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Non-equilibrium critical behavior of Heisenberg thin films

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Abstract.
In this work we study the non-equilibrium properties of Heisenberg ferromagnetic films using Monte Carlo simulations by short-time dynamic method. By exploring the short-time scaling dynamics, we have found thickness dependency of critical exponents z, θ' and β/ν for ferromagnetic thin film. For calculating the critical exponents of ferromagnetic films we considered systems with linear size $L = 128$ and layers number $N = 2$; 4; 6; 10. Starting from initial configurations, the system was updated with Metropolis algorithm at the critical temperatures

1 Introduction

It is well known now the fundamental role of competing interactions in the emerging features of low-dimensional systems. Among a wide number of numerical and theoretical investigations on equilibrium and dynamical properties of several model Hamiltonian of low-dimensional magnets, Heisenberg-like models are one of the most widely used to approach real magnetic materials. In fact, anisotropic versions of the Heisenberg model describe several compounds as K_2NiF_4 [1], $BaCo_2(AsO_4)_2$ [2], $CoCl_2$ – GIC [3] and Rb_2CrCl_4 [4].

Magnetic order in thin ferromagnetic films is very complex due to a strong influence of the shape and the magnetocrystalline anisotropies of the sample. In the past decade, a considerable amount of experimental results on different aspects of magnetism in ultrathin films has appeared [5]. Nevertheless it is difficult to reach general conclusions even in seemingly basic things such as the kind of magnetic order at low temperatures. In view of this complexity, theoretical work on simplified models and computer simulations are essential for rationalizing and guiding new experimental work.

In the vicinity of the critical temperature T_c, the thermodynamic observables associated with statistical models display universal characteristics, which may be parametrized in terms of critical exponents. These quantity tend to zero or infinity at the transition and depend only on the spatial dimensionality of the system, the range of the interactions and the number of components of the order parameter.

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2 Model and Methods

We have performed Monte Carlo simulations of macroscopic spin system with crystalline structure of ultrathin film which is described by anisotropic Heisenberg model [6] with Hamiltonian:

$$H = -J \sum_{i,j}^{N_s} \left[(1 - \Delta(N)) \left(S_i^x S_j^x + S_i^y S_j^y \right) + S_i^z S_j^z \right], \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is a unit vector in the direction of the classical magnetic moment at lattice site i; the sum is extended over nearest-neighbor pairs on the cubic lattice; $J > 0$ – ferromagnetic exchange constant; $N_s = L \times L \times N$ – size of film; Δ characterizes the amount of anisotropy; $\Delta = 0$ corresponds to the isotropic Heisenberg case; $\Delta = 1$ – the Ising case. Periodic and free boundary conditions are used for the in-plane and out-plane directions, respectively.

The effective anisotropy constant $\Delta(N)$ as a function of film thickness N was chosen from experimental studies of the Curie temperature T_C for thin films of $Ni(111)/W(110)$ [7] with different thicknesses of Ni film. It was proposed that Δ is proportional to the critical temperature for different film thicknesses. In approximation procedure it was used fact that Ni films with large number of layers demonstrate bulk critical properties of 3D isotropic Heisenberg magnets [8, 9]. The effective anisotropy constant $\Delta(N)$ as a function of film thickness N presented on figure 1.

According to the argument of Janssen et al. [10] obtained with the RG method and ε-expansion, one may anticipate a generalized scaling relation for the k-th moment of the magnetization

$$m^{(k)}(t, \tau, L, m_0) = b^{-k\beta/\nu} m^{(k)}(t/b^z, b^{1/\nu}\tau, L/b, b^{x_0} m_0). \quad (2)$$

And it is realized after a time scale $t_{\rm mic}$ which is large enough in a microscopic sense but still very small in a

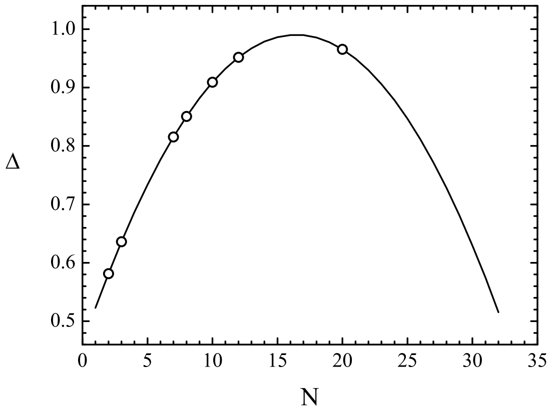

Figure 1. Anisotropy constant $\Delta(N)$ as a function of film thickness N

macroscopic sense. In (2) b is a spatial rescaling factor, β and ν are static critical exponents, z is the dynamic exponent, the new independent exponent x_0 is the scaling dimension of the initial magnetization m_0 and $\tau = (T - T_c)/T_c$ is the reduced temperature.

Since the system is in the early stage of the evolution the correlation length is still small and finite size problems are nearly absent. Therefore, we generally consider L large enough ($L = 128$) and skip this argument.

When system evolving from high-temperature state ($m_0 \ll 1$) we can choose the scaling factor $b = t^{1/z}$ and applying the scaling form (2) for $k = 1$ to the small quantity $t^{x_0/z}m_0$, one obtains

$$\begin{aligned} m(t,\tau,m_0) &\sim m_0 t^{\theta'} m(t^{1/\nu z}\tau, t^{x_0/z}m_0) = \\ &= m_0 t^{\theta'}(1 + a t^{1/\nu z}\tau) + O(\tau^2, m_0^2) \end{aligned} \quad (3)$$

where $\theta' = (x_0 - \beta/\nu)/z$ has been introduced. For $\tau = 0$ and small enough t and m_0, the scaling dependence for magnetization (3) takes the form $m(t) \sim m_0 t^{\theta'}$. For almost all statistical systems studied so far, the exponent θ' is positive. Time scale for this initial increase of magnetization is $t_0 \sim m_0^{-z/x_0}$. The increasing of the magnetization $m(t)$ from a high-temperature initial magnetization $m_0 \ll 1$ at short-time regime $t < t_{cr} \lesssim m_0^{-1/(\theta'+\beta/\nu z)}$ have the form $m(t) \sim t^{\theta'}$.

As the spatial correlation length in the beginning of the time evolution is small, for a finite system of dimension d with lattice size L the second moment $m^{(2)}(t, L) \sim L^d$. Combining this with the result of the scaling form in (3) for $\tau = 0$ and $b = t^{1/z}$, one obtains

$$m^{(2)}(t) \sim t^{-2\beta/\nu z} m^{(2)}(1, t^{-1/z}L) \sim t^{c_2}, \quad (4)$$

where $c_2 = (d - 2\beta/\nu)/z$. Until now, a completely disordered initial state has been considered as starting point, i.e., a state of very high temperature. The question arises how a completely ordered initial state evolves, when heated up suddenly to the critical temperature. In the scaling form (3), one can skip besides L, also the argument $m_0 = 1$,

$$m^{(k)}(t,\tau) = b^{-k\beta/\nu} m^{(k)}(b^{-z}t, b^{1/\nu}\tau). \quad (5)$$

The system is simulated numerically by starting with a completely ordered state, whose evaluation is measured at or near the critical temperature. The quantities measured are $m(t)$ and $m^{(2)}(t)$. With $b = t^{1/z}$, one avoids the main t dependence in $m^{(k)}(t)$ and for $k = 1$ one has

$$\begin{aligned} m(t,\tau) &= t^{-\beta/\nu z} m(1, t^{1/\nu z}\tau) = \\ &= t^{-\beta/\nu z}(1 + a t^{1/\nu z} + O(\tau^2)). \end{aligned} \quad (6)$$

In order to calculate the critical exponent z we have used the ratio $F_2(t) = m^{(2)}(t)|_{m_0=0}/m^2(t)|_{m_0=1} \sim t^{d/z}$ [11].

3 Results of Monte Carlo modeling

For calculating the critical exponents β/ν, z and θ' of ferromagnetic films we considered systems with linear size $L = 128$ and layers number $N = 2; 4; 6; 10$.

For ferromagnetic films the order parameter can be defined as magnetization

$$m^{(k)}(t) = \left\langle \left(\frac{1}{N_s} \left| \sum_{i=1}^{N_s} S_i(t) \right| \right)^k \right\rangle, \quad (7)$$

where angle brackets denote the statistical averaging. We have studied evolution of thin film both from high-temperature ($m_0 = 0.0001 \ll 1$) and from low-temperature ($m_0 = 1$) initial states. Starting from initial configurations, the system was updated with Metropolis algorithm at the critical temperatures $T_c = 1.03(8)$ for $N = 2$, $T_c = 1.25(5)$ for $N = 4$, $T_c = 1.35(4)$ for $N = 6$, $T_c = 1.57(8)$ for $N = 10$ [12, 13]. Simulations have been performed up to $t = 10000$ MCS/s. One would like to mention that measurements starting from a low-temperature initial state ($m_0 = 1$) are more favorable, since they are much less affected by fluctuations, because the quantities measured are rather big in contrast to those from a random start with zero or small initial magnetization ($m_0 \ll 1$).

In order to estimate values of critical exponents z, θ' and β/ν, we have measured the time evolution of the magnetization $m(t)$, the second moment $m^{(2)}(t)$ (figure 2*a*) from high-temperature and low-temperature initial states and autocorrelation function (figure 2*b*)

$$A(t) = \left\langle 1/N_s \sum_{i=1}^{N_s} S_i(t) S_i(0) \right\rangle - m(t)m(0) \sim t^{-c_a}, \quad (8)$$

where $c_a = d/z - \theta'$. In figure 3*a* the magnetization is plotted for a high-temperature initial state and a low-temperature initial state for different layer number $N = 2, 4, 6, 10$. It allowed to calculate the time-dependent cumulant $F_2(t)$ (figure 3*b*).

From slope of magnetization at high-temperature initial state on $t \in [710; 1800]$ we can estimate the value of critical non-equilibrium exponent θ'. The time interval $[t_{\text{left}}; 1800]$ for $t_{\text{left}} = 710$ gives the minimum of errors for exponent θ' for film thickness $N = 2, 4, 6, 10$ (figure 3*a*).

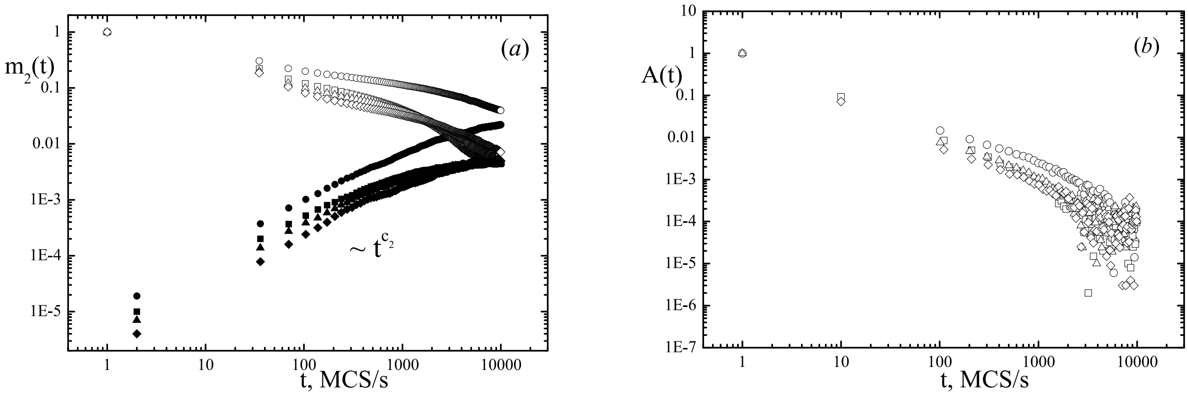

Figure 2. Time dependencies of second moment of magnetization $m^{(2)}(t)$ (*a*) for different initial state and autocorrelation function $A(t)$ (*b*) for film with $N = 2$ (○), $N = 4$ (□), $N = 6$ (△), $N = 10$ (◇)

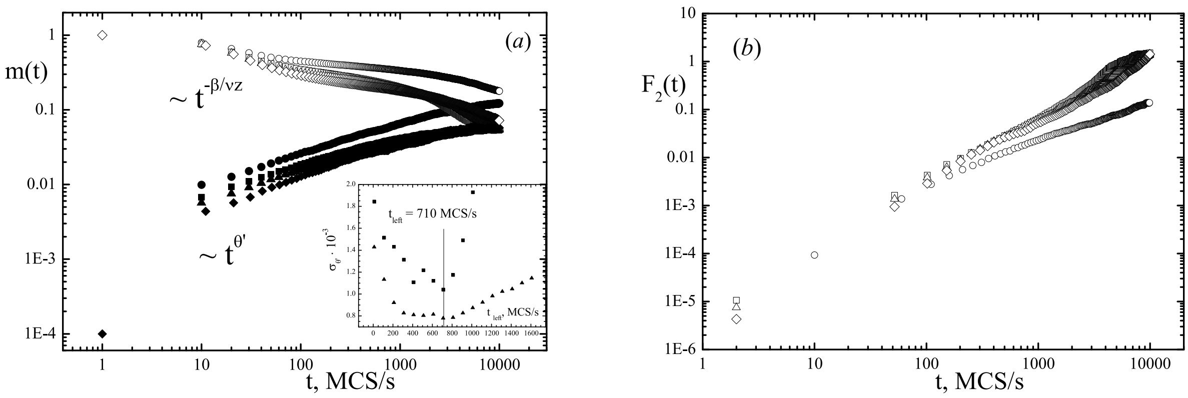

Figure 3. Time dependencies of magnetization $m(t)$ (*a*) for different initial state and cumulant $F_2(t)$ (*b*) for film with $N = 2$ (○), $N = 4$ (□), $N = 6$ (△), $N = 10$ (◇)

From the slope of time dependence of the cumulant $F_2(t)$ we can estimate the value of critical exponent d/z. Using the hyperscaling relation $\gamma/\nu + 2\beta/\nu = d$, the effective dimension of the system d_{eff} can be obtained [13]. This effective dimension $d_{\text{eff}} = 2.048$ for $N = 2$, $d_{\text{eff}} = 1.993$ for $N = 4$, $d_{\text{eff}} = 2.200$ for $N = 6$ and $d_{\text{eff}} = 2.199$ for $N = 10$ we use to estimate critical exponents z.

4 Conclusion

The dimensionality aspects of magnetic and structural phase transitions represent one of the key problems of ultrathin film [14, 15]. For magnetic systems, the spin dimensionality as well as the spatial extension determines the universality class, giving rise to a great number of ordering phenomena on different length scales. Furthermore, there are transition regions not represented by any universality class with corresponding critical exponents, but representing something in between. For example, the dependence of the critical exponents of thin magnetic films with thickness exhibit such a transition, in which the exponents are continuously changes with increasing film thickness of the layers, from two-dimensional (2D) Ising ($\beta = 0.125$) to three-dimensional (3D) Heisenberg ($\beta = 0.364$) [16] behaviour. The crossover from 2D to 3D critical exponents has been observed in thin films of Ni on W(110) [7] and of Co on Cu(111) [8] as their thickness is increased. Thus, studying the dimensional crossover of a system as its thickness is increased often provides a significant degree of insight.

In this paper we present result of Monte Carlo simulation of non-equilibrium critical behavior of Heisenberg thin film. We obtain values of $z = 2.187(16)$ for $N = 2$, $z = 2.197(33)$ for $N = 4$, $z = 2.300(26)$ for $N = 6$, $z = 2.108(21)$ for $N = 10$ and $\theta' = 0.248(5)$ for $N = 2$, $\theta' = 0.238(10)$ for $N = 4$, $\theta' = 0.225(8)$ for $N = 6$, $\theta' = 0.198(7)$ for $N = 10$. Comparing the calculated values z for $N = 2, 4$ with the results for 2D Ising model in various works $z = 0.191(1)$ [17], $z = 2.0842(39)$ [18], $z = 2.166(7)$ [19], $z = 2.1667(5)$ [20], $z = 2.14(2)$ [21],

$z = 2.12(6)$ [22] we see the very good agreement among them, i.e. thin ferromagnetic films belong to universality class non-equilibrium behaviour of 2D Ising model. Value of critical exponents $z = 2.300(26)$ for $N = 6$ and $z = 2.108(21)$ for $N = 10$ demonstrate the dimensional crossover to characteristic values for critical behavior of the 3D model.

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