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LETTER TO THE EDITOR

Scaling properties of the damage cloud in the 3D Ising model

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Abstract. We show that in the three-dimensional Ising model at the critical temperature the fractal dimension of the touching damage, determined by the box counting method, asymptotically converges to the expected value $d_f = d - \beta/\nu$. In contrast, the finite-size scaling analysis indicates for the touching damage an effective fractal dimension whose value is 20% smaller. The expected d_f is, however, recovered again when instead of the system size L the quantity $L/\ln L$ is used as a scaling variable. This behaviour could be explained by the recently discovered dynamical multiscaling.

In recent years a novel approach to the analysis of dynamical properties of spin systems has been successfully introduced. The basic ideas originated from cellular automata and dynamical systems theory and mainly consist of considering the wandering of a spin configuration in phase space to reach equilibrium as a dynamical process. In fact, once the dynamics of the system is chosen (e.g. Glauber, heat bath, Q2R, etc), this defines trajectories in phase space moving toward equilibrium. One can then study how much these trajectories are sensitive to the initial conditions, that is if two initially close configurations still remain close during their evolution and eventually merge or else they move apart to very different states. This type of analysis is often referred to as *damage spreading.*

The concept of damage spreading has been originally introduced in the Ising model [1] by analogy with cellular automata. Two configurations of Ising spins σ_i^A and σ_i^B, with $\sigma_i = \pm 1$, are considered on a lattice of N sites; then the damage or Hamming distance can be defined as

$$D(t) = \frac{1}{4N} \sum_i (\sigma_i^A(t) - \sigma_i^B(t))^2. \tag{1}$$

This quantity physically represents the fraction of spins that differ between the two configurations and therefore allows us to monitor the time evolution of the relative distance of the two configurations in phase space. In order to do this, the two configurations must be submitted to the same statistical noise, that is the same sequence of random numbers is used to update corresponding spins in the A and B configurations.

Depending on the chosen dynamics and the initial distance $D(0)$, very different results can be obtained [1-4]. In most cases, the damage shows some critical behaviour at or near the Ising critical temperature [1-6]. Furthermore, the concept of damage spreading has also given interesting insights into the study of spin glasses in a zero [2, 7] and non-zero [8] magnetic field.

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One of the major questions in the field was then to determine if any relation existed between the so-called dynamical transition, where the damage goes to zero, and the well known thermodynamical transition of the magnetic system. It has been shown [3] that for the Ising model submitted to the heat bath dynamics the damage between two configurations, respectively with plus and minus boundary conditions, is equal to the magnetisation. Moreover, the probability of damage to a site at a given distance from a fixed damage at the origin is proportional to the pair correlation function and that the sum over all sites of such probabilities is then proportional to the susceptibility. Looking at the damage spreading with heat bath dynamics is therefore a different way to study the thermodynamical transition in the Ising model and turns out to be a more efficient way to numerically evaluate correlation functions.

Within this scenario the cloud of damaged sites visualises the spin fluctuations, that is it contains those spins which are effectively correlated to the origin, cancelling contributions due to statistical noise. The damage cloud is therefore reminiscent of the droplet [9] in an Ising model, where neighbouring spins in the same state belong to the same droplet with a probability $p_B = 1 - e^{-2J/kT}$. It can, in fact, easily be derived by the following argument that the fractal dimension of the damage cloud is equal to $d_f = d - \beta/\nu$, the fractal dimension of the Ising critical droplet.

Let us consider a cloud of damaged sites spanning the system of size L and touching its boundaries. The mass of such a cloud, $D \sim L^{d_f}$, is given by all the damaged sites correlated to the origin kept damaged. Namely, $D = P(L) \int_0^L r^{-(d-2+\eta)} r^{d-1}\, dr$, where $P(L) = L^{d_f}/L^d$ is the probability for the cloud to touch the boundaries of the system. By performing the integration, one then obtains $D \sim L^{d+2-\eta-d_f}$, and using $2-\eta = d - 2\beta/\nu$ the relation $d_f = d - \beta/\nu$. To confirm this picture, the numerical determination of the fractal dimension of the damage cloud in the 2D ferromagnetic Ising model at its critical temperature has given a value $d_f = 1.87 \pm 0.02$, in good agreement with the exact value $d_f = d - \beta/\nu = 15/8$ of the fractal dimension of the droplets.

If the situation for the two dimensional Ising model is quite well established, the three-dimensional case still poses some open questions. A recent preprint [10] focusing on the finite-size scaling analysis of the damage cloud for the 3D Ising model at critical temperature with heat bath dynamics, indicates as a fractal dimension a value close to 1.9 as opposed to the expected value 2.5 predicted by $d_f = d - \beta/\nu$. In order to explain this discrepancy, it has been suggested [11] that the fractal dimension of a cloud of damage allowed to grow up to the boundaries of a box of fixed size, is indeed equal to $d_f = d - 2\beta/\nu$. Moreover, such an argument could also try to account for the predictions of the two-dimensional data, due to the small value of β in this case. However, the error bars estimated for the value of the fractal dimension seem actually to exclude the value 7/4 predicted by this argument.

The question of whether the fractal dimension of the damage cloud is actually given by $d - \beta/\nu$ has also been addressed for the two-dimensional Kauffman model. Previous numerical simulations [12] had in fact indicated that d_f was instead rather close to $d - 2\beta/\nu$. More recent calculations [13] have accurately determined the value of the critical threshold for the damage and finally re-established the agreement of d_f with $d - \beta/\nu$.

In this letter we attempt to clarify the question of whether the fractal dimension of the damage cloud in the three-dimensional ferromagnetic Ising model is indeed numerically given by $d_f = d - \beta/\nu$.

In order to do so, we considered a configuration of Ising spins on a cubic lattice of linear size L and with periodical boundary conditions. The time evolution of the spins follows the heat bath dynamics, namely the spin σ_i at site i will be up at time t with a probability

$$p_i(t) = 1 + \exp\left(\frac{-2J}{kT}\sum_j \sigma_j(t)\right) \tag{2}$$

the sum being over the spin's nearest neighbours at site i. All the spins belonging to each of the two sublattices, in which the cubic lattice splits, are updated in parallel. The initially random configuration is thermalised to equilibrium at the critical temperature $T = T_c = 4.51$, then two copies of such a configuration are made, σ_i^A and σ_i^B, where the spin at the origin is fixed up and down respectively. This damage at the origin will be kept at all times and it acts as a continuous source from which damage spreads out. The two parallel configurations then evolve following the heat bath dynamics with the same random number used to update corresponding spins.

The simulation is stopped when the damage finally touches the boundary of the lattice and a new configuration is generated. We analyse system sizes from $L = 10$ to $L = 98$, the thermalisation time ranging from 2000 to 5000 time steps and the statistics varying from 15 000 configurations for the smallest system size to five configurations for $L = 98$. The whole simulation took about 40 hours of CPU time on the Cray XMP.

To calculate the fractal dimension of the damage cloud, we first analysed the data by the box counting method. The mass of the cloud, that is the number of damaged sites, within a box around the origin is calculated for concentric boxes. The double logarithmic plot of the mass as a function of the box radius then provides the fractal dimension of the cloud. Figure 1 shows the data for two different system sizes. In the intermediate region the curves have a straight line behaviour, whose slope d_f^m is

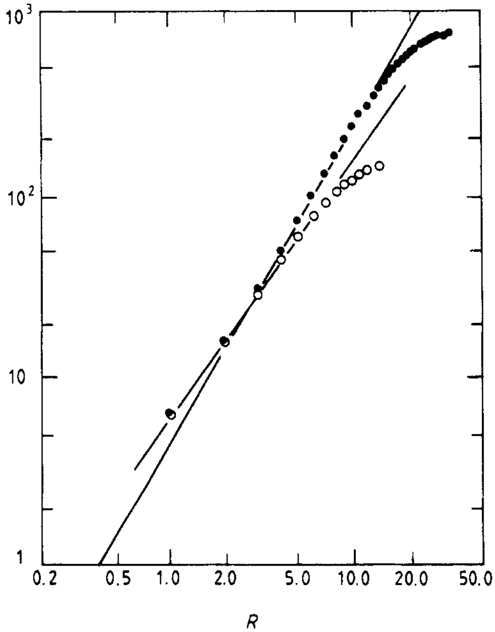

Figure 1. Log-log plot of the mass of the damage cloud D within a sphere of radius R against R for two different system sizes: 1900 configurations of $L = 30$ (○) with 4000 time steps of thermalisation and a slope $d_f^m \simeq 1.45$; 187 configurations of $L = 70$ (●) with the same thermalisation time and $d_f^m \simeq 1.73$.

substantially smaller than $d_f = d - \beta/\nu \simeq 2.5$ but increases slowly and steadily with the system size.

To account for this size dependence, we have analysed the corrections to scaling for the data. Figure 2 shows the value of the measured fractal dimension d_f^m for a given system size as function of $1/\ln L$, where a logarithmic correction to scaling of the form $d_f^m = d_f(1 + a(\ln L)^{-1})$ has been assumed. The data do indeed show a good linear behaviour and tend asymptotically to the value 2.5 in good agreement with $d_f = d - \beta/\nu \simeq 2.48$ [14]. We have also considered the possibility of a correction to scaling of the form $d_f^m = d_f(1 + aL^{-w})$. This form is also well satisfied by the data for quite a small correction exponent $w \simeq 0.3$, which numerically is not inconsistent with a logarithmic correction.

Since independent calculations [10] have indicated that in a finite size scaling plot d_f is rather closer to 1.9 than 2.5, we next analysed the scaling of the mass of the whole cloud at the time when it first touches the boundary of the lattice as function of the system size. The effective fractal dimension at a given size as function of $1/\ln L$ does indeed extrapolate asymptotically to a smaller exponent close to 1.9 (figure 3(a)).

We know from figure 2 that the numerical results can be reconciled to the theory if one assumes logarithmic corrections to scaling. For this reason we have tried to fit the data of figure 3(a) by a curve of the form $d_f^m = d_f + b/\ln L + \ln[1 + a/\ln L]/\ln L$, where the last term corresponds to the correction to scaling and $d_f = d - \beta/\nu$. We find

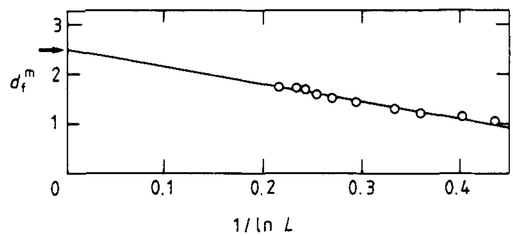

Figure 2. The effective fractal dimension d_f^m measured by the box counting method as function of $1/\ln L$. The arrow indicates the extrapolated value $d_f = d - \beta/\nu \simeq 2.5$.

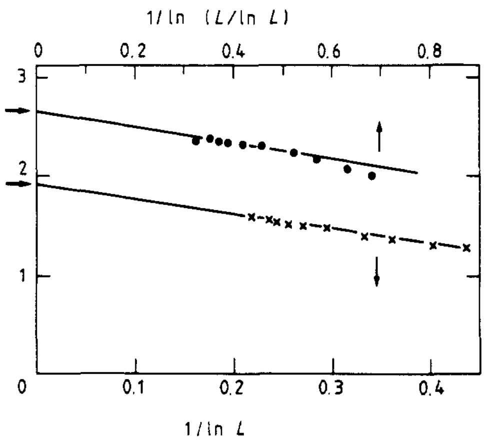

Figure 3. The effective fractal dimension $\ln D/\ln L$ as function of $1/\ln L$ (lower scale) giving an extrapolated value $d_f \simeq 1.9$ (×). The same data plotted by using, instead of L, the variable $L/\ln L$ (upper scale) recovering as extrapolated value $d_f = d - \beta/\nu \simeq 2.5$ (●).

that it is not possible to find any pair of constants a and b to convincingly fit the data so that the deviations from the expected value observed in figure 3(a) are not consistent in this case with logarithmic corrections to scaling.

Another possible explanation for the extremely slow convergence might be the existence of a logarithmic prefactor, namely a relation $D \sim (L/\ln L)^{d_f}$ for the mass of the cloud. In order to check this point, we have looked at the scaling of the mass of the damage cloud as a function of this new variable $L/\ln L$. The effective fractal dimension as function of $1/\ln(L/\ln L)$ does indeed extrapolate to the expected value 2.5 predicted by $d_f = d - \beta/\nu$ and obtained by the box counting method (figure 3(b)).

If, as the data indicate, a logarithmic prefactor exists for the effective fractal dimension of the damage cloud at the touching time, one should consistently also find this prefactor by the box counting method. For this reason we have also plotted the data of figure 1 in a log-log plot as a function of $R/\ln R$ instead of R. We find that the data do not fall on a straight line, seemingly excluding the possibility of a logarithmic prefactor in this case.

Moreover, a logarithmic prefactor cannot be explained by a relation such as $R = L/\ln L$ between the radius of gyration and the system size. In fact, the radius of gyration R of a damage cloud touching a box of size L is proportional to L itself and not to $L/\ln L$ (figure 4). As seen from figure 4(b), if a general relation of the type $R \sim (L/\ln L)^x$ is assumed, one finds $x \simeq 1.5$ and not unity.

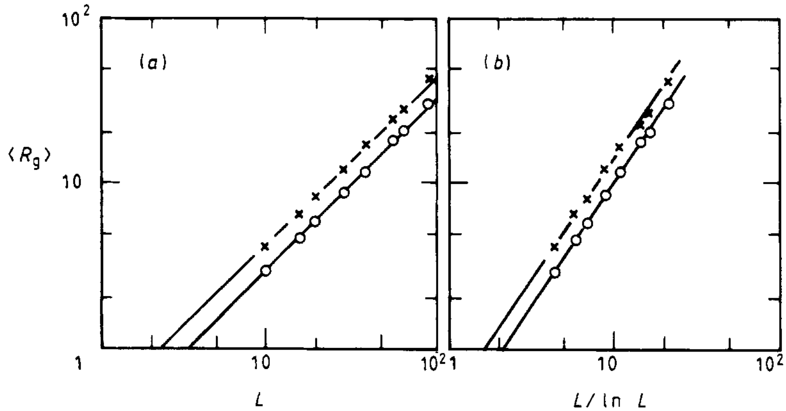

Figure 4. Log-log plot of the average radius of gyration against L with a slope $\simeq 1.0$ (a), and against $L/\ln L$ with a slope $\simeq 1.5$ (b). The symbols correspond to the two touching conditions: (○) at least one site on the boundary is damaged; (×) at least one site is damaged on each of the three boundary planes (100, 010, 001).

As a consequence, the situation seems rather contradictory: in order to reconcile our numerical data with the theory prediction we have to assume in one case logarithmic corrections to scaling, and in the other case a logarithmic prefactor, without being able to reach consistency using either logarithmic corrections or a logarithmic prefactor in both cases.

There could be, however, a possibility to explain this scenario. It has recently been shown [15] that the dynamical scaling of the structure function of growing domains in a nucleation problem has a much richer behaviour, also expected to be characteristic of other growth phenomena. By an exact analytical solution of the time-dependent

Ginzburg–Landau model a novel form of scaling has been detected, which finds its origin in the existence of two scaling lengths in the problem, one marginally different from the other. Because of the resulting so-called *multiscaling*, an infinity of growing exponents is then obtained by continuously varying a given characteristic parameter.

We assume now the possibility of a similar type of multiscaling to also hold in the damage spreading problem. In order to do so, for each cloud of a given radius of gyration R_g we fix the value of the parameter x and we calculate the mass $m(x)$ contained within a shell confined between $r = xR_g$ and $r' = (x+1)R_g$. We look then at the scaling dependence of the quantity $m(x)$ as function of R_g at a fixed value of x.

If dynamical multiscaling holds, a scaling of the form

$$\rho(r, R_g) = r^{-[d-d_f(r/R_g)]} f\left(\frac{r}{R_g}\right) \tag{3}$$

should be found for the density $\rho(r, R_g)$ and the fractal dimension d_f should continuously depend on the parameter $x = r/R_g$. The multiscaling would then reflect the rich internal structure of the cloud where shells with different x do exhibit independent scaling exponents. The expected value of d_f would then be recovered in the limit $x \to 0$.

One can evaluate the total mass of the cloud D by integrating (3)

$$D \propto \int_0^L \rho(r, R_g) r^{d-1}\, \mathrm{d}r = \int_0^{L/R} R^{d_f(x)} x^{d_f(x)-1} f(x)\, \mathrm{d}x \tag{4}$$

and assuming that $d_f(x) = d_f(0) - \beta x^2$, one finds by saddle point integration

$$D \propto \frac{R^{d_f(0)}}{(\ln R)^y} \tag{5}$$

where y depends on the form of $f(x)$. This is actually the general expression for a scaling variable of the log-prefactor type discussed above. If on the contrary $d_f(x)$ is constant for small x by similar arguments one finds a logarithmic correction. The form of $d_f(x)$ could well differ if the averages are taken over all the clouds or only over the touching ones. This difference in averaging could very well explain the discrepancy between the data of figure 1 and figure 3. The hypothesis of multiscaling made to obtain this result is currently the object of further investigation.

Since the physical picture behind the multiscaling behaviour is that the outer regions of the spreading damage cloud have lower fractal dimensions than the inner regions, we measure the number of sites in the damage cloud at touching distance, i.e. on the boundary of the system (figure 5). As a function of the system size the number of damaged sites on the boundary does remain constant and about equal to one. This is no longer valid if, for instance, one uses as a touching condition the requirement that the cloud touches the boundaries in all three directions at the same time. In this case, the damage at the boundary does show some power law dependence on the system size with an exponent roughly equal to 0.75 (figure 5). It is however worth stressing that the scaling behaviour of the whole damage cloud is independent of the touching condition, which only affects the amplitude factor in the mass-radius relation. The fact that different touching conditions show different scaling behaviours hints to the existence of the multiscaling given in (3).

In conclusion, we have found that the damage clouds introduced in [3] show a very slow convergence toward the expected fractal dimension $d_f = d - \beta/\nu$. This can be explained either by a logarithmic correction or by a logarithmic prefactor. The

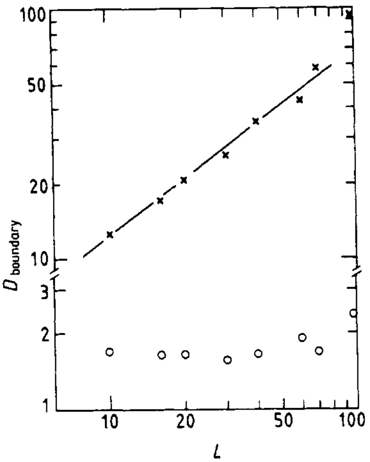

Figure 5. Log–log plot of the mass of the damage cloud on the boundaries of the lattice at the time of touching against L using the two touching conditions as in figure 4. For the touching condition in all three directions the scaling exponent is equal to about 0.75.

scenario is compatible with the multiscaling behaviour of the radial density of the clouds, a point which is currently under investigation.

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