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DYNAMICAL PHASE TRANSITIONS AND SPIN GLASSES

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Abstract:

By measuring the distance between two configurations subjected to the same thermal noise, one observes for spin glasses three phases: a high-temperature phase ($T > T_1$), where the distance between the two configurations vanishes in the long-time limit; an intermediate phase ($T_2 < T < T_1$), where this distance has a nonzero limit independent of the initial distance; a low-temperature phase ($T < T_2$), where the distance depends on the initial distance. For the 3d and 4d $\pm J$ spin glasses, the results of Monte Carlo simulations give clear evidence for the existence of these three phases. For the Sherrington–Kirkpatrick model, T_1 is infinite whereas T_2 is close to the equilibrium transition temperature. For the 2d $\pm J$ spin glass, the behavior at high and low temperature is similar to that of the 3d and 4d models but there is much less evidence for the presence of the intermediate phase and for well-defined transition temperatures between these phases.

1. Introduction

For a large class of spin models in statistical mechanics, one observes sharp dynamical phase transitions [1–6] when one compares the time evolution of two spin configurations subjected to the same thermal noise. These dynamical phase transitions usually separate two phases:

A high-temperature phase, where the two spin configurations become identical quickly. In this phase, the effect of thermal noise is strong enough to make the two configurations quickly forget their initial conditions and the distance between them vanishes.

A low-temperature phase, where the two configurations remain at a finite distance in the long-time limit (if the system size is large enough). Several effects can be responsible for this non-zero distance. Either phase space consists of several valleys separated by high free energy barriers and the two configurations do not meet because they fall into distinct valleys. Or the two configurations belong to the same valley in phase space but the dynamics is chaotic: two close configurations have the tendency to diverge (the dynamics has positive Lyapunov exponents).

This dynamical phase transition associated with the distance between two configurations has been studied up to now in a large class of systems: ferromagnets [1, 3, 4], 2d ANNNI model [2], spin glasses [1, 5], automata [6]. Several analytic results have been established concerning this dynamical phase transition. Firstly, one can calculate the time evolution of the distance exactly for some mean field models [3, 5] and one finds that above a certain temperature the distance tends to zero whereas at low temperature it does not. Secondly, one can show [7] that in the case of Ising spins with ferromagnetic interactions only, the dynamical transition coincides with the Curie temperature.

Numerical studies of other models (ANNNI model [2], spin glasses [1]) give a temperature for this dynamical transition which seems higher than the transition temperature which is observed when one studies the system at equilibrium. However, at least in the case of spin glasses [1], one can observe a second dynamical transition temperature below which the distance between the two configurations

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depends on their initial distance. In the case of the 3d spin glass [1], this second dynamical transition is rather close to the true spin glass phase transition.

In the present paper, the calculations of ref. [1] will be extended to the case of 2d, 3d, 4d, and infinite-dimension $\pm J$ spin glasses with sequential dynamics. We will see that the three phases can be observed in three and four dimensions. In infinite dimensions, the high-temperature phase disappears whereas in two dimensions the existence of sharp transitions and of the intermediate phase is much less clear.

2. The heat bath dynamics

For a system of N Ising spins $S_i = \pm 1$ interacting through the hamiltonian

$$\mathscr{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j \,, \tag{1}$$

the updating rule used here is the following. To obtain the configuration $\{S_i(t+\Delta t)\}$ of the system at time $t+\Delta t$, with

$$\Delta t = 1/N \,, \tag{2}$$

from its configuration $\{S_i(t)\}$ at time t, one chooses one spin i at random among the N spins and one updates it according to Glauber dynamics,

$$\begin{aligned} S_i(t+\Delta t) &= 1 \quad \text{with probability } \tfrac{1}{2} + \tfrac{1}{2}\tanh\Big(\sum_j \frac{J_{ij} S_j(t)}{T}\Big) \,, \\ &= -1 \quad \text{with probability } \tfrac{1}{2} - \tfrac{1}{2}\tanh\Big(\sum_j \frac{J_{ij} S_j(t)}{T}\Big) \,, \end{aligned} \tag{3}$$

where T is the temperature. With this dynamics, one can show that in the long-time limit, each spin configuration $\{S_i\}$ is visited with a probability $\exp[-\mathscr{H}(\{S_i\})/T]$. To implement this dynamics, at each time step Δt, one chooses a random number $z(t)$ uniformly distributed between 0 and 1 and one obtains $S_i(t+\Delta t)$ by

$$S_i(t+\Delta t) = \operatorname{sign}\Big[\tfrac{1}{2} + \tfrac{1}{2}\tanh\Big(\sum_j \frac{J_{ij} S_j(t)}{T}\Big) - z(t)\Big] \,. \tag{4}$$

In order to compare the time evolution of two configurations $\{S_i(t)\}$ and $\{\tilde{S}_i(t)\}$ subjected to the same thermal noise, one chooses at each time step Δt, the same site i for the two configurations and the same random number $z(t)$,

$$\begin{aligned} S_i(t+\Delta t) &= \operatorname{sign}\Big[\tfrac{1}{2} + \tfrac{1}{2}\tanh\Big(\sum_j \frac{J_{ij} S_j(t)}{T}\Big) - z(t)\Big] \,, \\ \tilde{S}_i(t+\Delta t) &= \operatorname{sign}\Big[\tfrac{1}{2} + \tfrac{1}{2}\tanh\Big(\sum_j \frac{J_{ij} \tilde{S}_j(t)}{T}\Big) - z(t)\Big] \,. \end{aligned} \tag{5}$$

In the limit $T \to \infty$, each time a spin is updated, this spin becomes identical in the two configurations. This means that the effect of using the same random numbers is to make the two configurations attract each other.

The first quantity one can measure to compare the two configurations is their distance $\Delta(t)$ at time t,

$$\Delta(t) = \frac{1}{2N} \sum^{N} |S_i(t) - \tilde{S}_i(t)| . \tag{6}$$

This distance $\Delta(t)$ counts the number of spins which are different in configurations $\{S_i(t)\}$ and $\{\tilde{S}_i(t)\}$ at time t. Usually, the calculations are repeated for many samples and the quantity which is measured is the average $\langle \Delta(t) \rangle$ over these samples.

If for any reason (finite size effects, fluctuations, etc.) the two configurations become identical at some time t, they remain identical at all later times. As a result it is more convenient to average the distance $\Delta(t)$ only over those samples which have survived at time t, i.e., such that $\Delta(t) \neq 0$. To do so, one can introduce the survival probability $P(t)$ defined as the fraction of samples for which the two configurations $\{S_i(t)\}$ and $\{\tilde{S}_i(t)\}$ are still different at time t. Then the distance $\langle D(t) \rangle$ obtained by averaging over those samples only is given by

$$\langle D(t) \rangle = \langle \Delta(t) \rangle / P(t) . \tag{7}$$

3. Distances in spin glass models

In this section, the results of numerical simulations done to measure $\langle D(t) \rangle$ for four spin glass systems are presented. The models studied here are the Sherrington–Kirkpatrick [8] model with interactions $J_{ij} = \pm 1/\sqrt{N}$ and the $\pm J$ spin glass model on a 4d hypercubic, 3d cubic and 2d square lattice.

In all cases $\langle \Delta(t) \rangle$ and $P(t)$ were calculated by averaging over 100 samples. For each system, two lattice sizes were used ($N = 256$ and 512 for the SK model, $N = 4^4$ and 6^4 for the 4d model, $N = 8^3$ and 12^3 for the 3d model, $N = 16^2$ and 32^2 for the 2d model).

For each model, the following three initial conditions were considered:
- situation A: $\{S_i(0)\}$ is random and $\{\tilde{S}_i(0)\} = -\{S_i(0)\}$;
- situation B: $\{S_i(0)\}$ and $\{\tilde{S}_i(0)\}$ are random and uncorrelated;
- situation C: $\{S_i(0)\}$ is random and $\{\tilde{S}_i(0)\}$ is identical to $\{S_i(0)\}$ except for one spin: $\tilde{S}_i(0) = S_i(0)$ for $i \geq 2$ and $\tilde{S}_1(0) = -S_1(0)$.

Similar calculations had been done [1] for the 3d $\pm J$ spin glass in the case of parallel dynamics.

Lastly, all the results shown in the present paper correspond to the time $t = 500$ Monte Carlo steps per spin.

Figure 1 shows $\langle D(t) \rangle$ for the SK model. We see that the distance $\langle D(t) \rangle$ does not vanish at any temperature (this has been checked up to $T \simeq 4$ and $\langle D(t) \rangle$ seems to decrease like T^{-2}). So the temperature T_1 above which $\langle D(t) \rangle$ vanishes is infinite for the SK model. We see also that (as for the 3d spin glass [1]), there exists a phase $T_2 < T < T_1 = \infty$ where the distance $\langle D(t) \rangle$ does not depend on the initial distance. From fig. 1, one can estimate $T_2 \simeq 0.9$. This estimate is rather close to the spin glass transition $T_c = 1$ of the SK model and it is plausible that T_2 and T_c are the same temperature since the data corresponding to different distances come together in a tangential way. Of course it would be very

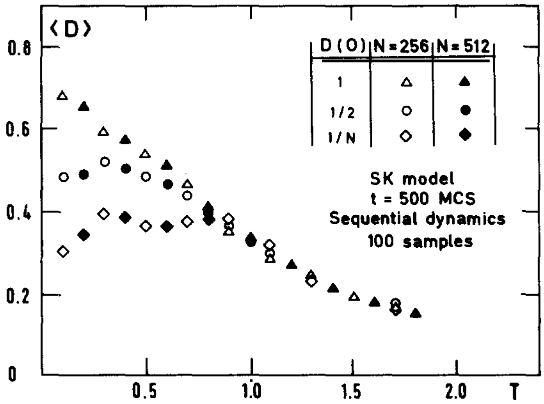

Fig. 1. SK model. The distance $\langle D(t)\rangle$ versus temperature T for three initial distances; opposite initial conditions $[D(0)=1]$, uncorrelated initial conditions $[D(0)=1/2]$, identical initial conditions except for one spin $[D(0)=1/N]$.

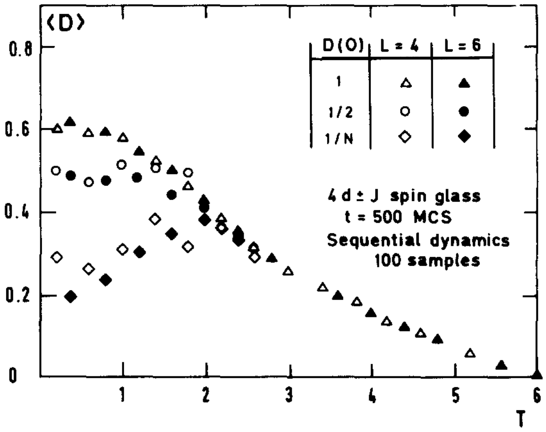

Fig. 2. The distance $\langle D(t)\rangle$ versus temperature (as in fig. 1) for the 4d $\pm J$ spin glass.

interesting to improve the data for the SK model in order to know whether T_2 and T_c coincide. This would require a careful analysis of the time and size dependence of T_2.

Figure 2 shows the data obtained for the four-dimensional $\pm J$ spin glass. The statistics (100 samples) is clearly not sufficient to get a good estimate of T_2. One can, however, see that the distance $\langle D(t)\rangle$ vanishes above T_1 with $T_1 \simeq 6$, and that $\langle D(t)\rangle$ is nonzero but independent of $\langle D(0)\rangle$ for $T_2 < T < T_1$ with $T_2 \simeq 2.0 \pm 0.4$. For $T < T_2$, $\langle D(t)\rangle$ depends on $D(0)$.

Figure 3 shows the distance $\langle D(t)\rangle$ for the 3d $\pm J$ spin glass. The fluctuations are smaller than in four dimensions. One finds again three phases: For $T > T_1$, $\langle D(t)\rangle$ vanishes. For $T_2 < T < T_1$, $\langle D(t)\rangle$ is nonzero but independent of $D(0)$. For $T < T_2$, $\langle D(t)\rangle$ depends on $D(0)$. From fig. 3, one can estimate $T_1 \simeq 4.0$, $T_2 \simeq 1.5 \pm 0.2$. These results (and the estimates of T_1 and T_2) for the 3d problem with sequential dynamics are almost identical to those obtained for 3d problem with parallel dynamics. The temperature $T_c \simeq 1.2$ of the spin glass transition [9] is again close to T_2.

Figure 4 shows the data for the 2d case. An important difference with the previous cases is that one does not observe the intermediate phase $T_2 < T < T_1$, where the distance $\langle D(t)\rangle$ depends neither on

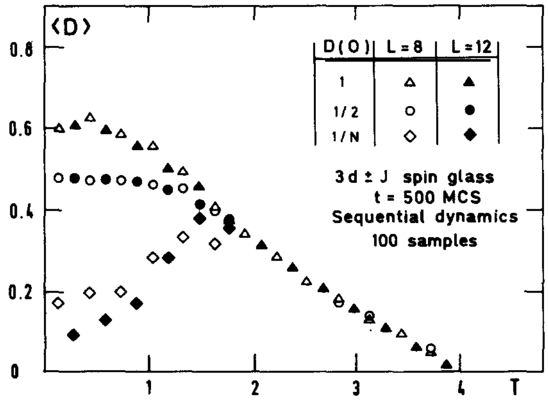

Fig. 3. The distance $\langle D(t)$ versus temperature (as in figs. 1 and 2) for the 3d $\pm J$ spin glass.

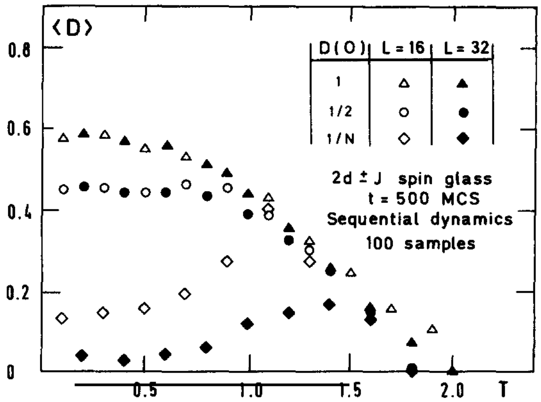

Fig. 4. The distance $\langle D(t)\rangle$ versus temperature (as in figs. 1, 2 and 3) for the 2d $\pm J$ spin glass.

the size nor on the initial distance $D(0)$. We see nevertheless on fig. 4 that $\langle D(t) \rangle$ vanishes above a temperature $T \sim 1.8 \pm 0.2$ and does not vanish below. At low temperature, the results are very similar to those of the 3d and 4d models. This means that at least after 500 MCS, the data on the distance $\langle D(t) \rangle$ at low temperature do not show any evidence for a different behavior in two dimensions and in more dimensions. In this two-dimensional case as well, a careful study of the time and size dependence of the data would be very useful in order to decide whether the 2d and higher-dimensional systems are similar or not.

4. Conclusion

In this paper, some preliminary results concerning the distance between two configurations subjected to the same thermal noise were presented. In three and four dimensions, three different phases can be observed: a high-temperature phase $T > T_1$, where the distance vanishes; an intermediate phase $T_2 < T < T_1$, where the distance does not vanish but is independent of the initial distance; a low-temperature phase $T < T_2$, where the distance depends on the initial distance. In two dimensions, the results look very similar to those of $d = 3$ and 4 at high and low temperatures but the existence of the intermediate phase is much less clear than in $d = 3$ and 4. For the SK model, the results look very similar to the 3d case except that the high-temperature phase disappears ($T_1 = \infty$).

In the numerical results shown here (in $d = 3$ and for the SK model) the temperature T_2 (which is defined as the temperature below which the distance starts to depend on the initial distance) seems to be close to the spin glass phase transition. Since the curves $\langle D(t) \rangle$ always depend on the system size and on the time t at which the distance is measured, it is hard to know whether T_2 and the spin glass transition are the same or not. To answer that question, a careful study of the time and size dependence of T_2 would be needed.

A finite size scaling method has been developed [4] which allows one to determine T_1 rather accurately. The method consists in measuring the time $\tau(L, T)$ it takes for the distance to vanish as a function of the system size L and of the temperature T, and in using finite size scaling ideas to estimate T_1 where $\tau(L, T)$ diverges as $L \to \infty$. In the case of T_1, the time $\tau(L, T)$ can be calculated easily because for a given sample, one knows that once the distance vanishes, it remains zero for ever.

It seems that it would be possible to use similar ideas to estimate T_2. Since T_2 is the temperature where remanence effects associated with the distance appear, one can start with three initial conditions $\{S_i^{(1)}(0)\}$, $\{S_i^{(2)}(0)\}$ and $\{S_i^{(3)}(0)\}$, such that the distance $D_2(0)$ between $\{S_i^{(1)}(0)\}$ and $\{S_i^{(2)}(0)\}$ is $\frac{1}{2}$ and the distance $D_3(0)$ between $\{S_i^{(1)}(0)\}$ and $\{S_i^{(3)}(0)\}$ is 1. Then for each sample, one can define a remanence time $\tau(L, T)$ as the time such that $D_2(\tau) = D_3(\tau)$ for the first time. From the data on this remanence time $\tau(L, T)$, one should be able to measure T_2 rather accurately using finite size scaling ideas.

It would be interesting to do these finite size scaling calculations of T_2 because one could know how the dynamical phase transition T_2 associated with the remanence effects (which are purely dynamical effects) is related to the spin glass phase transition.

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