d = 3$; equivalently $\underline{r}_{ij} = \underline{i} - \underline{j}$. When $g = 0$, the uniform state has the lowest energy. If $g \neq 0$, the creation of one domain wall in the uniform state causes an increase of the exchange energy of $2J$ and a net decrease of the long-range interaction energy ΔE_{LR}. The scaling of ΔE_{LR} with the number of spins in the lattice N can be easily estimated in the continuum limit. For $d = 1$, integrating over the sites on the left- (dx) and right-hand (dx') side of the domain wall yields

$$\Delta E_{LR} \sim \frac{1}{r^{\sigma+d}} \overset{\int dx}{\Rightarrow} \frac{1}{r^{\sigma+d-1}} \overset{\int dx'}{\Rightarrow} \frac{1}{r^{\sigma+d-2}}.$$

This estimation can be generalized to any lattice dimension to get

$$\Delta E_{LR} \sim \left[\frac{1}{r^{\sigma-1}} \right]_1^N \underset{N\to\infty}{\sim} \begin{cases} \infty & \text{for } \sigma \leq 1 \Rightarrow \text{domain ground state} \\ < \infty & \text{for } \sigma > 1 \Rightarrow \text{domain/uniform ground state.} \end{cases}$$

When $\Delta E_{LR} \to \infty$ (in the thermodynamic limit $N \to \infty$), the system prefers to split into domains and the ground state turns out to have a mono-dimensionally modulated structure [1,2]. The half-period of modulation h_{gs} depends on the ratio $\frac{J}{g}$. For $\sigma > 1$ a more detailed analysis is required to define the threshold $\hat{\sigma}$ which separates the uniform- from the patterned-ground-state phase[1]. We represent [6] the ground-state configuration in the regime $\sigma \leq \hat{\sigma}$ with a square-wave profile of period $2h$ modulated along the x direction $\sigma_{\underline{j}} = \mathrm{Sq}(k_0 j_x) = \sum_{m \geq 0} a_m \sin(k_m j_x)$ (with $k_0 = \frac{\pi}{h}$, $k_m = (2m+1)k_0$ and $a_m = \frac{4}{\pi} \frac{1}{2m+1}$). Exploiting the orthogonality relation $\sum_{j_x=1}^{N_x} e^{-i(k-k')j_x} = N_x \delta_{k,k'}$ (with $j_x + N_x = j_x$), two-point correlations at $T = 0$ can be computed by averaging over the site variables $\underline{j}$ ($\langle \ldots \rangle_j$ henceforth)

$$\langle \sigma_{\underline{j}+\underline{r}} \sigma_{\underline{j}} \rangle_j = \frac{1}{N_x} \sum_{j_x} \mathrm{Sq}(k_0(j_x + r_x)) \mathrm{Sq}(k_0 j_x) = \frac{1}{2} \sum_{m \geq 0} a_m^2 \cos(k_m r_x). \tag{2}$$

The form of Eq. (2) suggests the observation of a peak in the structure factor located at every odd higher-harmonic of $k_0 = \frac{\pi}{h}$ at sufficiently low temperatures. This is actually observed in MC simulations performed for $d = 1$ [6], in spite of the fact that no long-range order is expected to occur at any $T \neq 0$ [1]. Eq. (2) allows writing the energy per spin for a square-wave profile

[1] For $\sigma > 1$, $\hat{\sigma}$ depends on the ratio $\frac{J}{g}$. In $d = 1$, a straightforward discrete-lattice calculation gives a closed equation involving the Riemann zeta function: $\zeta(\hat{\sigma}) = \frac{J}{g}$ [6].

$$\mathcal{E}_h = 2J\frac{1}{h} + \frac{g}{2}\sum_{m\geq 0} a_m^2 \sum_{r_\nu}\sum_{r_x\geq 1}\frac{\cos\left(k_m r_x\right)}{|\underline{r}|^{d+\sigma}} = 2J\frac{1}{h} + \sum_{m\geq 0} a_m^2 f_\sigma(k_m); \qquad (3)$$

the exchange contribution comes just from counting the number of domain walls, $\frac{N_x}{h}$, while the sum $\sum_{r_\nu}$ is performed over $d-1$ integer variables according to the lattice dimension. The whole energy (3) depends parametrically on the half-period of modulation, h, so that the ground-state is found by minimizing it with respect to this variable to obtain h_{gs} [1,2,6].

MF Approach and Experiments. An experimental counterpart of our model (1) with $d = 2$ and $\sigma = 1$ is represented by ultrathin Fe films grown epitaxially on Cu(001) [3]. For these specific d and σ, the ground state is expected to be a striped pattern [2]. In the experimental system such a magnetic-domain pattern is indeed encountered together with a variety of different ones [3]. Throughout all these patterns a significant domain width reduction is observed as T is increased [4]. Fig. 1a shows how this experimental fact is well reproduced by a MF treatment of Hamiltonian (1) [5]. In the shadowed region slow-dynamics effects become important so that the equilibrium-thermodynamic description does not apply anymore. In Fig. 1b a typical MF magnetization profile inside a single stripe domain is reported for different T. Apart from $T \sim 0$, the average magnetization of the domain-wall spins (full triangles), is systematically lower than that of inside-domain spins. Consequently, the creation of new domain walls "costs" less and less as T is increased: the balance between exchange and long-range interaction is thus biased with respect to what happens at $T = 0$ and domains with smaller equilibrium size are ultimately favored.

Elastic Model. To the aim of recovering the same phenomenology as with the MF approach but with an alternative treatment of thermal fluctuations, let us consider first the effect of a perturbative displacement field along x, u_{j_x}, of the whole square-wave profile:

$$\sigma_j = \mathrm{Sq}\left(k_0(j+u_j)\right) = \sum_{m\geq 0} a_m \sin\left(k_m(j+u_j)\right). \qquad (4)$$

After some algebra [6] and recalling the definition of $f_\sigma(k_m)$ (3), the perturbed energy can be written as

$$\Delta\mathcal{E}_h = \frac{1}{N}\sum_q\sum_{m\geq 0}\left\{a_m^2 k_m^2\left[\frac{1}{2}f_\sigma(k_m-q) + \frac{1}{2}f_\sigma(k_m+q) - f_\sigma(k_m)\right]|\tilde{u}_q|^2\right\}, (5)$$

where $\tilde{u}_q$ is the Fourier transform of the displacement field. As far as the large-distance behavior is concerned, Eq. (5) can be expanded for $q \ll k_0$:

$$\Delta\mathcal{E}_h = \frac{1}{N}\sum_q\left[\frac{1}{2}k_0^2\frac{\partial^2\mathcal{E}_h}{\partial k_0^2}q^2|\tilde{u}_q|^2\right]. \qquad (6)$$

Eq. (6) is formally equivalent to a Planar Degenerate System Hamiltonian. For such systems and $d = 1$ the correlation length is expected to behave like $\xi \sim \frac{1}{T}$, which is in good agreement with our MC results [6]. Even in the absence of

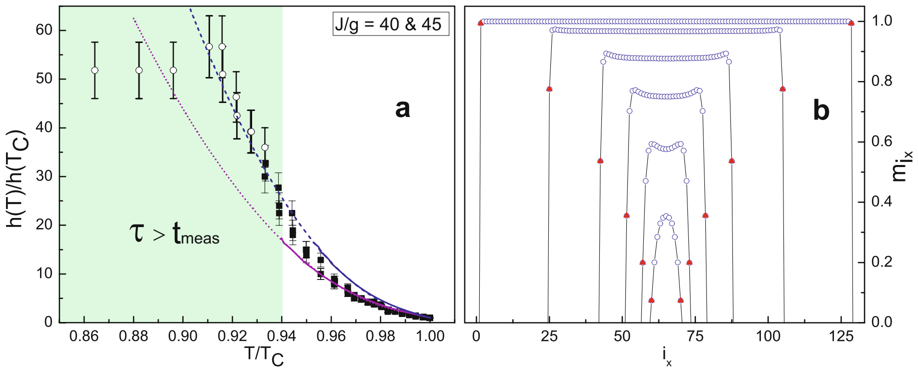

Fig. 1. a) Relative domain width variation as a function of the reduced temperature, T_C being the Curie temperature. Experimental points correspond to labyrinthine (open circles) and striped (full square) patterns. Lines correspond to MF calculations with $d = 2$ and $\sigma = 1$ performed for $\frac{J}{g} = 40$ (violet) and $\frac{J}{g} = 45$ (blue): exact (solid), parabolic extrapolation (dotted). In the shadowed region the relaxation time – estimated independently – becomes larger than the characteristic time of the measurements. **b)** MF magnetization profile inside a striped domain. The average magnetization on each site m_{i_x} is plotted *versus* the site index i_x itself.

long-range order, a characteristic length scale is preserved at finite temperatures in the form of the modulation period of the two-point correlation function. In the limit $T \to 0$, this period approaches h_{gs} continuously from below so that it can be considered the $d = 1$ counterpart of the temperature-dependent domain width in ultrathin Fe/Cu(001) films [4,5].

Justifying – in the framework of the elastic model – the decrease of the modulation period with the increase of T independently of the lattice dimensionality d and of the occurrence of long-range order is a goal for future work.

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