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LETTER TO THE EDITOR

Relaxation of an isolated droplet in pure and random Ising magnets: Monte Carlo simulation

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Abstract. By Monte Carlo simulation we have investigated the relaxation of an isolated droplet in the two-dimensional pure Ising model below the ordering temperature T_c. For system sizes 180^2 and 240^2 we have observed a stretched exponential decay, namely $C(t) \sim \exp[-(t/\tau)^{1/2}]$, of the temporal spin autocorrelation function $C(t)$ in the intermediate and long time regimes (of the order of 10^4 Monte Carlo steps spin^{-1}). We have also computed the correlation function $C(t)$ for the two-dimensional Ising model with quenched random site disorder out to 10^5 Monte Carlo steps spin^{-1} for system sizes up to 180^2. The relaxation is much slower in the latter model than in the pure Ising model.

The decay of metastable and unstable states in thermodynamic systems has been studied quite extensively over the last two decades [1, 2]. The kinetic Ising model and its appropriate generalisations have been considered as prototype systems for studying such non-equilibrium phenomena. It is now well known that quite often the dynamics of such systems, evolving from non-equilibrium initial states, is dominated by the 'droplets' (e.g. droplets of down spins surrounded by up spins or vice versa). The dynamical evolution of such systems is complicated by the 'splitting' and 'coalescence' of the droplets [3, 4]. However, during the late stages of growth, quite often the system consists of an isolated domain in a sea of oppositely oriented spins. In this letter we shall focus our attention on an idealised Ising spin system where a single large domain of down spins, surrounded by a sea of up spins, begins to relax. Safran *et al* [5] studied the decay law for the area $A(t)$ of such isolated droplets. In this letter we shall compute the corresponding time dependence of the spin autocorrelation function $C(t)$ by Monte Carlo (MC) simulation of the two-dimensional Ising model with nearest-neighbour exchange interactions. We shall also study the effects of non-magnetic quenched impurities on the time dependence of $C(t)$. We would like to emphasise here that we are investigating a non-equilibrium phenomenon in contrast to the phenomenon of droplet fluctuation in the Ising model at equilibrium [6].

Let us denote an Ising spin at an arbitrary site $\boldsymbol{r}_i$ by S_i, where S_i can be in one of two possible states, namely $S_i = +1$ and -1. We define the spin autocorrelation function

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$C(t)$ in an N-spin Ising system by

$$C(t)=\left[(1/N)\sum_{i=1}^{N}(S_i(t)S_i(0)-\langle S_i(\infty)\rangle^2)\right]_{\mathrm{av}} \tag{1}$$

where

$$\langle S_i(\infty)\rangle=(1/N)\sum_{i=1}^{N}S_i(\infty)$$

is the magnetisation per spin in equilibrium. The symbol $[\ ]_{\mathrm{av}}$ denotes an average over a large number of initial configurations.

We have carried out MC simulations of two models:

(i) the two-dimensional pure Ising model, and

(ii) the two-dimensional dilute Ising model (DIM), which is an Ising spin system where a finite fraction of the spins are replaced randomly by non-magnetic quenched impurities [7]. We assumed that each spin interacts only with the other spins on the nearest-neighbour lattice sites. All the systems simulated were in the ferromagnetic regime ($T<T_c$).

So far as the simulations are concerned, the initial configuration always consisted of a droplet of down spins of linear size L_d surrounded by up spins where the linear size of the whole system was $L(L>L_d)$. Rigid boundary conditions were employed to simulate an effectively infinite sea of up spins surrounding an isolated finite domain of down spins. Then the spin configurations were updated using the Metropolis algorithm. We have used the multi-spin coding technique. Computer programs for simulating the pure Ising model and the DIM using multi-spin coding were developed earlier [8, 9]. Suppose t_{eq} is the number of Monte Carlo steps per spin (MCS spin^{-1}) required for the decay of the droplet so that the correlation function $C(t)$ does not alter significantly beyond t_{eq}. Assuming that $\langle S_i(\infty)\rangle$ can be replaced by $\langle S_i(t_{eq})\rangle$, we have computed the correlation function $C(t)$ defined through the relation (1). In the DIM each of the lattice sites is occupied randomly by an Ising spin with probability p and empty (i.e. occupied by a non-magnetic impurity) with probability $1-p$. Our simulations were carried out on several mainframe CDC computers. The production of the data (including those not shown explicitly in the figures) required more than 200 h of CPU time.

We have simulated two-dimensional pure Ising systems of various sizes L^2 ($120\leqslant L\leqslant 240$). We have always started with a square droplet at the centre of the system. We have investigated the effects of varying the linear size L_d ($60\leqslant L_d\leqslant 100$) of droplets for $L=120$. Since the relaxation is very fast at low temperatures, the decay law inferred from the data over such a short timescale may not be reliable. On the other hand, temperatures too close to T_c are plagued by critical fluctuations and are, therefore, extremely time consuming. Thus, in order to stretch the timescale of relaxation to the order of 10^3-10^4 MCS spin^{-1} without appreciable complications from critical fluctuations we have carried out most of our simulations of the pure Ising model at an optimum value $T=0.6T_c$. So far as the DIM is concerned, the higher the temperature is, the faster the relaxation for a given concentration of the impurities. Therefore in order to equilibrate the systems within the available computer time one should choose a sufficiently high temperature. However, since dilution reduces the transition temperature (i.e. $T_c(p)<T_c(1)$ for all $p<1$), one has to be careful not to choose any temperature too close to the corresponding $T_c(p)$.

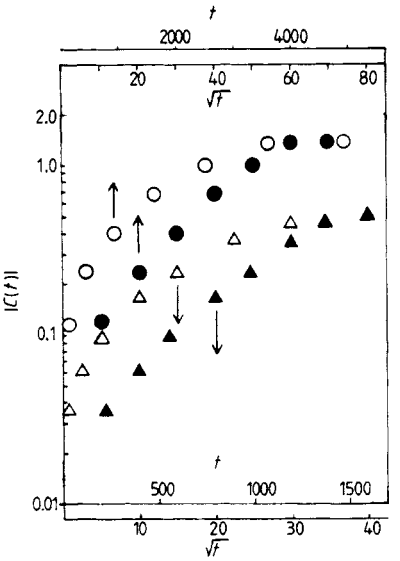

Figure 1. Log$|C(t)|$ plotted against t (open symbols) and $\sqrt{t}$ (full symbols) for the pure Ising model with system size $L = 120$ at $T = 0.6T_c$. The circles and triangles correspond to $L_d = 100$ and $L_d = 60$, respectively. Each of the data points is obtained by averaging over 25 configurations.

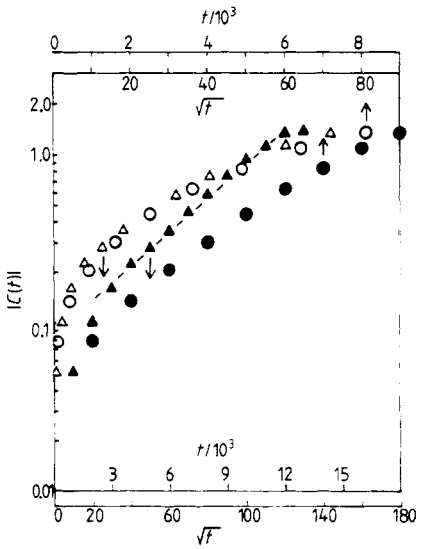

Figure 2. Log$|C(t)|$ plotted against t (open symbols) and $\sqrt{t}$ (full symbols) for the pure Ising model. The circles and triangles correspond to $L = 180$, $L_d = 150$ and $L = 240$, $L_d = 200$, respectively at $T = 0.6T_c$. Each of the data points is obtained by averaging over five configurations. The broken line is just a guide to the eye to emphasise the stretched exponential decay of $C(t)$.

In figures 1 and 2 we have plotted $\ln|C(t)|$ for the pure Ising model as functions of t and $t^{1/2}$ for different values of L and L_d. Note that for all L and L_d the fit with $t^{1/2}$ is much better than that with t. Moreover, as L increases the fit with $t^{1/2}$ becomes better, thereby providing further support to our claim that for the pure Ising model $C(t)$ decays as a stretched exponential in an infinitely large system, i.e.

$$\ln|C(t)| \sim t^{1/2}. \tag{2}$$

Note that stretched exponential decay is observed only for intermediate and long timescales; the relaxation is much faster in the early time regime.

There are two possible interpretations for the different growth rates in the early time and later regimes. First, this early time regime possibly exists for droplets of all possible shapes and sizes and the corresponding fast decay is a real effect. Second, the stretched exponential form (2) holds only for approximately spherical droplets and the square droplets become approximately spherical only after an initial period of time during which the relaxation is much faster.

The stretched exponential decay of $C(t)$ can be interpreted as a consequence of curvature-driven shrinking of the droplet [10]. The probability that a spin retains its original orientation at time t is proportional to $\exp(\Delta E/k_B T)$, where ΔE is the corresponding barrier height. For the pure Ising model in d dimensions $\Delta E \sim R^{d-1}\sigma$ where σ is the surface tension and R is the radius of the droplet. Since $(R^2(t) - R^2(0))\alpha - t$ for curvature-driven shrinking [10] one gets stretched exponential decay (2) in $d = 2$.

It is well known [11-15] that the quenched impurities tend to pin the interfaces. The slower decay of $C(t)$ in the DIM than in the pure Ising model observed in our simulation (figure 3) is a consequence of such pinning effects of the impurities. However, the curvature, although small, of the plots of $\ln|C(t)|$ against $\ln t$ in figure 3 indicates that the decay of $C(t)$ cannot be fitted to a simple power law.

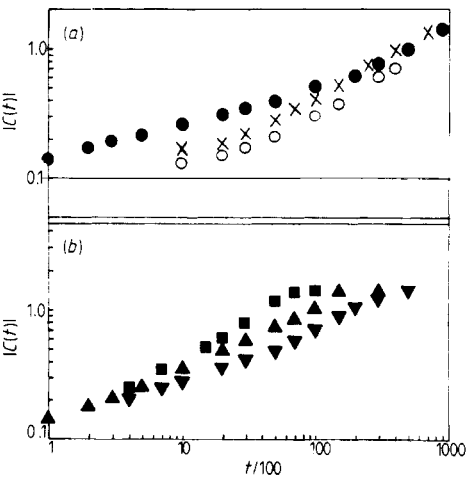

Figure 3. Log-log plots of $|C(t)|$ against t for the Ising model with quenched random site dilution. (*a*) The full circles correspond to $L = 96$, $L_d = 80$, $p = 0.9$, $T = 0.5T_c$, the open circles to $L = 180$, $L_d = 150$, $p = 0.925$, $T = 0.6T_c$, the crosses to $L = 180$, $L_d = 150$, $p = 0.95$, $T = 0.65T_c$. (*b*) The squares correspond to $L = 96$, $L_d = 80$, $p = 0.975$, $T = 0.55T_c$, the inverted triangles to $L = 96$, $L_d = 80$, $p = 0.95$, $T = 0.45T_c$, the triangles to $L = 72$, $L_d = 60$, $p = 0.95$, $T = 0.35T_c$. Each of the data points is obtained by averaging over five configurations.

We conclude that the decay of the spin autocorrelation function $C(t)$ corresponding to the relaxation of a single isolated droplet in the pure Ising model is a consequence of the curvature-driven shrinking mechanism. The tendency of the quenched random non-magnetic impurities to pin the interfaces leads to much slower decay of $C(t)$ in the DIM than in the pure Ising model.

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