Violation of the fluctuation-dissipation theorem in a two-dimensional Ising model with dipolar interactions

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The violation of the fluctuation-dissipation theorem (FDT) in a two-dimensional Ising model with both ferromagnetic exchange and antiferromagnetic dipolar interactions is established and investigated via Monte Carlo simulations. Through the computation of the autocorrelation $C(t+t_w,t_w)$ and the integrated response (susceptibility) functions we obtain the FDT violation factor $X(t+t_w,t_w)$ for different values of the temperature, the waiting time t_w and the quotient $\delta=J_0/J_d$, J_0 and J_d being the strength of exchange and dipolar interactions, respectively. For positive values of δ this system develops a striped phase at low temperatures, in which the nonequilibrium dynamics presents two different regimes according to the value of δ. In each regime $C(t+t_w,t_w)$ displays different scaling laws. Our results show that such different regimes are not reflected in the FDT violation factor, where X goes always to zero for high values of t_w in the aging regime, a result that appears in domain growth processes in nonfrustrated ordered systems.

The competition between long-range antiferromagnetic dipolar interactions and short-range ferromagnetic exchange interactions can give rise to a variety of unusual and interesting macroscopic phenomena. Recent 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.[1,2] and nonequilibrium dynamical properties.[3] Moreover, recent results have shown some similarities between the nonequilibrium dynamical properties of these kinds of ordered systems and that of glassy systems.[4]

Magnetization processes in these kinds of systems are of interest due to aspects related to information storage in ultrathin ferromagnetic films. For instance, the magnetization size unit and its thermal stability are of great importance for magneto-optical recording performance. These factors depend on the pattern and dynamics of the magnetic domains (see Ref. 3 and references therein). There are also several contexts in which a short-ranged tendency to order is perturbated by a long-range frustrating interaction. Among others, model systems of this type have been proposed to study avoided phase transitions in supercooled liquids[5] and charge-density waves in doped antiferromagnets.[6–8]

The above-mentioned systems can be described by an Ising-like Hamiltonian of the type

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

where the spin variable $\sigma_i=\pm1$ is located at the site i of a square lattice, the sum $\Sigma_{\langle i,j\rangle}$ runs over all pairs of nearest-neighbor sites, and the sum $\Sigma_{(i,j)}$ runs over all distinct pairs of sites of the lattice; r_{ij} is the distance (in crystal units) between sites i and j; δ represents the ratio between the exchange J_0 and dipolar J_d coupling parameters, where the energy is mesured in units of J_d, which is assumed always antiferromagnetic $(J_d>0)$. Hence, $\delta>0$ means the ferromagnetic exchange copling.

There are few numerical results concerning the equilibrium statistical mechanics, i.e., the finite-temperature phase diagram of this model. MacIsaac and co-workers[2] have shown that the ground state of Hamiltonian (1) is the antiferromagnetic state for $\delta<0.85$. For $\delta>0.85$ the antiferromagnetic state becomes unstable with respect to the formation of striped domain structures, that is, to state configurations with spins aligned along a particular axis forming a ferromagnetic strip of constant width h, so that spins in adjacent strips are antialigned, forming a super lattice in the direction perpendicular to the strips. They also showed that striped states of increasingly higher thickness h become more stable as δ increases from $\delta=0.85$. Moreover, they showed that the striped states are also more stable than the ferromagnetic one for arbitrary large values of δ, suggesting such a phase to be the ground state of the model for $\delta>0.85$. Monte Carlo calculations on finite lattices at low temperature[2,3] gave further support to this proposal, at least for intermediate values of δ. Furthermore, such simulations have shown that striped phases of increasingly higher values of h may become thermodynamically stable at *finite* temperatures for intermediate values of δ. This results are in agreement with other analytic results.[1,6] For small values of δ the system presents an antiferromagnetic phase at low temperatures. At high temperatures, of course, the system becomes paramagnetic.

The dynamics of the model in the striped region is characterized by the formation and growth of magnetic domains, dominated by the competition between the exchange and the dipolar interactions. Monte Carlo studies of the dynamics at low temperatures have shown the existence of two different dynamical regimes, according to the value of δ. First, for $\delta > \delta_c \sim 2.7$ the magnetization relaxes exponentially,[3] with a relaxation time that depends both on the temperature and δ. For $\delta < \delta_c$ the magnetization presents a power-law decay, with an exponent independent of δ. Second, strong hysteresis effects appear[3,4] for $\delta > \delta_c$, which are almost absent for $\delta < \delta_c$. Finally, different types of aging behaviors have been observed in both regimes.[4]

Aging effects, that is, history dependence in the time evolution of correlations and response functions after the system has been quenched into some nonequilibrium state, appear in a variety of ordered and disordered systems which are essentially out of equilibrium on experimental time scales.[9] Aging can be observed in real systems through different experiments. A typical example is the zero-field-cooling[10] experiment, in which the sample is cooled in zero field to a subcritical temperature at time t_0. After a waiting time t_w a small constant magnetic field is applied and subsequently the time evolution of the magnetization is recorded. It is then observed that the longer the waiting time t_w the slower the relaxation.

Although aging can be detected through several time-dependent quantities, a straightforward way to establish it in a numerical simulation is to calculate the spin autocorrelation function

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

where $\langle \cdots \rangle$ means an average over different realizations of the thermal noise and t_w is the waiting time, measured from some quenching time $t_0=0$.

A second quantity of interest is the conjugated response function to an external magnetic field $h_i(t)$:

$$R(t+t_w,t_w)=\frac{1}{N}\sum_i \frac{\partial\langle \sigma_i(t+t_w)\rangle}{\partial h_i(t_w)}. \tag{3}$$

In a variety of disordered systems and also in some domain growth processes in ordered ones $C(t+t_w,t_w)$ and $R(t+t_w,t_w)$ are found to satisfy the generalized fluctuation-dissipation relation proposed by Cugliandolo and Kurchan:[11]

$$R(t+t_w,t_w)=\frac{X(t+t_w,t_w)}{T}\frac{\partial C(t+t_w,t_w)}{\partial t_w}. \tag{4}$$

At equilibrium $C(t+t_w,t_w)$ and $R(t+t_w,t_w)$ satisfy time translational invariance (TTI), the functions depend only on the times difference t, and $X(t+t_w,t_w)=1$, that is, Eq. (4) reduces to the usual fluctuation-disspation theorem (FDT). Out of equilibrium such properties are not expected to hold depending on the observation time scales. The following scenario has been proposed in the context of spin glasses:[11] for small values of $t(t/t_w \ll 1)$ the system is in quasiequilibrium and equilibrium properties hold; in the aging regime $t/t_w \gg 1$ both TTI and FDT do not hold, i.e., $C(t+t_w,t_w)$ depends explicitly on t and t_w and $X(t+t_w,t_w)\neq 1$. Moreover, for large values of t_w, $X(t+t_w,t_w)$ becomes a function of time only through $C(t+t_w,t_w)$: $X(t+t_w,t_w)=X[C(t+t_w,t_w)]$. This function $X(C)$ has been interpreted in terms of an effective temperature.[12]

At high temperatures X equals one since the system always equilibrate at large times and the equilibrium properties hold. At low temperatures, where aging phenomena appear, the departure of $X(C)$ from 1 characterizes the FDT violation.

This scenario has been verified in several models of spin glasses,[13] in the Lennard-Jones glass,[14] in kinetic Ising models,[15] and in polymers in random media.[16] It has also been verified in the domain growth dynamics of ferromagnetic systems[17] in dimensions $d=2$ and 3, where X has been found to be zero in the aging regime.

Instead of analyzing the response $R(t+t_w,t_w)$ we look at the integrated response function (proportional to the magnetic susceptibility), that is, in a zero-field-cooling numerical experiment we observe the growth of the magnetization under a constant external field applied at t_w:

$$M(t+t_w,t_w)=\int_{t_w}^{t+t_w} R(t+t_w,s)h(s)ds. \tag{5}$$

Using Eq. (4) we can rewrite Eq. (5) for long times as

$$\frac{T}{h}M(t+t_w,t_w)=\int_{C(t+t_w,t_w)}^{1} X(C)dC. \tag{6}$$

If FDT is satisfied Eq. (6) reduces to a linear relation

$$\frac{T}{h}M(t+t_w,t_w)=1-C(t+t_w,t_w), \tag{7}$$

while a departure from this straight line in an M vs C parametric plot indicates a violation of FDT and gives information about $X(C)$.

In this work we present the results of Monte Carlo simulations in the two-dimensional Ising model defined by the Hamiltonian (1) on an $N=30\times 30$ square lattice with free boundary conditions. We chose the heat-bath algorithm for the spin dynamics and time is measured in Monte Carlo steps per site. For each run the system is initialized in a random initial configuration corresponding to a quenching from infinite temperature to the temperature T at which the simulation is done. We compute $C(t+t_w,t_w)$ as a function of the observation time t, for different values of t_w, δ, and T. In the striped phase at low temperatures this function decays quickly from $C(t_w,t_w)=1$ to a constant value that persists for $t/t_w \ll 1$; at $t>t_w$ it decays more slowly towards zero with a scaling law that depends on the ratio[4] $h(t)/h(t_w)$. The scaling function $h(t)$ appears to be linear for $\delta > \delta_c \sim 2.7$ and logarithmic for $\delta < \delta_c$. It was also observed[3] that the magnetization (for a fully magnetized initial state) relaxes exponentially for $\delta > \delta_c$, with a relaxation time that depends both on the temperature and on δ, while it presents a power-law decay for $\delta < \delta_c$, with an exponent independent of δ. These behaviors suggest a different domain growth dynamics in every one of the dynamical regimes.[4] Hence, it is of interest to check whether such different dynamics are reflected in the FDT violation factor or not.

At time t_w we take a copy of the system, to which a random magnetic field $h(i)=h\epsilon_i$ is applied, in order to avoid favoring one of the different phases;[17] ϵ_i are taken from a bimodal distribution ($\epsilon_i=\pm 1$) and the strength h of the field

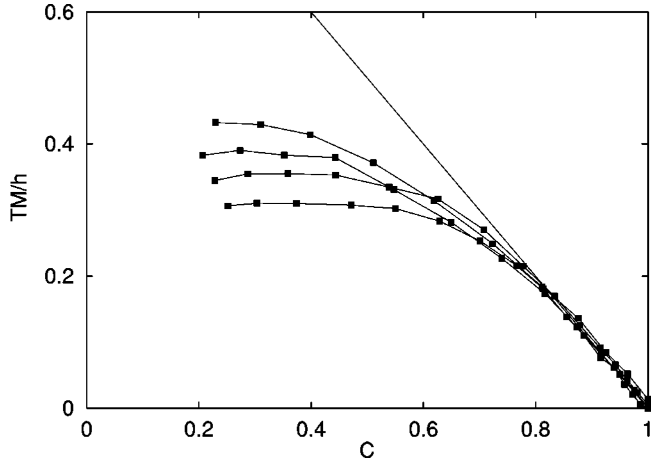

FIG. 1. Integrated response versus autocorrelations for $T=0.5$ and $\delta=2$. The different curves correspond, from top to bottom, to waiting times $t_w=2^5,2^7,2^9,2^{11}$. The straight line corresponds to the FDT relation $TM/h=1-C$.

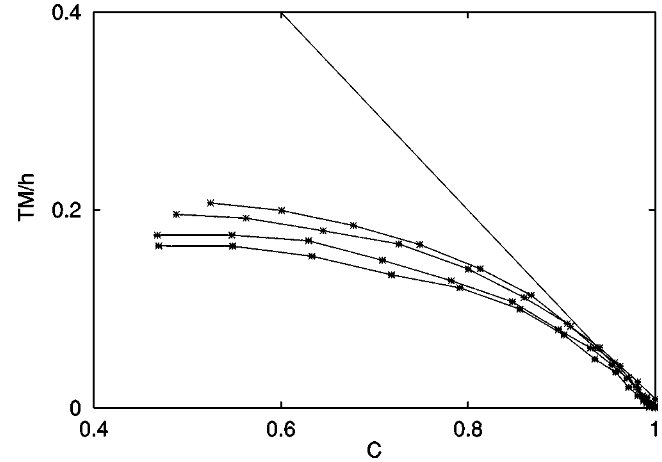

FIG. 2. Integrated response versus autocorrelations for $T=0.5$ and $\delta=4$. The different curves correspond, from top to bottom, to waiting times $t_w=2^5,2^7,2^9,2^{11}$. The straight line corresponds to the FDT relation $TM/h=1-C$.

is taken small ($h=0.01$) to ensure linear response. We then compute the staggered magnetization[17]

$$M(t+t_w,t_w)=\frac{1}{N}\sum_i \overline{\langle \sigma_i(t+t_w)\epsilon_i\rangle}, \qquad (8)$$

whose conjugate field is h and where the overline means an average over the random variables ϵ_i. We then obtain parametric plots of $TM(t+t_w,t_w)/h$ vs $C(t+t_w,t_w)$ for several values of the temperature, the waiting time $t_w=2^n(n=5,7,9,11)$, and for $\delta=2<\delta_c$ and $\delta=4>\delta_c$. We first made some checks at high temperatures where the system equilibrates quickly, verifying that both TTI and FDT are satisfied.

In Fig. 1 a parametric plot of the integrated response vs autocorrelation is shown for $\delta=2$, $T=0.5$ and waiting times $t_w=2^n(n=5,7,9,11)$ from top to bottom. We made an average over 400 realizations of the random field. The straight line corresponds to the FDT relation (7) with constant slope -1. For fixed t_w and observation times $t\ll t_w$ FDT holds, and the system is in the stationary regime. For times $t\sim t_w$ the curves begin to depart from the FDT line signaling a crossover region where the system begins to fall out of equilibrium. Finally, when $t\gg t_w$ the system is out of equilibrium with the correlations decaying to zero as $t\to\infty$. In this last regime the integrated response keeps growing for the small t_w but, as t_w grows it tends to stabilize in a constant value. Furthermore, this value decreases as t_w grows. The older the system the smaller the memory of the past history. This behavior is similar, e.g., to what happens in the coarsening dynamics of ferromagnets.[17,18] It is not at all obvious that this would be the case. It is important to note that the system is in a region ($\delta=2$) where the ground state is the striped phase with stripe width h which grows with[2] δ. For this value of δ the scaling of the autocorrelations in the out of equilibrium regime is logarithmic:[4] $C(t+t_w,t_w)\propto \log(t)/\log(\tau(t_w))$. This slow decay is typical of activated dynamics in systems with a broad distribution of relaxation times. This may be a consequence of the degeneracy of the striped ground state, a problem that deserves further study. So naively one would expect rather strong memory effects as a consequence of the slow logarithmic decay in the correlations, at variance with what is observed in the simulations.

The flatness of the integrated response for long times implies an FDT violation factor $X(t+t_w,t_w)=0$ for $t_w\to\infty$. If we interpret T/X as the "effective temperature" for the system in this time regime, this implies an infinite effective temperature.[12]

The FDT plot for $\delta=4$ is presented in Fig. 2. This is qualitatively similar to the plot for $\delta=2$. The main difference is that the integrated response flattens to a value which is roughly half of that corresponding to $\delta=2$. In this case the ferromagnetic term of the Hamiltonian is clearly dominant. This is reflected, e.g., in the scaling form of the autocorrelations in the aging regime,[4] i.e., $C(t+t_w,t_w)\propto t/\tau(t_w)$. We must note, however, that the stable phase still corresponds to the striped one[2] but with increasing value of the width of the stripes as δ increases. For a fixed t_w in the aging regime, the striped domains are wider with $\delta=4$ than with $\delta=2$. Consequently, the domain walls have smaller total length in the latter case. This implies a smaller contribution for the stag-

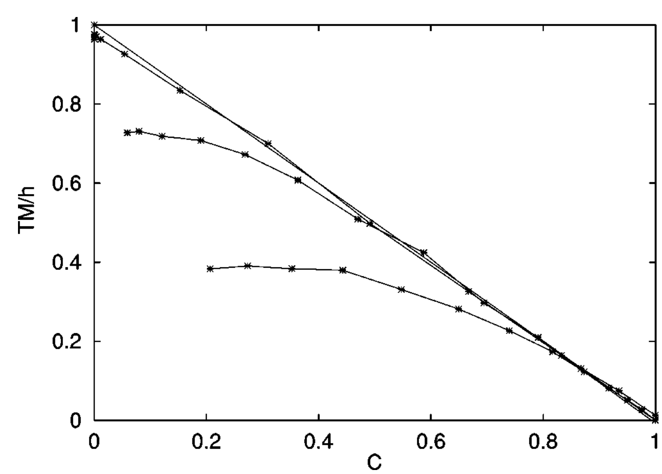

FIG. 3. Integrated response versus autocorrelations for $t_w=2^7$ and $\delta=2$. The different curves correspond, from top to bottom, to temperatures $T=1,0.7,0.5$. The straight line corresponds to the FDT relation $TM/h=1-C$.

gered magnetization while the bulk contributions are roughly the same. So it is reasonable to expect a smaller response in this case. In other words, as the systems become more ''ferromagnetic'' the long term memory becomes weaker. A detailed analysis of the bulk and domain walls contributions to the response has been recently done for a ferromagnet by Berthier *et al.*[18]

In Fig. 3 we show a parametric plot for different values of the temperature $T=1$, 0.7, and 0.5 (from top to bottom) and a fixed $t_w=2^7$ for $\delta=2$. Equilibrium dynamics is restored at $T=1$. It would be interesting to know if the change of dynamical regime at this temperature coincides with a thermodynamic phase transition or is a purely dynamic effect.

We have studied the FDT violation in the coarsening process of an Ising model with dipolar long-range interactions. Going through $\delta_c \sim 2.7$ the aging dynamics of the autocorrelations presents a crossover from a logarithmic decay for $\delta < \delta_c$ to an algebraic decay for $\delta > \delta_c$, probably related to some dynamical phase transition related with the change of the strips width. We asked weather this difference would manifest itself in the responses and FDT violation factor X. It turns out that this is not the case. For long waiting times in the aging regime $X \to 0$ in both cases, signaling that the long term memory is weak in both regimes. In fact, recent work on the connection between equilibrium and nonequilibrium properties of systems with short-range interactions indicate that $X(C)$ should go to zero asymptotically in systems which do not present replica symmetry breaking, like the one we have studied in this work.[19]

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