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LETTER TO THE EDITOR

Damage spreading in a three-dimensional Ising model in a magnetic field

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Abstract. The time evolution of two ferromagnetic Ising cubic systems, which differ by the orientation of a single spin at t = 0, has been studied in a magnetic field B by computer simulation. The critical field $B_c(T)$, above which the previous initial damage does not spread, has been determined. The magnetisation for $B = B_c$ is very well approximated by $M(B_c) = 1 - \exp(-T_c/T)$ in the range of T values investigated. The concentration of minority spins at $B_c(T)$ differs strongly from the corresponding concentration for percolation at T.

Studies of the dynamics of statistical systems have been recently performed in various models in order to characterise dynamical phase transitions [1-5] and to understand their relations to thermodynamical properties [4, 5]. The spread of a small perturbation, called the damage, has been studied by Stanley *et al* [1] in two-dimensional Ising models and by Costa [2] in a three-dimensional Ising model using Metropolis dynamics (see also Derrida and Weisbuch [3, 4] for the heat bath method). Costa [2] has observed a dynamical phase transition at about 0.96 T_c ($T_c = 4.5116$ [6] in units of J/k) which is, as he emphasised, in agreement with the critical temperature for the Ising-correlated site percolation [10].

We report here the main results of a simulation study similar to [1, 2] of the time evolution of a three-dimensional ferromagnetic Ising system on a cubic lattice in a magnetic field B (in units of J/μ) as a function of temperature T. Starting from a ferromagnetic system on a simple cubic lattice of L^3 sites, a configuration $\{S_i^A\} = \pm 1$ is obtained at equilibrium in the applied field B. At t = 0, a twin configuration $\{S_i^B\}$ of $\{S_i^A\}$ is created and a single spin is flipped at the centre of the twin. The two systems are processed with Glauber dynamics with helical boundary conditions. The spin updating is done either sequentially going through the lattice in a regular fashion [7] or simultaneously [8] with identical pseudorandom numbers for both lattices and with a flip probability of $1/(1 + \exp(-\Delta E/T))$, where ΔE is the energy change of the flip [7]. Sequential processing is performed on an IBM 3090 for L = 10 while parallel processing is performed on a Cray-XMP/416 for L up to 144 with a fully vectorised multispin coding program (10 updatings per microsecond, details to be presented in a future publication). All programs give magnetisation values M in precise agreement with the magnetisation calculated by using the Padé approximants of Essam and Fisher [9] for $T < T_c$, and the mean-field approximation at large temperatures and fields.

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At the end of each sweep, the damage D is characterised by a normalised Hamming distance between the two updated configurations:

$$D(t, T, B) = \sum_{i} (|S_{i}^{A}(t, T, B) - S_{i}^{B}(t, T, B)|)(2L^{3}).$$

The study is repeated for one hundred to several thousand systems for L = 10 and for about ten to some hundreds for larger sizes. An average distance $\langle D(t, T, B) \rangle$ is calculated over the samples which have survived $(D \neq 0)$ at time t. Two different studies have been performed in order to characterise the evolution of the systems.

(i) After a transient period of time, D(t, T, B) fluctuates around a stationary value and

$$\langle D(T, B) \rangle = \left\langle \left(\sum_{t_1}^{t_2} D(t, T, B) \right) (t_2 - t_1 + 1)^{-1} \right\rangle$$

is observed to be independent of t_1 and t_2 in wide time intervals. We have calculated the field $B_c(\langle D \rangle)$ at which $\langle D(T, B) \rangle$ extrapolates to zero (figures 1 and 2). Figure 1 shows a range of fields (~0.7 to ~0.95) in which $\langle D \rangle$ varies almost linearly with B, being well approximated by $\langle D \rangle = 0.5(1 - B/B_c)$. Figure 1 also shows the rounding effect close to B_c due to finite size [6] for T = 10 and L = 10.



Figure 1. Mean damage $\langle D \rangle$ as a function of B/B_c for various values of T and L: T = 7, L = 20, 80 (\blacklozenge); T = 10, L = 10, 20 (\Box); T = 20, L = 10 (\blacktriangle); T = 40, L = 10 (\blacksquare).

(ii) We, like Costa [2], have calculated the time $t_d(T, B)$ needed to damage all sites at least once. The study is repeated for N systems, among which only N_d are damaged in the previous sense while the remaining systems $N - N_d$ are never fully damaged and have all the damage healing out completely at some finite time. The mean $\langle t_d \rangle$ is calculated over the N_d systems, as is the field $B_c(\langle t_d \rangle)$ (figure 2) at which $\langle t_d \rangle^{-1}$ extrapolates to zero. The mean damage $\langle D(t_d, T, B) \rangle$ has also been calculated (figure 1, for L > 10). We have observed that both $\langle t_d \rangle^{-1}$ and $\langle D(t_d, T, B) \rangle$ have almost linear field dependences in the vicinity of B_c and that they extrapolate to zero at the same field within experimental error.

For study (i) the spins have been updated sequentially while for study (ii) almost all simulations have been performed with simultaneous updating. Both studies give



Figure 2. Critical field B_c as a function of temperature T for: L = 10, $B_c(\langle D \rangle)$, sequential updating (\blacksquare) ; L from 48 to 112, $B_c(\langle t_d \rangle)$, simultaneous updating (\Box) ; B_c calculated from $M(B_c) = 1 - \exp(-T_c/T)$ (full curve).

similar critical fields, as seen in figure 2, the time t_d being large enough for the damage to have its stationary value at that time. The number of damaged sites is proportional to either L^3 or to zero for both studies. In the content of study (i), we have also determined the survival probability P(t, T, B) [3]. This probability goes more and more rapidly to zero when B is closer and closer to B_c . For T = 10 and L = 10, we have also calculated P(t, T, B) for the heat bath method [3, 4] (with, in that case: $\{S_i^B\} = -\{S_i^A\}$ at t = 0) for B between 0 and 3, but we have just observed that P decreases more rapidly from 1 to 0 when B increases without noticing any particular behaviour at B_c .

Figure 3 shows the concentration of minority spins X_c for $B = B_c$, i.e.

$$X_{\rm c}(T) = \frac{1}{2}(1 - M(B_{\rm c}))$$

as a function of reciprocal T. We have empirically observed that X_c is very well approximated by

$$X_{\rm c}(T) = 0.5 \exp(-T_{\rm c}/T)$$

in the temperature range investigated ($5 \le T \le 40$, shown by the full curve in figure 3), i.e.

$$M(B_{\rm c}) = 1 - \exp(-T_{\rm c}/T).$$
(1)

The B_c values calculated from equation (1) are also shown as a full curve on figure 2. Extrapolating on both sides of the investigated temperature range, we note that B_c given by (1) goes to zero at $T^*/T_c = 0.94$ where $M(B_c)$ is equal to the spontaneous magnetisation. Equation (1) may therefore be valid at most down to T^* , but may become invalid when T decreases below T = 5. When $T \to \infty$, we deduce from (1) that $B_c \to T_c$ not in contradiction with a reasonable trend that can be observed on figure 2. In any case, we observe that B_c increases much less rapidly than T, i.e. $M = B_c/T \to 0$ when $T \to \infty$. We therefore expect that $X_c(\infty) = 0.5$, X_c varying thus between 0.5 at $T = \infty$ and 0.20 at T = 5.



Figure 3. Concentration of minority spins $X_c = \frac{1}{2}(1 - M(B_c))$ as a function of T_c/T for: $L = 10, X_c(\langle D \rangle)$, sequential updating (\blacksquare); L from 48 to 112, $X_c(\langle t_d \rangle)$, simultaneous updating (\square); $X_c = 0.5 \exp(-T_c/T)$ (full curve); results of Heermann and Stauffer [10] for Ising-correlated site percolation (broken curve).

Equation (1), which summarises our results, and the fact that $X_c(T)$ differs from the corresponding curve for the percolation of minority spins (figure 3, X_c between 0.3117 for $T = \infty$ and 0.22 for $T/T_c = 0.96$ [10]) constitute the main conclusions of the present work.

In a paper to be submitted, we will present a study of damage spreading in a zero field as well as scaling behaviours and more detailed results on time evolutions.

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