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Autor(en): **Ariosa, D. / Droz, M. / Malaspinas, A.**

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Numerical study of a long range Ising spin-glass: exact results for small samples and Monte-Carlo simulations

by D. Ariosa, M. Droz and A. Malaspinas, Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

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Abstract. A long range Ising spin-glass, in which the spins have a random position and interact, through a Ruderman–Kittel–Kasuya–Yosida interaction, is studied. Chains of $N = 8, 12$ and 16 spins are exactly solved while a chain with 48 spins is analysed by Monte-Carlo technique. Extrapolation to infinite chain is performed and it is shown that this system has a clear paramagnetic spin-glass transition. The qualitative features of this transition are shown to agree with the predictions of the Parisi–Toulouse hypothesis.

I. Introduction

Despite the vast amount of efforts that have been expended in recent years to explain the nature of the paramagnetic spin-glass phase transition, several important questions have not yet received a clean cut answer [1]. For example, one does not have a complete mean field theory for a spin glass. One way of defining a mean field theory consists in considering a model with infinite range interactions. The most studied model of this type is the Sherrington Kirkpatrick [2] (SK) model in which, Ising spins on a lattice interact through a random interaction J_{ij}. Although this model has not been solved completely, Parisi [3] gave a convincing approximate solution to it. The physical content of Parisi's solution has been reformulated in simple terms by Parisi and Toulouse [4]. The so-called Parisi and Toulouse (or PaT) projection hypothesis can be stated as follows: the parameter space (T, h), where T is the temperature and h the magnetic external field, is divided into two domains by the Almeida Thouless instability line [5]. In the high temperature domain, the spins behave as free spins. However in the low temperature phase, i.e., the spin-glass phase, the system is suddently frozen and the magnetization $m(T, h)$ is independent of the temperature T. Thus the thermodynamic properties of the spin-glass phase are obtained by projection from the instability line. Recent experiments on CuMn and AgMn [6] show a behaviour of the magnetization in agreement with the PaT hypothesis. These results suggest that the type of ordering predicted by PaT is not particularly to the SK model but may be a general feature for a spin-glass. It is thus legitimate to study other models of spin-glass than the SK model in this perspective.

It is well known that in substances like CuMn for example, the magnetic ions interact via the indirect exchange interaction of Ruderman–Kittel–Kasuya–Yosida (RKKY) [7]. The positions $\{\mathbf{x}_i\}$ of the impurities are random but the interactions

between them are deterministic. Most of the theoretical descriptions of spin-glass assume that the positions of the magnetic impurities are well defined (the sites of a lattice) while the interactions are random variables. It is not obvious that this later description is totally equivalent to the physical one and thus it is interesting to test this point.

In this paper, we consider a model which allows us to address ourselves to the above questions, namely, the behaviour of the system in its low temperature phase (by comparison with the PaT hypothesis) and the role of the positional disorder. The model consists of an one dimensional assembly of spins interacting via a long range one dimensional RKKY like interaction, the positions of the spins on the chain being random.

The paper is organized as follows. In Section II, the model is defined and the methods used for solving it are discussed. Section III is devoted to the exact statistical mechanics of small chains and the extrapolation to the thermodynamic limit. The internal energy, magnetization and the susceptibility are computed. The problem of the order parameters associated with the ordered phase is discussed and the order parameter Q is explicitly computed for different values of N. The results obtained are compared with similar results obtained recently for SK model [8, 9]. In Section IV, a 48 spins chain is analyzed by Monte-Carlo simulation. The simulation exhibits clearly two types of susceptibilities: the reversible and the irreversible one. These two types of behaviour are explained in terms of metastable states and breaking of the ergodicity in the spin-glass phase. Finally, in the conclusion, the results obtained are analyzed by comparison with the PaT hypothesis.

II. The model

We consider an assembly of N Ising spins $s_i = \pm 1$ randomly distributed on a chain in an external magnetic field h. The distances between the spins $\{\mathbf{x}_i - \mathbf{x}_{i-1}\}$ are random and the spins interact through a one dimensional RKKY-like interaction. It is easy to extend the original derivation of RKKY [7] to an arbitrary dimension. In particular, for $d = 1$, one finds

$$J_{ij} = J_0 \frac{\cos(\alpha |\mathbf{x}_i - \mathbf{x}_j|)}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{II.1}$$

for $\alpha |\mathbf{x}_i - \mathbf{x}_j| \gg 1$ where α is twice the Fermi wave vector of the host metal and is taken as a parameter in our calculation.

The position $\{\mathbf{x}_i\}$ being distributed randomly, we have to avoid the situation where $|\mathbf{x}_i - \mathbf{x}_j|$ becomes too small, making the interaction J_{ij} to diverge. This is easily obtained by changing slightly the denominator of (II.1). The interaction chosen is then:

$$J_{ij} = J_0 \frac{\cos(\alpha |\mathbf{x}_i - \mathbf{x}_j|)}{|\mathbf{x}_i - \mathbf{x}_j| + 1} \equiv J_0 V_{ij} \tag{II.2}$$

and the hamiltonian reads:

$$H = \sum_{i<j}^{N} J_{ij} S_i S_j - h \sum_{i}^{N} S_i \tag{II.3}$$

To avoid ambiguities with the boundary conditions and the symmetry of the interaction (II.2), we work with an open chain.

The quantities of interest are quenched averages. Let $\{J_{ij}\}$ a given configuration of the interactions and $P(\{J_{ij}\})$ the probability distribution of $\{J_{ij}\}$. The quenched free energy is defined as:

$$\bar{F} = -k_B T \langle F(\{J_{ij}\})\rangle_J \tag{II.4}$$

where

$$\bar{A} = \langle A(\{J_{ij}\})\rangle_J \equiv \int \prod_{ij} dJ_{ij} P(\{J_{ij}\}) A(\{J_{ij}\}) \tag{II.5}$$

and

$$F(\{J_{ij}\}) = \ln \operatorname{Tr}_{\{S_i\}} \exp\left[\frac{-H(\{J_{ij}\})}{k_B T}\right] \tag{II.6}$$

is the free energy for the configuration $\{J_{ij}\}$.

The numerical results for the average ground state energy $\bar{E}_0(N)$, (see Section III.D), indicate that the model as defined by (II.2) does not yield an extensive free energy. To have a well defined thermodynamic limit, we must then replace the coupling J_0 by $J_0/\rho(N)$, $\rho(N)$ being such that the free energy becomes extensive. By studying a non-frustrated version of the model, obtained by replacing V_{ij} by $|V_{ij}|$ in (II.2), one can show that $\rho(N) \leq \ln N$. However, we were not able to find $\rho(N)$ analytically and we shall determine it numerically in the following sections.

Other quantities of interest for our problem are the internal energy per spin

$$u(\{J_{ij}\}) = \frac{1}{N} \frac{\operatorname{Tr}_{\{S_i\}}\left[\exp\left(\frac{-H}{k_B T}\right) H\right]}{\operatorname{Tr}_{\{S_i\}} \exp\left(\frac{-H}{k_B T}\right)} = \frac{1}{N}\langle H\rangle_T \tag{II.7}$$

and its configuration average

$$\bar{u} = \frac{1}{N}\langle\langle H\rangle_T\rangle_J, \tag{II.8}$$

the magnetization per spin given by

$$m(\{J_{ij}\}) = \frac{1}{N}\left\langle \sum_i s_i \right\rangle_T = \frac{1}{N} \frac{\operatorname{Tr}_{\{S_i\}}\left[\sum_i s_i \exp\left(\frac{-H}{k_B T}\right)\right]}{\operatorname{Tr}_{\{S_i\}} \exp\left(\frac{-H}{k_B T}\right]} \tag{II.9}$$

and its configurational average

$$\bar{m} = \frac{1}{N}\left\langle\left\langle \sum_i s_i \right\rangle_T\right\rangle_J \tag{II.10}$$

The magnetic susceptibility $\chi(T)$ is defined by

$$\chi(T) = \lim_{h \to 0} m(\{J_{ij}\}, h)/h \tag{II.11}$$

and similarly its configurational average $\bar{\chi}(T)$. As we shall see in the next section, the limit $h \to 0$ in (II.11) only makes sense for infinite systems. For finite systems, the limit in (II.11) should be reinterpreted.

We can now proceed and compute the above quantities for our model. Due to the complicated form of the interaction, it is not possible to solve the problem analytically and thus, we used two different methods:

i) Exact numerical solution for small chains ($N = 8, 12, 16$) and extension to large N.
ii) Monte-Carlo simulation for a large chain ($N = 48$).

III. Exact results for small chains

The procedure is the following. Given N, and given a distribution of the impurities, i.e., a distribution of the interactions $\{J_{ij}\}$, one can compute numerically the quantities of interest by taking explicitly the trace over the 2^N states, for several fields and temperatures. More delicate is the average over the configurations. Although it is not a problem of principle, for computing time reasons, we cannot average over too many configurations (10 for the 16 spin chains). Accordingly, we selected some representative configurations of the spin glass state according to the following criteria.

i) Small ground state magnetization, typically $m_0 \leq 1/\sqrt{N}$ [9].
ii) Average nearest neighbour interaction $\sum_{i<j} J_{ij}$ (i, j nearest neighbours) as small as possible.
iii) Average interaction $\sum_{i<j} J_{ij'}(\forall\, i, j)$ as small as possible.

The parameters entering into the interaction (II.2) are the following: $x_i = x_{i-1} + 20 \cdot r$, r being a random number, $0 \leq r \leq 1$,

$$\begin{aligned} \alpha &= 7\pi \\ J_0 &= -10 \end{aligned} \tag{III.1}$$

The average spacing between two spins is thus 10.

In order to ensure that the model describes indeed a kind of spin-glass, we have to make sure that the system is neither too frustrated nor totally non-frustrated [1]. This can be achieved by comparing the ground state energies for a given configuration $\{x_i\}$ with the corresponding non-frustrated and fully frustrated cases. The first case corresponds in replacing V_{ij} by $|V_{ij}|$ in (II.2) and the second by replacing $J_0 V_{ij}$ by $|J_0 V_{ij}|$. All the samples chosen for averaging have a ground state energy well between these two extreme values. The numerical exacts results obtained are then the following.

α. Case $N = 16$

A. *Ground states properties and internal energy*

For a 16 spins chain the configurational average has been performed over ten samples. Each sample can be in 65536 different states. For each of these states,

Table I
Ground state energies and the corresponding magnetizations and spin configurations for the 10 samples used for the averaging in the $N = 16$ case.

	E_0	M	Spin configuration
1	−18.73	0	− + + − − + + − + − + + − + − −
2	−13.87	−4	− + + + − + − + − − − − − − + −
3	−29.32	+4	− + + + + + + + − + − + − − − +
4	−31.75	−4	− − − + − − + − − + + − − − + +
5	−25.51	0	− + + − + + − − − + + − − + + −
6	−24.67	4	− − + + − + + + + − − + + − + +
7	−24.16	−2	− − − + − + + + − + + − − − − +
8	−25.29	0	− − + + + − − − − + − + + + − +
9	−17.72	+4	− + + + − + + + − + − + + + − −
10	−30.26	−2	− + − − + + − − − + + − − − + +

the energy has been computed, and thus the ground state identified. Table I gives the 10 grounds states with their explicit configuration, energy and magnetization. Note that each ground state is twice degenerated (inversion of all the spins). The average ground state energy plus or minus its standard deviation is:

$$\bar{E}_0 = -24.13 \pm 5.49 \qquad \text{(III.2)}$$

The ground state magnetization M is $\leq\sqrt{N}$ for each sample. One also notes that,

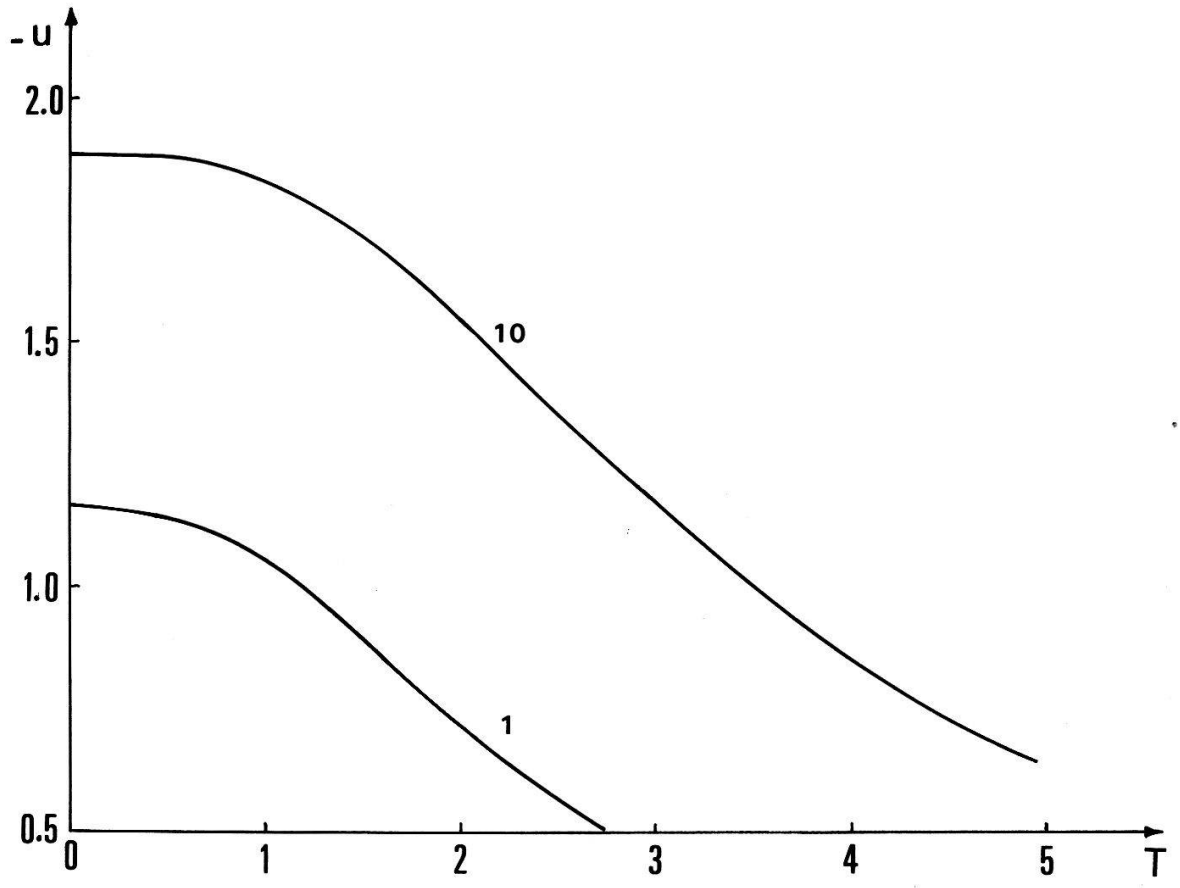

Figure 1
Internal energy as a function of temperature for two samples (No. 1 and 10 in Table I) for the N = 16 case.

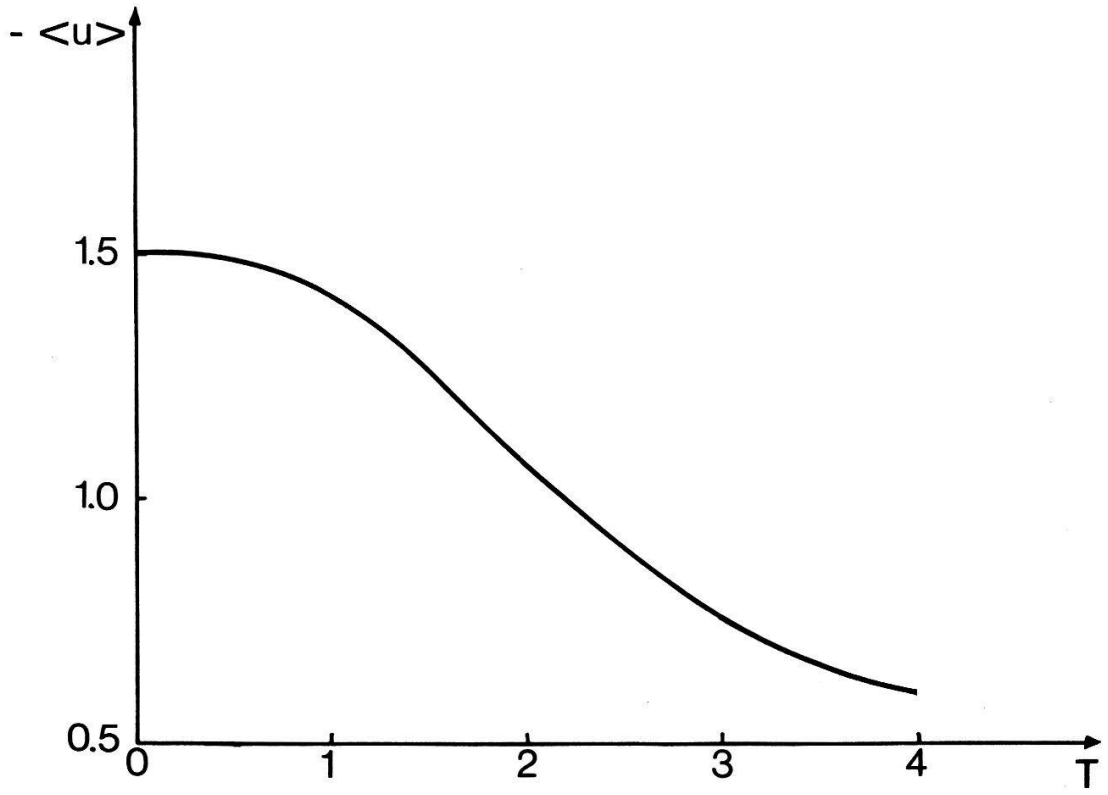

Figure 2
Average internal energy as a function of temperature for the $N = 16$ case.

besides the natural twofold degenerary already mentioned, the ground states were never degenerated; a typical example of the ground and first excited states is given for the configuration number 1:

$$E_0 = -18.73 \qquad E_1 = -18.51 \qquad E_2 = -18.24$$

Typically, the first excited state is not obtained by flipping only one spin in the ground state but corresponds rather to the excitation of a small cluster of spins (1, 2 or 3). Typical value for $\sum_{i<j} J_{ij}$ for J_{ij} nearest neighbour or for the sum over all sites is $\sim 5 \cdot 10^{-2}$.

The easiest quantities to compute are the ones in zero field. Using (II.7), (II.8) we can compute the internal energy as a function of temperature. Figure 1 shows this internal energy for the configurations number 1 and 10. Both curves show an inflexion point corresponding to a maximum of the specific heat at temperatures respectively $T_{m^1} = 2.37$ and $T_{m^{10}} = 1.69$. Thus, there are important variations of T_m from sample to sample. Figure 2 shows the average internal energy over all samples. Here $T_m = 1.75$.

B. *Magnetization as a function of the external field*

A crucial quantity to test the PaT hypothesis is the magnetization as a function of the magnetic field and the temperature. Using relation (II.9) one gets $m(h, T)$ for the different configurations. The results are shown on Figs. 3, 4 and 5. Figure 3 shows the typical behaviour for a given sample (the number 10 in Table I). At low temperatures ($T = 0.3$), the magnetization increases by jumps from one

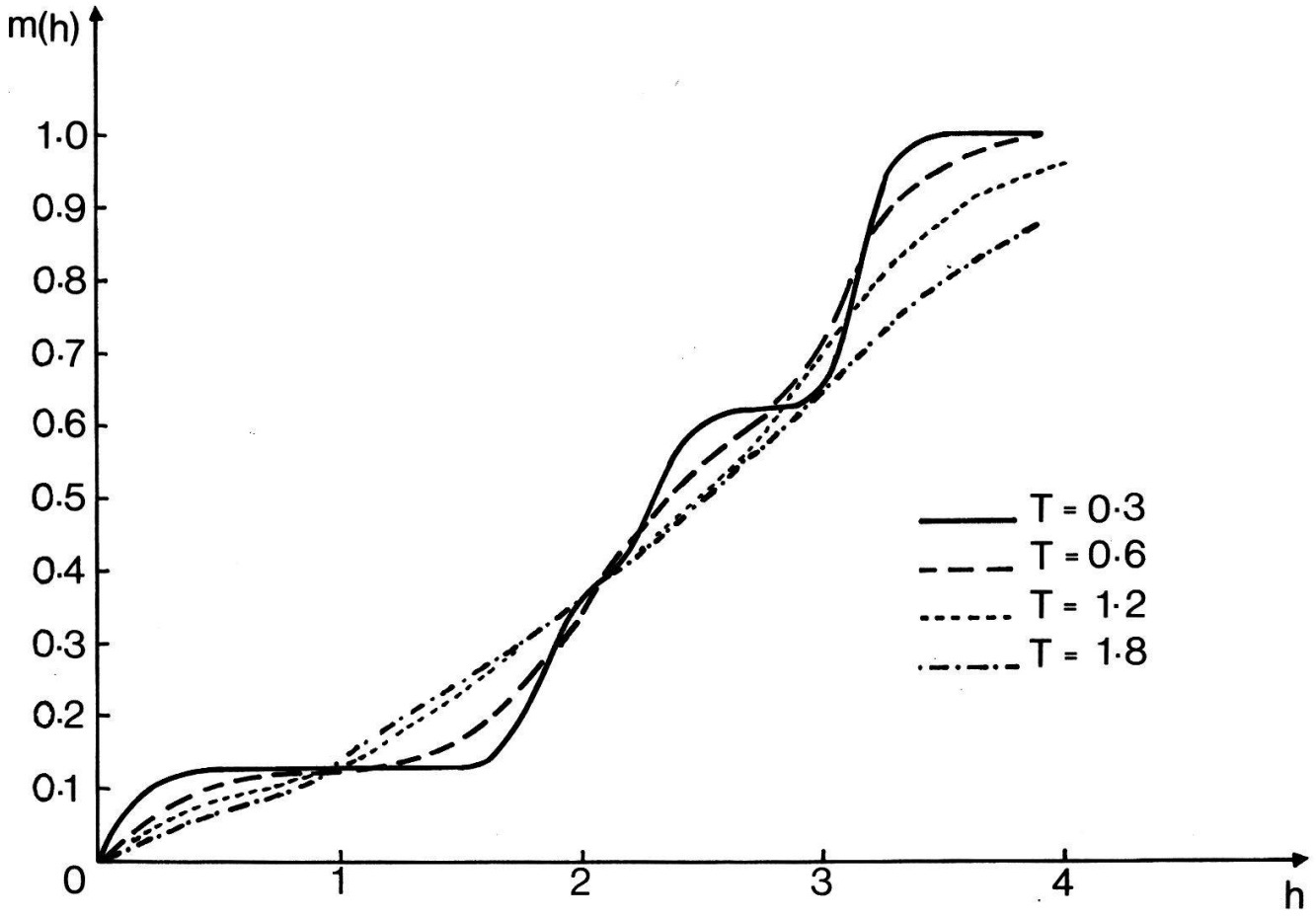

Figure 3
Magnetization at given temperatures as a function of the magnetic field for a typical sample (No. 10 in Table I) for the $N = 16$ case.

plateau to the other. As the temperature increases, the general behaviour is smoother and, for high temperatures ($T = 1.8$), the magnetization increases smoothly with the field. This behaviour is easily explained in terms of the results of Table I and the energies and magnetizations of the first excited states. Indeed, the energy gap between two states is $\Delta E_{ij} = (E_i(h=0) - E_j(h=0)) - h(M_i - M_j)$. At very low temperatures, the excited states are populated only when the external field is large enough such that $\Delta E_{0i} \simeq 0$. Once an excited state can be occupied then the magnetization jumps. As the temperature increases, the role played by the energy gaps is smoothed out by the product $k_B T$ in the Boltzman factor $\exp -\Delta E_{0i}/k_B T$. Thus the magnetization becomes a smooth function of the field. Figure 4 shows the behaviour of different samples at low temperature. The important differences from sample to sample reflect the differences in the energy spectrums from sample to sample. Figure 5 shows a similar behaviour at a higher temperature ($T = 1.2$). Note that this step like behaviour for the magnetization as a function of the field, suggest that the spin-glass ordering may be described as a succession of first order transitions.

Here again, in order to get a meaningful information, one has to average over the different samples. Figure 6 shows the average $\bar{m}(h)$ for different temperatures. The striking feature is that, for small temperatures, the average magnetization $\bar{m}(h)$ is almost independent of the temperature, while for high temperatures

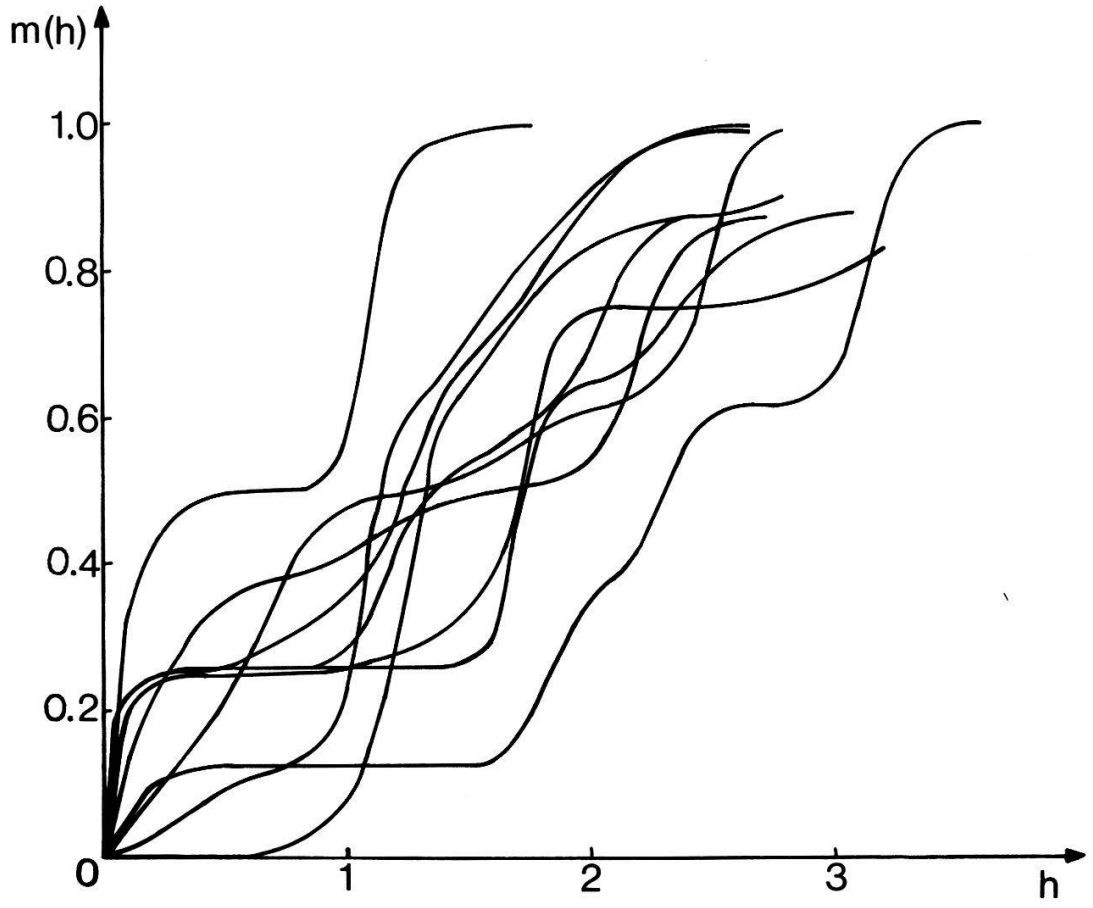

Figure 4
The magnetizations of all samples at $T = 0.3$ as functions of the magnetic field ($N = 16$).

($T \geqslant 1.8$), a clear temperature dependence develops. The results of Figs. 4, 5 and 6 show that the differences from sample to sample are quite important and that, in order to be able to make a precise determination of the transition temperature, one would need better statistics, i.e., to average over a much larger number of samples. The results obtained for our model are qualitatively similar to the ones obtained for the *SK* model [9]. Another useful way to look at those results consists in computing the magnetic susceptibility as defined by formula (II.11). However, for our finite system we cannot take the limit $h \to 0$ because, due to the structure of the first excited states, $m(h)$ may be zero for small fields. Accordingly, the relevant quantity is $m(h, T)/h$ for small h. This quantity is plotted on Fig. 7. For fields not too small, the susceptibility for fixed field and varying temperature shows two regimes. For $T < T_c(h)$ a plateau type of behaviour while for $T > T_c(h)$, $\bar{\chi}$ is falling down to follow a Curie–Weiss law at high enough temperature. The critical temperature $T_c(h)$, determined by the end of the plateau, is decreasing as the field increases. Again, due to the rather poor statistic, it is difficult to make a precise determination of $T_c(h)$. However, in view of the curves as estimation of $T_c(h = 0) = 1.6 \pm 0.1$ seems reasonable. Qualitatively, the behaviour of our system agrees with the PaT hypothesis.

Note finally that $T_c(h = 0)$ is smaller than the temperature at which the internal energy has its inflexion point. i.e. the specific heat has its maximum.

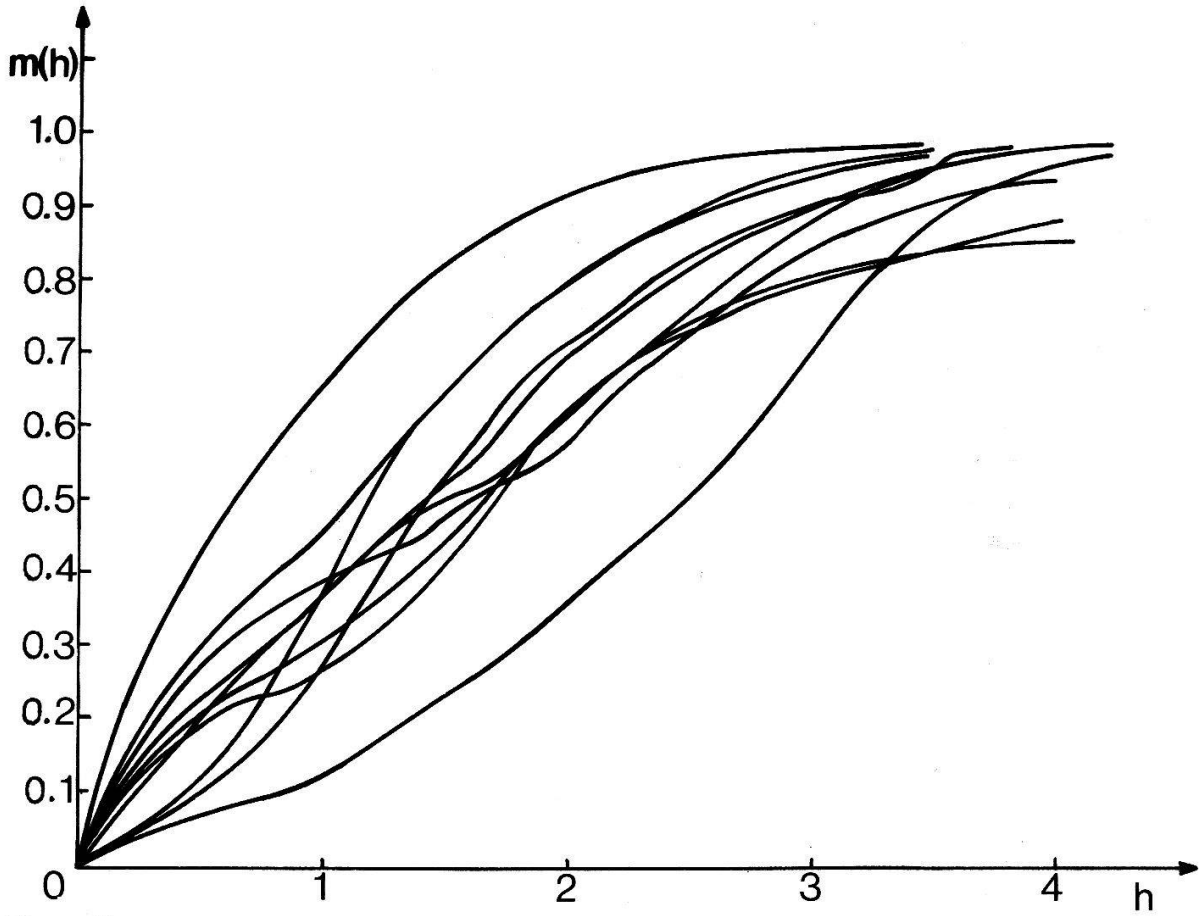

Figure 5
The magnetizations of all samples at $T = 1.2$ as functions of the magnetic field ($N = 16$).

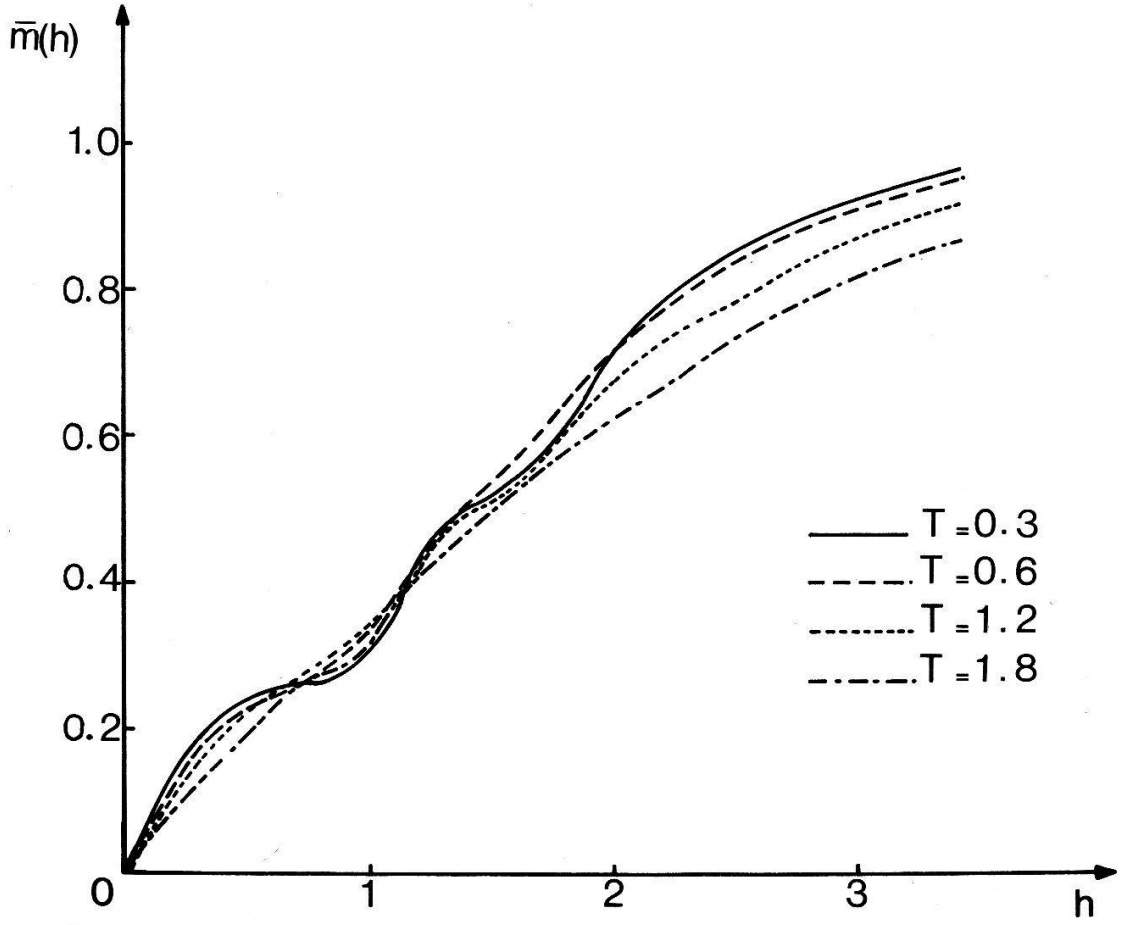

Figure 6
Average magnetization at given temperatures as a function of the magnetic field ($N = 16$).

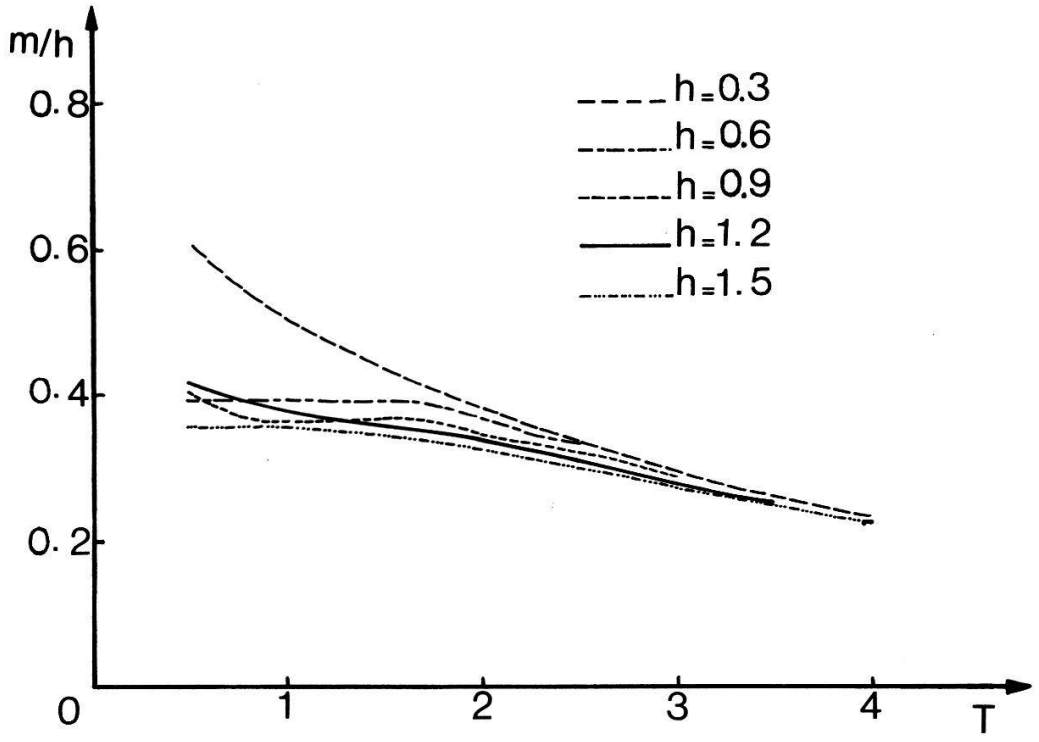

Figure 7
Average susceptibility at given magnetic fields as a function of temperature ($N = 16$).

C. *Order parameter*

In order to give a firmer justification for the existence of a phase transition at T_c, we would like to define an order parameter for our system. Assuming that the ordered phase is a spin-glass, one may ask what would be a good order parameter to compute. Since the works of Parisi [3] and Sompolinsky [10], we know that the spin-glass phase cannot be simply described by a scalar order parameter but, at best, by an infinite number of order parameters. However if not all the properties of the ordered phase can be described by a simple order parameter, the qualitative behaviour of some scalar quantities can be taken as the signature of a spin-glass phase. The most used order parameter is the so-called Edwards Anderson order parameter q_{EA} defined as [11] $q_{EA} = \langle \langle s_i \rangle_T^2 \rangle_J$. However, this is not a suitable quantity to compute for finite systems because $\langle s_i \rangle_T = 0$ is zero field and finite N. Another order parameter, which does not suffer of this drawback, has been proposed by Morgenstern and Binder [12] for models with short range interactions. We suggest the following generalization of their definition for our long range interaction model:

$$Q(T) = \frac{1}{N(N-1)} \left\langle \sum_{i<j} \langle s_i s_j \rangle_T^2 \right\rangle_J \tag{III.3}$$

For the *SK* model, where $\langle \langle s_i s_j \rangle_T \rangle_J$ is the same for all pairs $i \neq j$, Q reduces to the $q^{(2)}$ discussed by Young and Kirkpatrick [9]. In our case, in the limit $T \to 0$, $Q \to 1$, since the ground state is not degenerated. Moreover, if for $T > T_c$, the spins behave as free spins (as suggested by the susceptibility), then Q is zero. In

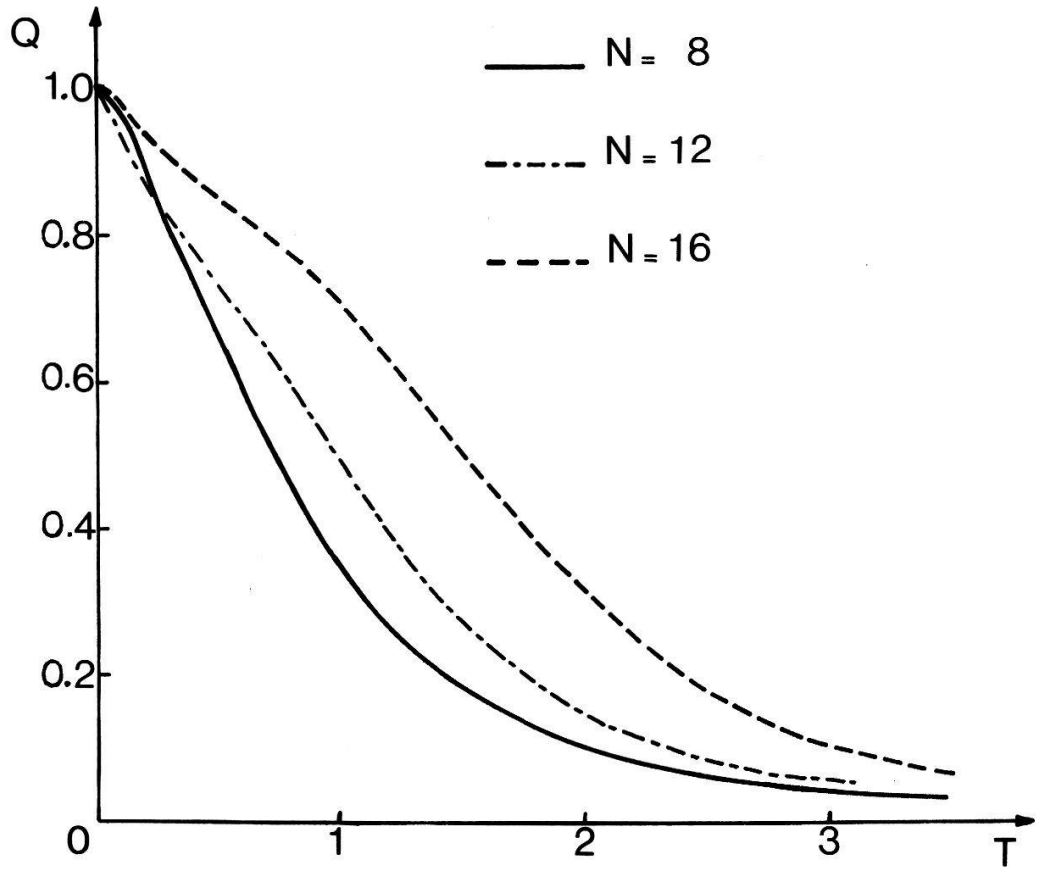

Figure 8
The order parameter Q, defined in (III.3), as a function of temperature for $N=8$, 12 and 16.

between, Q should decrease smoothly. The numerical results obtained for $Q(T)$ are shown on Fig. 8. Note however that, for computer time reasons, the average has been performed only over three samples (the numbers 4, 6 and 10). The average T_c for these three samples, T_c', is somehow higher than the average T_c for the 10 samples, namely $T_c'=1.8$. We see on Fig. 8 that the qualitative behaviour is correct, although some important finite size effects are showing up. A better analysis of the size dependence is clearly needed and will be performed in Section III.D.

β. Case $N=12$

For the 12 spin chains, the averages have been performed over ten samples choosen according to the same criteria than before. All that has been said for $N=16$ can be qualitatively repeated in this case. Thus we will not enter into all the details. The susceptibility versus field and temperature results are shown of Fig. 9. We see that the extrapolated zero field critical temperature is now $T_c=1.0\pm0.1$. Here also, a better statistics would be useful to give better quantitative results. The results for $Q(T)$ are plotted on Fig. 8. The average has been performed over all the ten configurations.

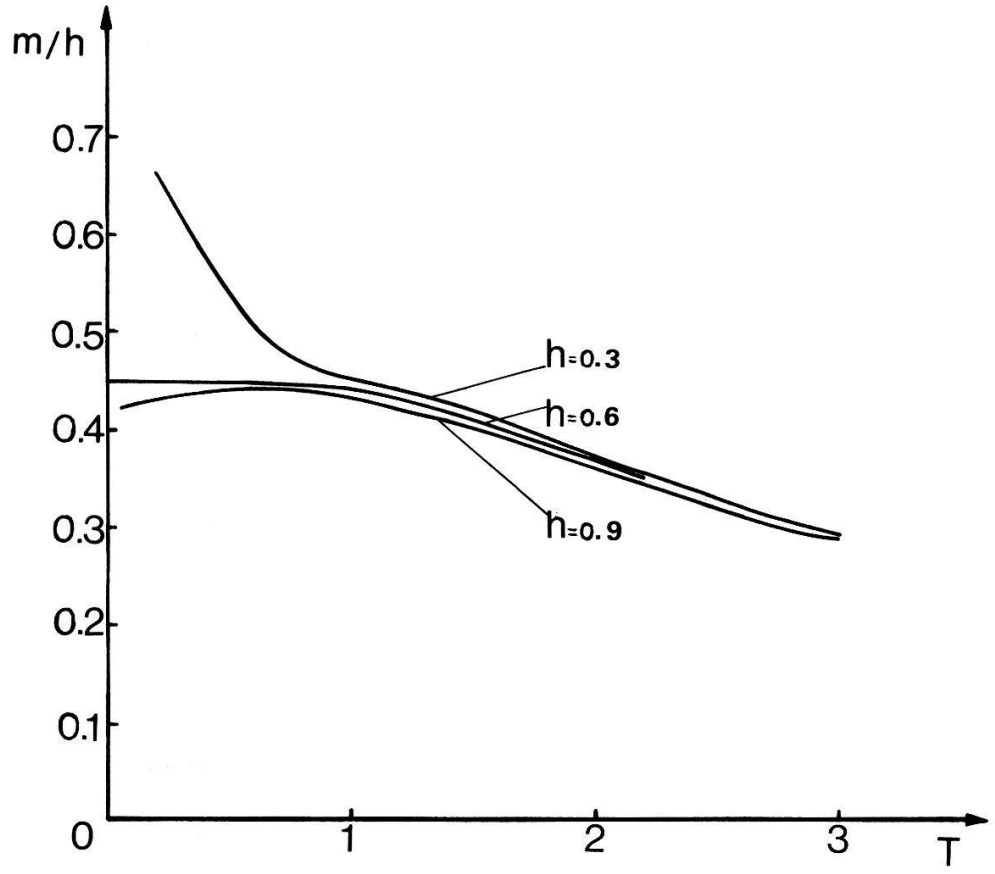

Figure 9
Average susceptibility for $N = 12$.

γ. Case $N = 8$

For the 8 spin chains, the averages have been performed over 20 samples. Susceptibility versus field and temperature is plotted on Fig. 10, leading to a value of $T_c = 0.75 \pm 0.1$. $Q(T)$ given on Fig. 8, is also obtained by averaging all the 20 samples.

D. *Size effects and extrapolation to infinite chains*

In order to interpret properly our results, we have to study their size dependence and draw some conclusions for the infinite chain.

a. *Size dependence of* J_0

The first question we have to address ourself is the determination of the factor $\rho(N)$, introduced in Section II, which ensures the existence of the thermodynamic limit. We can determine $\rho(N)$ by looking at the average ground state energies $\bar{E}_0(N)$, which should be extensive. The average ground state energies can be fitted by the following power law:

$$\bar{E}(N) = N\varepsilon_0 N^a, \qquad a = 0.35 \tag{III.4}$$

and

$$\rho(N) = N^{0.35} \tag{III.5}$$

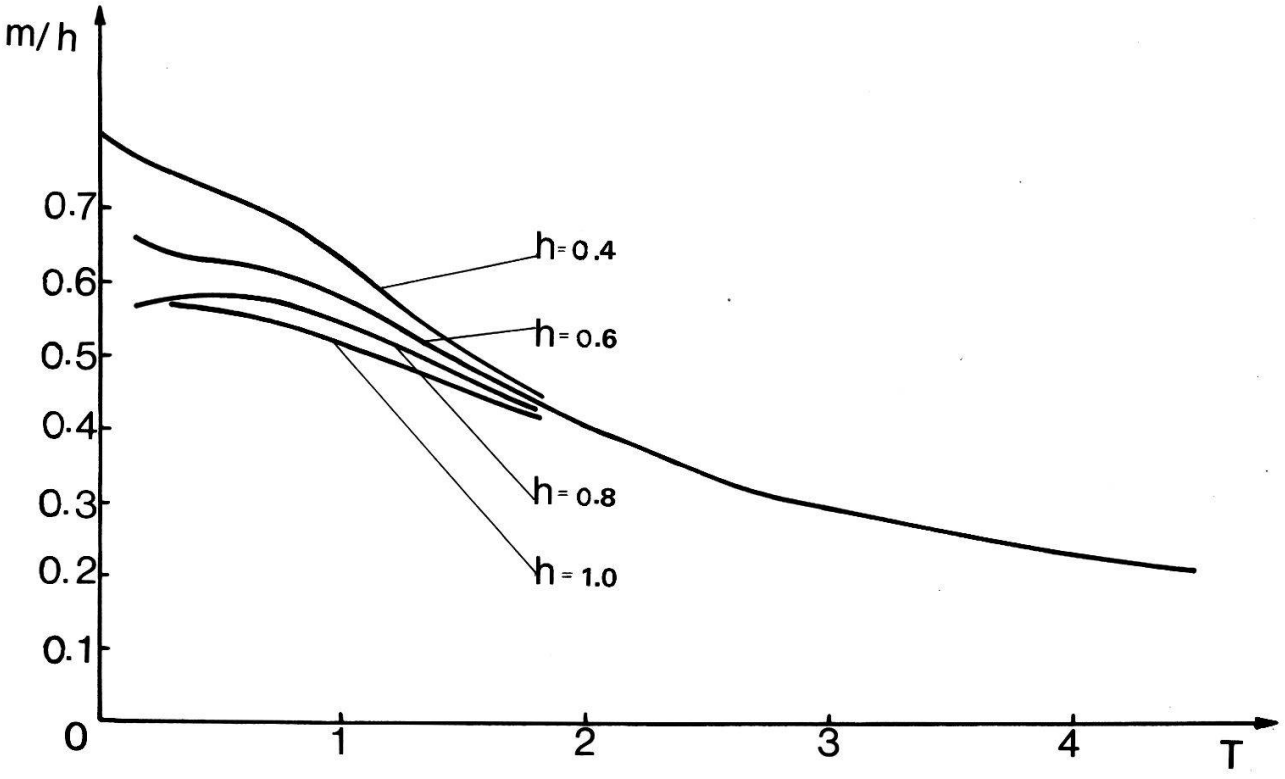

Figure 10
Average susceptibility for $N=8$.

Note that for $N=8, 12$ and 16, $N^{0.35}$ is only slightly smaller than $\ln N$, relative difference being smaller than 5%. Accordingly, we assume that $\rho(N)=\ln N$. The energies and temperatures have to be rescaled by this factor.

Let us consider now the critical temperatures obtained numerically $T_{c,n}(N)$, they are

$$\begin{aligned} T_{c,n}(16) &= 1.6 \pm 0.1 \\ T_{c,n}(12) &= 1.0 \pm 0.1 \\ T_{c,n}(8) &= 0.75 \pm 0.1 \end{aligned} \tag{III.6}$$

Besides the rescaling of the temperature scale given by (III.5), the $T_{c,n}$ should exhibit an explicit finite size effect. One may fit the numerical critical temperatures by the following law:

$$T_{c,n}(N) = \rho(N) T_{c\infty}\left(1-\frac{\alpha}{N^b}\right) \tag{III.7}$$

The best fit is for $\alpha=1.3$, $b=0.35$, with $T_{c\infty}=1.03$.

b. *Size dependence of Q*

In order to compare the Q obtained for different sizes we have firstly to rescale the critical temperatures according to the above analysis. The values of $Q(T/T_c)$ for $N=8, 12$ and 16 are plotted in Fig. 11. One notes that for low

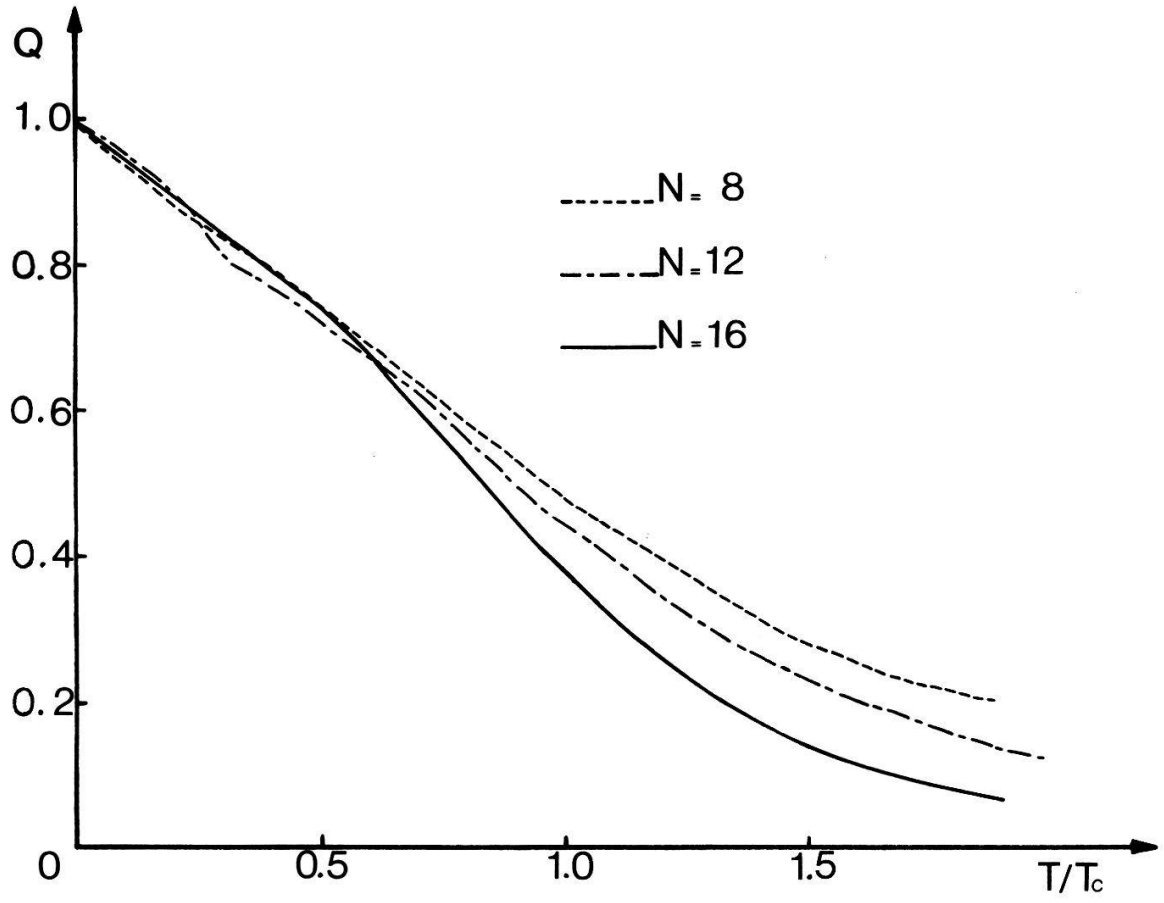

Figure 11
The order parameter Q as a function of T/T_c for $N=8$, 12 and 16.

temperatures one gets:

$$Q = 1 - \gamma(T/T_c) \tag{III.8}$$

with $\gamma \simeq 0.5$. Moreover, we see that Q decreases more rapidly with increasing N. At low temperatures, Q is going to 1 in a similar way for all values of N, although our statistic does not allow us to see more subtle N dependence in this domain. These qualitative features are similar in the *SK* model.

Looking at $T = T_c$, one sees that Q does not vanish at the critical point. However, the value $Q(T_c, N) = Q_c(N)$ decreases when N increases. One can extrapolate to $N \to \infty$ by fitting again the data with a power law. One gets:

$$Q_c(N) = Q_{c\infty}/N^x \tag{III.9}$$

with $x \simeq 0.31$.

This leads to a vanishing Q for $T < T_c$ in the thermodynamic limit, indicating the presence of a clear cut transition for infinite chain.

c. *Scaling form for $Q(t, N)$*

We can do more than the prediction (III.9) by returning to the definition (III.3) for Q. Indeed, if we consider the Edwards Anderson order parameter $q = \langle\langle s_i \rangle_T^2\rangle_J$, then in the high temperature phase $Q(T)$ is simply related to the

susceptibility χ_q associated to q. One has, for large N (i.e. $N^{-1} \ll 1$),

$$Q(T) \sim N^{-1} k_B T^2 \chi_q(T) \tag{III.10}$$

But if q is describing, at least partially, the ordering then χ_q diverges at T_c. In terms of the reduced temperature $t = (T - T_c)/T_c$ one has:

$$\chi_q \sim t^{-\gamma} \tag{III.11}$$

γ being the critical exponent associated to χ_q, and thus

$$Q(t, N) \sim N^{-1} t^{-\gamma} \tag{III.12}$$

Just below T_c, one expects:

$$Q(t, N) \sim |t|^{\beta} \tag{III.13}$$

where β is the critical exponent for this order parameter.

These two behaviours can be reproduced by assuming for $Q(t, N)$ the following scaling form:

$$Q(t, N) = N^{-x} f(tN^{y}) \tag{III.14}$$

To reproduce the t dependence of (III.12) one should have $f(tN^{y}) \sim (tN^{y})^{-\gamma}$ for $t > 0$ and thus

$$x + \gamma y = 1. \tag{III.15}$$

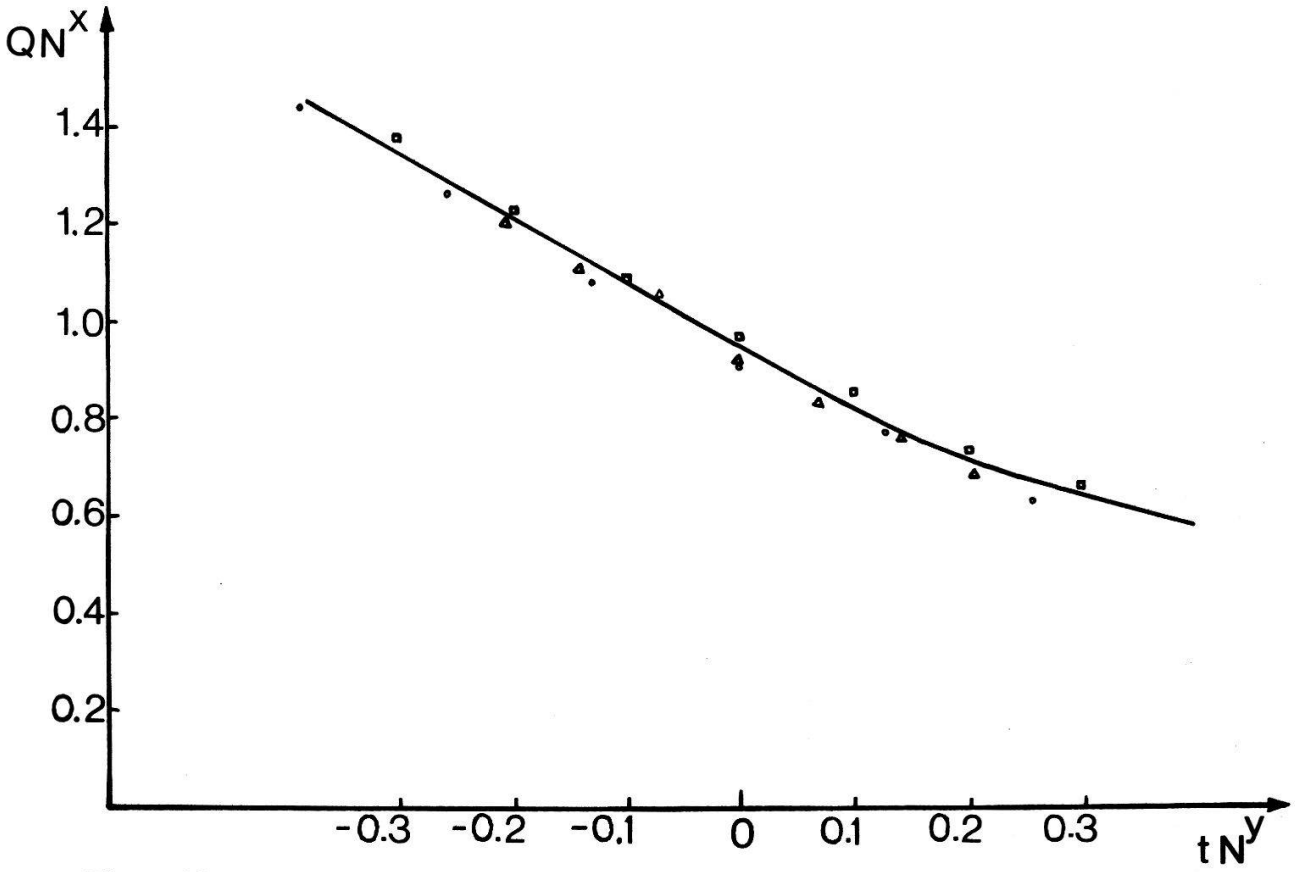

Figure 12
Fit of the numerical data with a form $Q(t, N) = N^{-0.31} f(tN^{0.9})$ (see (III.14)). (Δ, $\square$ and $\cdot$ are for $N = 8$, 12 and 16).

For $t<0$ one should have $f(tN^y)\sim(tN^y)^\beta$, and thus $Q(t,N)\sim N^{-x+\beta y}|t|^\beta$. Hence

$$\beta y - x = 0 \tag{III.16}$$

thus x and y are given in terms of β and γ by

$$x=\frac{\beta}{\gamma+\beta}, \qquad y=\frac{1}{\gamma+\beta} \tag{III.17}$$

For the *SK* model, γ and β are known to be representively 1 and 2. Thus Young and Kirkpatrick were able to test the scaling form (III.14) [8]. In our case, we do not have an *a priori* knowledge of γ and β and thus, x and y are to be taken as fitting parameters. Note that the exponent x entering in (III.14) is the same x which is in (III.9). Thus we have $x=0.31$. One can then fit the numerical data with a scaling form like (III.14), and determine y. Figure 12 shows such a fit with $y=0.9$. It turns out that our datas do not allow a very precise determination of y. The most reasonable fit is obtained for $y=0.85\pm0.15$, giving $\gamma=0.82\pm0.15$ and $\beta=0.36\pm0.06$.

IV. Monte-Carlo simulations

The study of longer chains by the exact method described in Section III implies a too long computational time. Accordingly, we approached the problem by another way, the Monte-Carlo method [13].

The strategy is very similar to the one used in Section III. Given N, one distributes the spins along the chain according to (III.1). Then, for a given field h and temperature T, one applies the standard Monte-Carlo procedure [12]. The time evolution of the system is given by the usual master equation associated to the hamiltonian (III.3). Starting from an arbitrary spins configuration C_0, one lets the system evolve in such a way that after N_f Monte-Carlo steps per spin (MCS/spin) one reaches a configuration C_1. If N_f is large enough, then C_1 will be an (or close by to an) equilibrium configuration. From this state one computes equilibrium quantities (thermodynamic quantities or correlations functions) by invoking the ergodic theorem. Averages over the phase space are replaced by averages over time, the dynamics being always defined by the master equation. Starting from configuration C_1 one runs N_i more MCS/spin to reach a new configuration C_2. One computes the quantities of interest in the configuration C_2. Then one repeats the same procedure N_p times, to reach a final configuration C_{N_p}. The thermal averages of interest are then given by the average over the values associated to the configurations C_i i.e.:

$$\langle A\rangle_T=\frac{1}{N_p}\sum_i A(C_i) \tag{IV.1}$$

The overall number of Monte-Carlo steps per spin is thus $N_{\text{tot}}=N_f+N_i\cdot N_p$. Note that one key point of the Monte-Carlo method is the validity of the ergodic theorem.

Once the above program has been performed for one sample, i.e., one distribution of the spins on the chain, one should in principle repeat it for other samples and then average over the samples. However, as the size of the chain gets larger, one expects to have to average on a smaller number of samples to obtain a

good answer for the quenched averages. Indeed, it has been proven, see Ref. [14], that for some general classes of disordered spin systems, a particular configurational free energy $F(J)$ was equal, with probability one, to the quenched free energy, in the thermodynamic limit.

According to the above remarks, we have studied an unique chain of 48 spins. The choice of the sample has been performed according to the criteria explained in Section III for the small chains. The total number of MCS/spin performed was between 10^3 and 10^4. This number was choosen in such a way that doubling the number of Monte-Carlo steps did not change significantly the results. At high temperatures, less steps are needed than at low temperatures. The main quantity that we have been looking at in the simulation is the magnetization M as a function of the temperature T for different fields h. Typical results are given on the Figs. 13, 14 and 15 for magnetic fields of 0.3, 0.5 and 0.6. Two different regimes have to be distinguished:

a. *Irreversible regime*

This regime corresponds to the following situation. Starting in zero field, one reaches the ground state of the system. Once the ground state is reached, one switches on the magnetic field and then one increases the temperature step by

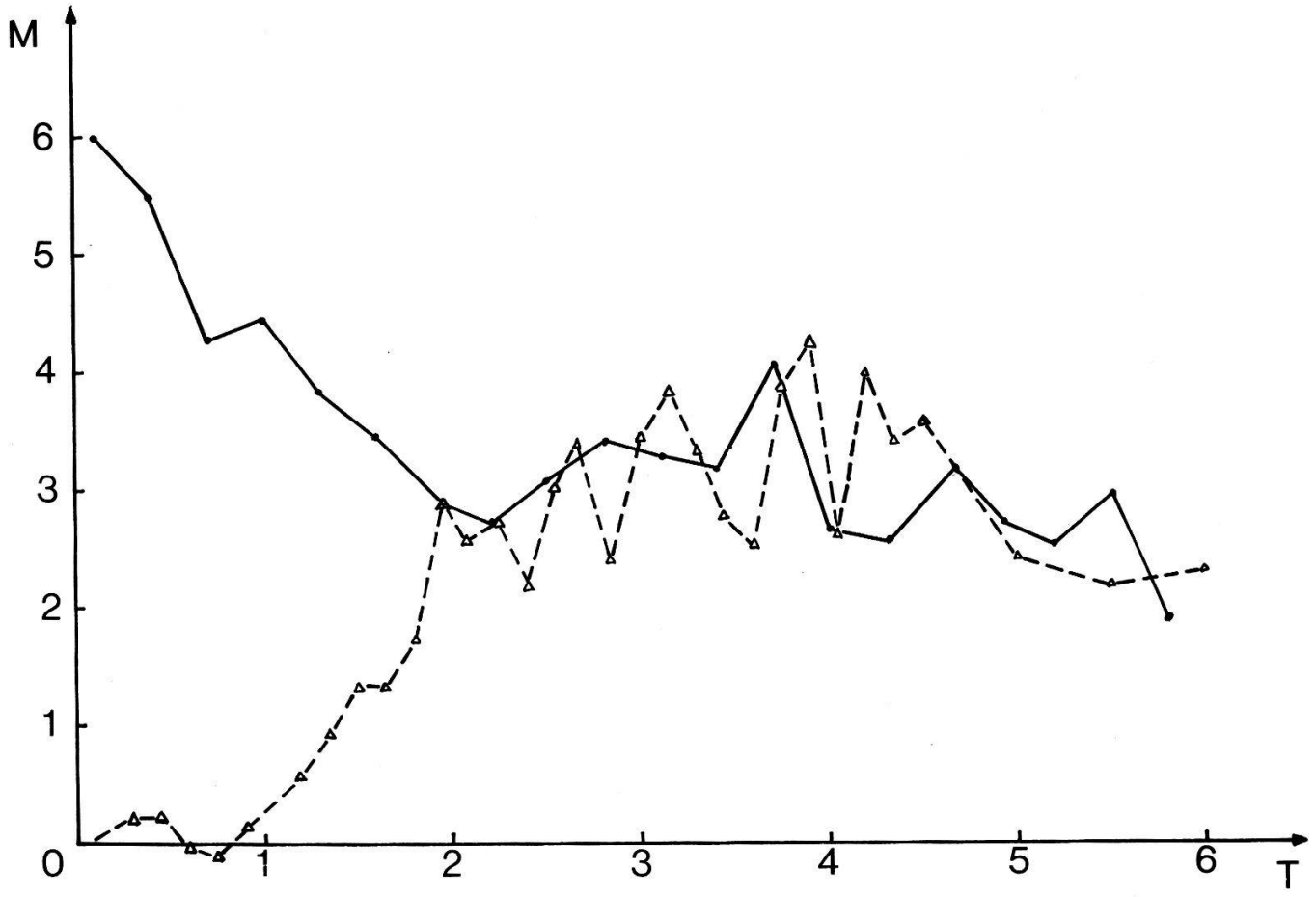

Figure 13
Monte-Carlo magnetization versus temperature at $h = 0.3$ ($N = 48$). The dotted line corresponds to a field heating experiment and the full line to a field cooling one.

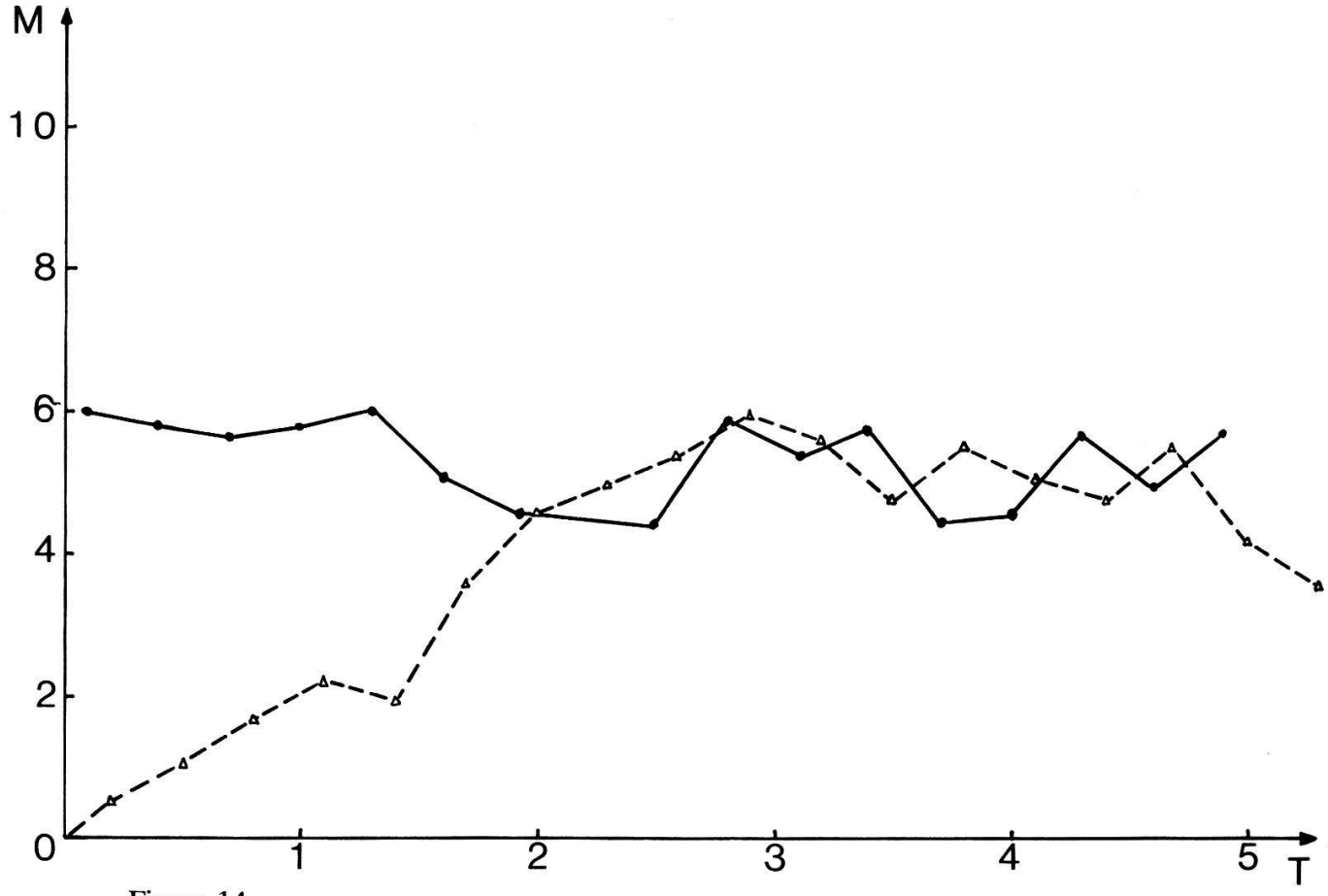

Figure 14
Monte-Carlo magnetization versus temperature at $h = 0.5$.

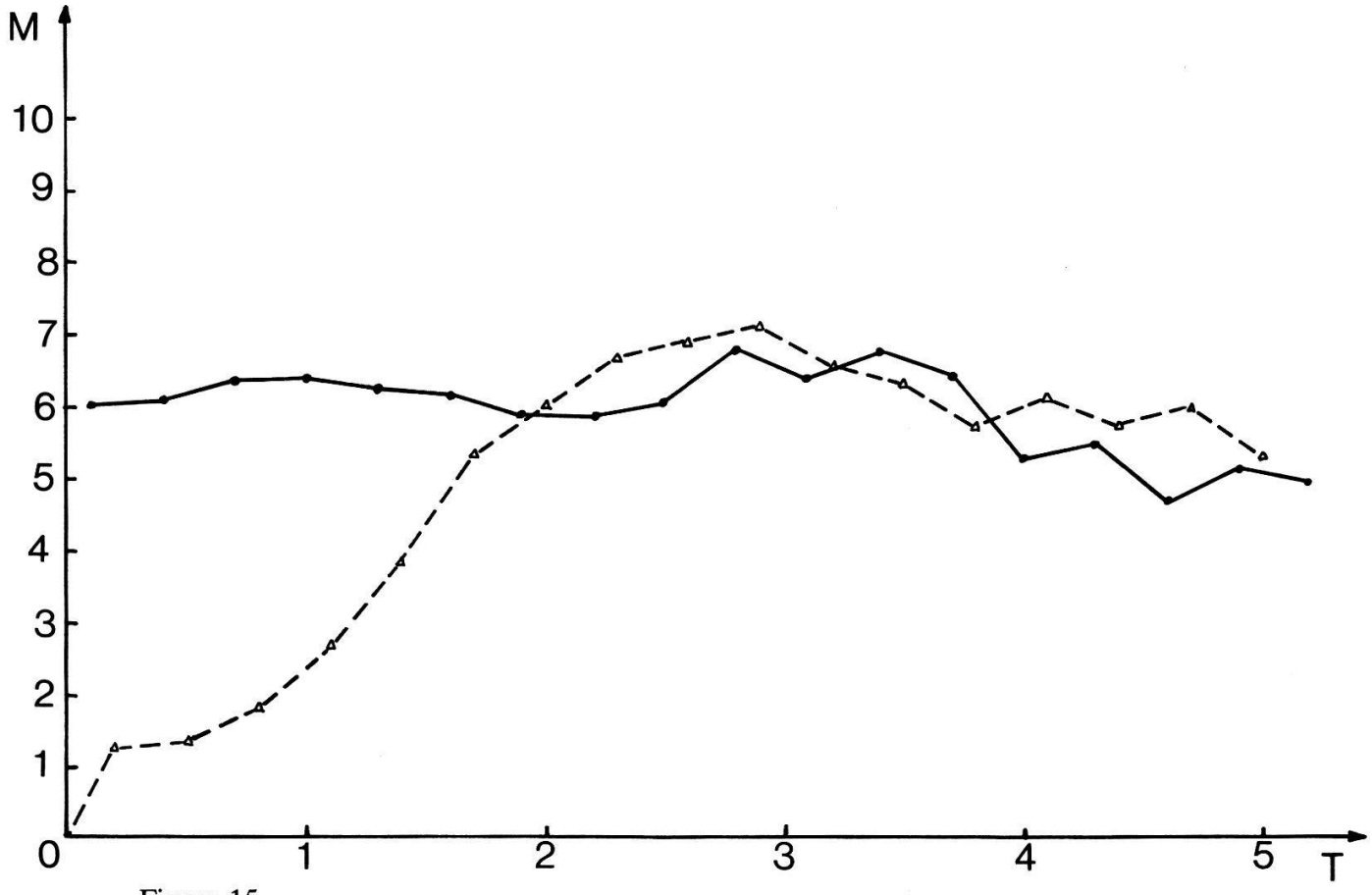

Figure 15
Monte-Carlo magnetization versus temperature at $h = 0.6$.

step. The magnetization (or the susceptibility χ which is just M/h) is then given by the dotted line on the figures. The magnetization increases smoothly till $T=3$ where its shows a slight, but systematic bump; as T increases, the magnetization remains approximatively constant until $T=5$ where it starts to decrease again.

b. *Reversible regime (or field cooling)*

Here, the procedure is different. Starting from the high temperature state in the field h, one decreases step by step the temperature, i.e., one proceeds to a field cooling type of experiment. In this case, the behaviour of the magnetization, shown by the full line in the Figs. 13 to 15, is quite different. Until a temperature of about $T=2$, the magnetization follows the plateau type behaviour observed in Case a. But, for T below 2, the magnetization remains about constant to reach a ground state with finite magnetization. Thus we see indeed a plateau like structure for the magnetization.

The reason of this irreversible behaviour is essentially the following. When the field is switched on at low temperatures, the systems lies in its zero field ground state φ_0. For fields not to large, this state remains a relative minimum of the energy but is no longer the true ground state φ_{0h}. Moreover the states φ_0 and φ_{0h} are separated by large energy barriers in the phase space [15]. Accordingly, at low temperatures, the system remains close to the state φ_0 in the phase space, and thus the behaviour of the system is governed only by the states in the vicinity of this "wrong" ground state. There is breaking of the ergodicity. Only when the temperature is high enough, the system is able to jump the energy barriers and reach the portion of phase space to which φ_{0h} belongs. This irreversible line is clearly metastable. On the other hand, when the system is cooled in the presence of a field, it may return to its "correct" ground state φ_{0h}. It could also, in principle, return to a metastable state, but we have observed that within the number of MCS/spin used, the system was always returning to its "correct" ground state φ_{0h}. Moreover, the behaviour of the system was perfectly reversible. thus, the field cooling line must be interpreted as the equilibrium line.

Note finally that due to the important fluctuations in the Monte-Carlo simulation, we were not able to locate precisely the critical temperature T_c, above which the system behaves paramagnetically.

V. Conclusions

The study of this long range Ising model with positional disorder has shown that its qualitative properties are similar to the one found for the *SK* model. Thus positional disorder with deterministic interactions or random interactions on an ordered lattice lead to the same qualitative features.

The exact numerical study of small chains has shown that the specific heat exhibits a maximum at a temperature T_{cm}. The study of the magnetization in a field exhibited the presence of two regimes: a low temperature one, with a susceptibility more or less independent of the field, and a high temperature regime with a Curie–Weiss type of susceptibility. The transition from one regime to the other occurs at a rather well defined temperature T_c. This picture agrees qualitatively with the Parisi–Toulouse projection hypothesis, which validity does

not seem to be restricted to the *SK* model. Moreover, we found systematically that $T_{cm} > T_c$, results observed in all experiments on spin-glass [1].

The extrapolation of the finite size results to the thermodynamic limit has shown that the transition is well described by the order parameter Q, which scaling form allowed us to extract the critical exponents β and γ. However, due to the imprecisions resulting from the restricted number of samples used in the averages, we do not think that such subtle quantitative results are meaningful.

The Monte-Carlo study of the 48 spins chain, has shown the crucial role played by the metastable states and the breaking of ergodicity in a spin-glass. Moreover, the results for the reversible susceptibility have qualitatively confirmed the behaviour observed for small chains.

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