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LETTER TO THE EDITOR

Gradient method for thermal phase transitions

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Abstract. We present a new numerical method of obtaining critical temperatures and exponents for ferromagnetic spin models and dynamical transitions. This method is based on the spreading of damage in a temperature gradient. We illustrate the method on the two-dimensional Ising model and present new results on the ± Ising spin glass in two dimensions. We also obtain new critical exponents, describing the behaviour of the width and the length of the damage front.

The numerical determination of critical temperatures and critical exponents has led to the invention of many different techniques and algorithms over the last twenty years. Nevertheles, in this letter, we are proposing a new method based on recent understanding about the spreading of 'damage' in a thermal model [1-4], and applying it to a temperature gradient.

'Damage' is defined as the 'Hamming' distance between two configurations that evolve under exactly the same dynamics. In the case of Ising variables $\sigma = 0, 1$ the damage D between two configurations A and B is given by the fraction of sites having different values (i.e. being damaged):

$$D(t) = \frac{1}{N} \sum_i |\sigma_i^{\mathrm{A}}(t) - \sigma_i^{\mathrm{B}}(t)| \tag{1}$$

where N is the number of sites of the system.

It has been shown [1] that if one uses, in a ferromagnetic model, heat bath dynamics with the same random numbers for both configurations, the probability of having a damaged site equals the spontaneous magnetization. In particular, all initial damage disappears in the paramagnetic phase after a time proportional to the relaxation time. In the ferromagnetic phase, however, a finite amount of damage survives in the thermodynamic limit and one then has $D(\infty) \to M$. If one has in a system a temperature gradient such that one end is in the paramagnetic phase ($T > T_c$) and at the other end is in the ferromagnetic phase ($T < T_c$) the initial damage in the ferromagnetic phase will only spread until it reaches the critical temperature T_c. Similarly, if initially one has damage at all temperatures, it will only completely heal within a region $T > T_c$.

We consider a square lattice of size $L_\parallel (L_\perp)$ in the x- (y-) direction and impose periodic boundary conditions in the y-direction and fixed boundary conditions in the x-direction. Each line of fixed x-coordinate has a different temperature. On the left (right) boundary we impose a temperature $T_f < T_c$ ($T_p > T_c$) and on line j:

$$T(j) = T_f + \frac{T_p - T_f}{L_\parallel - 1}(j-1). \tag{2}$$

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This means that on each line perpendicular to the x-axis one has other values for the Boltzmann factors, so that technically speaking each line has its own look-up table in the Monte Carlo algorithm. We also consider a zeroth and a $(L_\parallel+1)$th line on which the spins are fixed.

Take two lattices A and B of the type described above. On lattice A(B) we initially set all the spins to 1(0), i.e. $D(0)=1$. On the zeroth line the spins are fixed in the same way while on the $(L_\parallel+1)$th line the fixed spins are randomly chosen but have the same value for both configurations A and B. We then let both systems evolve towards equilibrium using heat bath dynamics with the same random number sequence applied to A and B. After waiting several times the (nonlinear) correlation time, τ_{nl}, the system is considered to be in equilibrium. In our case the dominant correlation time is the one at T_c which should scale as a power law in $L_\perp$.

At equilibrium one finds for each Monte Carlo iteration damaged sites in the region $T<T_c$. If one says that two neighbouring damaged sites belong to the same cluster there is one (infinite) damage cluster connected to the left end (since on the zeroth line one has a fixed source of damage). To this cluster one can define an outer boundary or front (see figure 1) consisting of all the bonds between sites of the cluster and undamaged sites that are connected to the right end of the system by a path of nearest neighbouring undamaged sites (i.e. belonging to the infinite cluster of undamaged sites). The number of these bonds, l, is the length of the front. Since each bond k of the front has a well defined temperature T_k one can define

$$T_m=\frac{1}{l}\sum_k T_k \qquad \text{and} \qquad w=\sqrt{\frac{1}{l}\sum_k (T_k-T_m)^2} \tag{3}$$

as the average temperature and the width of the front. We expect $T_m \to T_c$ and $w \to 0$

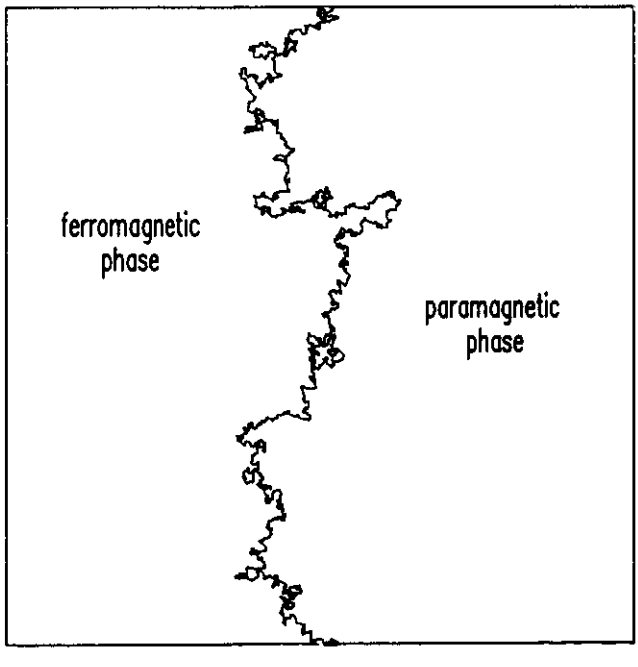

Figure 1. Front of the infinite damage cluster as obtained in an Ising model on a square lattice with $L_\parallel = L_\perp = 512$.

when the gradient

$$\Delta = (T_p - T_f)/L_\parallel \tag{4}$$

vanishes, i.e. in the thermodynamic limit.

We implemented the above algorithm using multispin coding, i.e. putting 16 sites in one single computer word of 64 bits of a Cray-XMP. The infinite cluster was obtained by burning [5], i.e. by letting a front of labelled ('burned') sites spread on the cluster over nearest neighbours such that a site can at most be burned at one time step. If the burning starts at the left end, exactly the infinite damage cluster will be burned. The burning can also be implemented in multispin coding by putting on one bit iff the site is damaged and a second one iff the site is burning at that time step. The second bit at the next time step is then obtained as a logic AND of the first bit with an OR over the second bits of all the nearest neighbours. These logical operations are executed for all the bits in parallel, speeding up the process by a factor of 16. Contrary to the Monte Carlo update the burning cannot, however, be vectorized.

In order to extrapolate to the thermodynamic limit we will consider our quantities as a function of Δ and $L_\perp$. We can expect:

$$T_m(L_\perp, \Delta) = aL_\perp^{-1/\nu} + b\Delta^x \qquad \text{and} \qquad w(\Delta) = c\Delta^y \tag{5}$$

where x and y are *a priori* unknown exponents and a, b and c are constants.

It turns out that $x < 1$ so that the second term dominates the behaviour of T_m. This is reflected numerically in the fact that the data depend much more strongly on the gradient than on $L_\perp$. This can be seen in figure 2 where we plotted T_m for the Ising model, obtained through various methods as shown by different symbols: the squares and diamonds were made for $L_\parallel = L_\perp$ in the first case with the same T_p and T_f for all $L_\perp$ and in the second case by adjusting T_p and T_f such that the front nearly touches the boundary. The stars are data for $L_\parallel \ll L_\perp$. The same notation of symbols is also used in figure 3.

The data in figure 2 collapse on a straight line for $x = 0.55 \pm 0.05$ which extrapolated to $T_c = 2.269 \pm 0.001$, in good agreement with the exact value. In figure 3 we see that indeed w has the power law behaviour of (5) with an exponent $y = 0.51 \pm 0.01$.

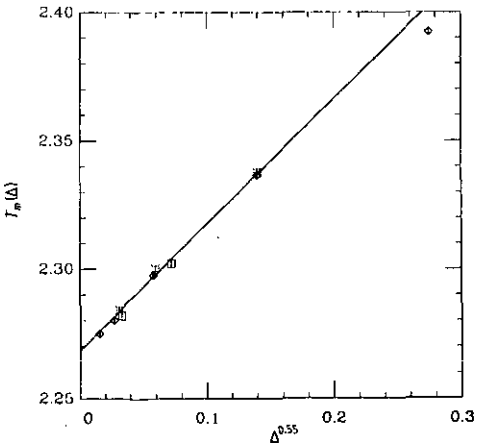

Figure 2. Average temperature T_m of the front as a function of $\Delta^{0.55}$ for the Ising model. The statistical error bars can be seen to fall inside the symbols.

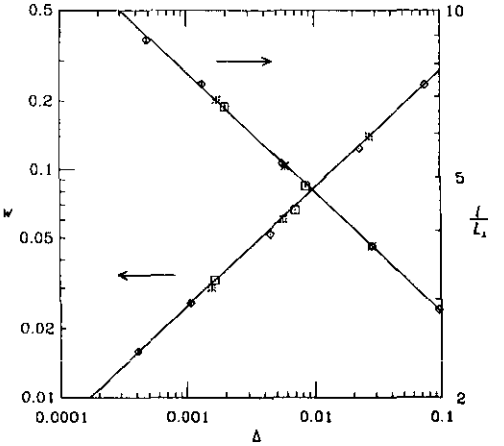

Figure 3. Log-log plot of the width (right axis) and $l/L_\perp$ (left axis) as a function of the gradient for the Ising model.

This is in good agreement with

$$y = \frac{1}{1+\nu} \tag{6}$$

which can be obtained by the following argument [6]. One considers that the width of the front comes from damage clusters at $T_0 \neq T_c$ of size $\xi(T_0)$ that touch the front so that the condition $w \propto \Delta\xi(T_m \pm w)$ should be fulfilled. Using the fact that the correlation length goes like $\xi(T) \propto |T - T_c|^{-\nu}$, and making a Taylor expansion around the critical temperature gives $w \propto \Delta w^{-\nu}$ and thus (6).

Let us investigate next if the front shown in figure 1 is self-affine:

$$l(L_\perp, \Delta) \sim L_\perp \Delta^{-\delta}. \tag{7}$$

In figure 3 we see in a log-log plot of $l/L_\perp$ against Δ that one obtains a straight line of slope $\delta = 0.214 \pm 0.003$ in agreement with (7). By considering that the front lives in a box of size $L_\perp \times w/\Delta$ one can define a fractal dimension d_f [7] through $l \sim L_\perp (w/\Delta)^{d_f - 1}$ and this gives, using (6) and (7):

$$d_f = 1 + \frac{1+\nu}{\nu}\delta \tag{8}$$

so we have $d_f = 1.43 \pm 0.01$. This number does not coincide with the dimension of the hull of the critical clusters [8] or with that of the hull of the spin-up clusters at T_c [9].

We also made the same analysis for the ± Ising spin glass on the square lattice. In this case no theorem is available relating the damage to thermodynamic quantities. Although it is generally believed that there is no thermodynamic transition for this model in two dimensions it has been numerically observed [10] that using a heat bath there is a dynamic phase transition between a 'frozen' phase, where all damage heals as in the paramagnetic phase of the ferromagnetic model and, at low temperatures, a 'choice' phase in which any infinitesimally small damage spreads to infinity. In figure 4 we show the results we obtained for the spreading of damage in a gradient. The relaxation times are much longer for the spin glass compared with the ferromagnetic model so we started for each data point from an ordered, as well as from a disordered, initial configuration and made sure that both converged to the same value. From

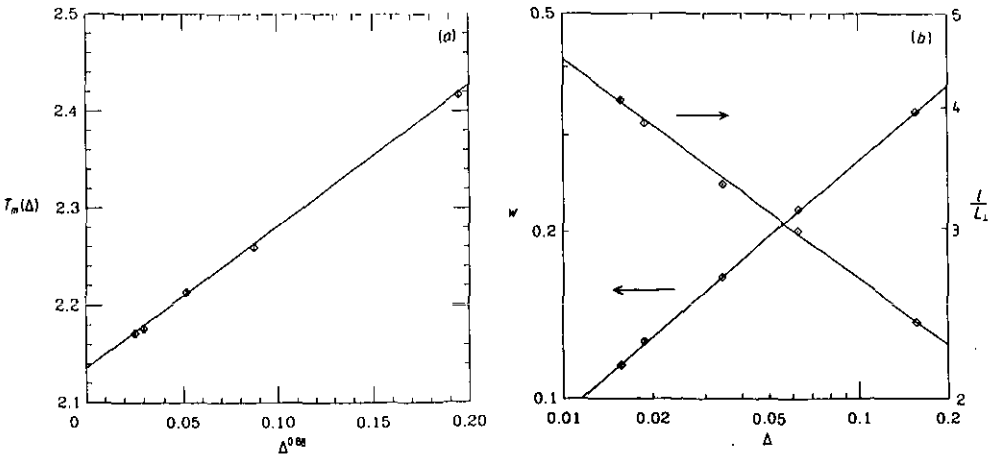

Figure 4. Same as figures 2 and 3 for the ± Ising spin glass on a square lattice.

figure 4 we obtain $T_d = 2.137 \pm 0.005$ for the dynamic transition temperature, a larger value than found previously [10], excluding from its error bars the critical point of the pure Ising model. For the exponents we find: $x \approx 0.88$, $y = 0.458 \pm 0.005$ and $\delta = 0.225 \pm 0.005$. These values give using (6) and (8): $\nu = 1.18 \pm 0.02$ and $d_f = 1.72 \pm 0.02$.

We have proposed a method of obtaining precise transition temperatures and critical exponents of the dynamical damage spreading transition. We do this by considering a temperature gradient similar to the gradient in the probability that was applied to percolation [6, 11] and to the Kauffman model [12], and which in both cases also gave very accurate results. For the ferromagnetic Ising model, where an exact relation to the thermal phase transition is available, our method agrees with high precision with the exactly known numbers. We have, however, not yet found a relation between the fractal dimension of the damage front and known critical exponents. For the spin glass we confirm the existence of a damage phase transition and obtain values for the transition temperature, ν, and the fractal dimension of the front.

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