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The de Almeida-Thouless line in the four dimensional Ising spin glass

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Abstract . — We confirm recent results obtained in a previous work by studying the Ising spin glass at finite magnetic field in four dimensions. Different approaches to this problem suggest the existence of a critical line similar to that found in mean-field theory but in a universality class different of the transition at zero magnetic field. Problems due to the strong nature of the finite-size corrections within a magnetic field are also discussed.

1. Introduction.

Spin glasses have received much attention because they are representative of a large class of models with disorder and frustration [1, 2, 3]. Up to now a complete understanding of spin-glass field theory is lacking because of the enormous theoretical difficulties one encounters when studying short ranged systems [5]. The main success of spin glass theory is mean-field theory [4]. Even though there are some problems in mean-field theory which we do not fully understand (i.e. some finite-size corrections) the nature of a phase transition from a paramagnetic phase to a replica broken symmetry phase is widely accepted. The difficulties one encounters when studying finite dimensional systems using field theoretical methods have provoked the appearance of other different approaches. Among them we recall the phenomenological droplet model firstly developed by W.L. Mc Millan [6] and finally collected by D.S. Fisher and D.A.

Huse [7, 8] in a series of papers. Nevertheless, some predictions of these phenomenological models are substantially different from those found in short-ranged systems if a mean-field picture were valid in this case.

From the experimental point of view recent cycling temperature experiments have been interpreted within the mean-field picture [9, 10]. It has also been claimed that they are inconsistent with predictions of the droplet model even though there is not general agreement on this point.

One of the most striking differences among droplet models and mean-field theory is the response of the system to an applied magnetic field. If the droplet theory predicts that a magnetic field should destroy the spin glass phase, the mean-field picture suggests that, even though some pure states are suppressed by the magnetic field, an infinite number of them will survive to the perturbation. In this case a transition line in finite magnetic field (de Almeida-Thouless -AT- line [11]) is expected.

Recently this issues has been adressed in a previous work in the four dimensional Ising spin glass [12]. The advantages of studying the Ising spin glass in four dimensions are mainly numerical and we believe it captures the main features of spin glasses below the upper critical dimension and (we hope) those at three dimensions. In that work [12], it was found evidence of a phase transition at finite field using standard finite-size scaling methods. A different approach was used in [13].

Also numerical work in zero magnetic field [14, 15] has shown that the spin glass phase seems to consist of an infinite number of pure states and that these states cannot be considered as excitations (droplets) due to inversion of local compact domains.

The problem of the existence of the AT line in short-ranged spin glasses is important because it is one of the very features of an ordered phase with replica symmetry breaking.

This work is divided as follows. In section 2 we present general theoretical predictions on the expected critical behaviour within a magnetic field. Section 3 presents some finite-size scaling results for the spin-spin overlap and for the link to link energy overlap. Section 4 investigates some predictions of mean-field theory in a magnetic field for the overlap probability distribution $P(q)$ in large systems. Section 5 show results on the dynamics of large samples within the spin-glass phase with a finite magnetic field. Finally, section 6 presents the conclusions.

2. General predictions.

One of the most important consequences of a spin-glass phase with replica symmetry breaking (RSB) features is the existence of a lot of thermodynamic states N_s whose number grows enormously with the size ($N_s \propto N^\alpha$ with $\alpha < 1$). All these states have the same free energy and because its number does not grow exponentially with the size they do not contribute with an extra entropy to the system. Theoretical results are well know in case of mean field theory (SK model) in which all is more or less under control.

The SK model is defined by the hamiltonian

$$H = - \sum_{i < j} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i \quad (1)$$

where the J_{ij} are quenched variables with zero mean and $1/N$ variance. The order parameter is defined by

$$q_{\sigma\tau} = \frac{1}{N} \sum_i \sigma_i \tau_i \quad (2)$$

where $\{\sigma_i, \tau_i\}$ are the spins of two independent replicas of the hamiltonian equation (1) with the same realization of the disorder. From this overlap we construct its probability distribution

$$P(q) = \overline{P_J(q)} = \overline{\left\langle \delta \left(q - \frac{1}{N} \sum_i \sigma_i \tau_i \right) \right\rangle} \quad (3)$$

where $\langle (\dots) \rangle$ means thermodynamic average and $\overline{(\dots)}$ means average over samples. The thermodynamic average is defined by

$$\langle (\dots) \rangle = \frac{1}{Z} \sum_{\sigma \tau} (\dots) \exp(-\beta H_2[\sigma, \tau]) \quad (4)$$

with

$$H_2[\sigma, \tau] = H_1[\sigma] + H_1[\tau] \quad (5)$$

and the partition function is

$$Z = \sum_{\sigma \tau} \exp(-\beta H_2[\sigma, \tau]) \quad (6)$$

Replica theory computes all moments $\overline{P_J^k(q)}$ from which one can construct its probability distribution [16]. One of the most important results of mean field theory regard the form of the $P(q)$ function. It consists of a continuous non self-averaging part plus a delta-type singularity at the maximum overlap $q = q_{\max} = q(1)$ where $q(x)$ is related to $P(q)$ by

$$P(q) = \frac{dx(q)}{dq} \quad (7)$$

and $x(q)$ is the invers of the monotonous function $q(x)$ [17, 18].

The function $P(q)$ is symmetric. This means that for a given pure state there is another one related by the inversion of the spins. When a finite magnetic field h is applied to the system we add to the Hamiltonian equation (1) a perturbation $h \sum_i \sigma_i = N h m$ proportional to the size of the system N where m is the magnetization. Since all pure states have zero magnetization the external field does not couple to any particular state and there is no reason why only one state should be selected. In fact, this is what happens in the infinite-ranged model where an infinite number of states still survive to the applied field. In that case, $P(q)$ is non zero only for q positive and it consists of a continuous part $P_0(q)$ limited by two singularities at $q = q_{\min}$ and $q = q_{\max}$ [19].

$$P(q) = a\delta(q - q_{\min}) + P_0(q) + b\delta(q - q_{\max}) \quad (8)$$

and $P_0(q)$ non-zero within the interval $q_{\min} < q < q_{\max}$.

Recently, finite-size corrections to both singularities have been analitically computed. It has been found [20, 21] that

$$P(q > q_{\max}) \sim N^{1/3} f(\lambda_+ N (q - q_{\max})^3) \quad (9)$$

$$P(q < q_{\min}) \sim N^{1/3} f(\lambda_- N (q_{\min} - q)^3) \quad (10)$$

with $f(x) \sim \exp(-x)$ for $x \gg 1$ and λ_+ approximately one order of magnitude greater than λ_- [20]. This means that finite-size effects for the singularity at $q = q_{\min}$ should be stronger than those at $q = q_{\max}$. For a finite size one also would expect that the height of $P(q)$ at $q = q_{\min}$ should be smaller than the height of $P(q)$ at $q = q_{\max}$. Then we expect to find in the SK model that the $P(q)$ has a left tail with strong finite-size corrections extending down to negative values of q . Only for very large sizes the singularity at $q = q_{\min}$ would be seen. In fact, we do not know of any numerical work which has tested this point.

The problem we pose in this work regards the determination of the AT line in short-ranged models. These are given by the Hamiltonian

$$H = - \sum_{(i,j)} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i \quad (11)$$

and the sum (i,j) runs over nearest neighbours on a simple lattice in d dimensions. In order to increase the speed of the simulations it is usually taken $J_{ij} = \pm 1$ with equal probability.

Recently we have found that finite-size scaling techniques are useful in order to discover the AT line [12]. The main idea is to find a divergence in the non-linear susceptibility. Finite-size scaling techniques are useful in spin glasses because one is able to discover the phase transition qualitatively studying relatively small systems. The danger is that one is not able to discern between a true divergence in the infinite size limit and a transient behaviour for small sizes.

At zero magnetic field these techniques produce good qualitative results [22]. In general, in order to locate the transition one introduces the Binder parameter (plainly speaking it is the curtosis of the order parameter distribution $P(q)$). This is defined by

$$g = \frac{1}{2} \left(3 - \frac{\overline{\langle q^4 \rangle}}{\overline{\langle q^2 \rangle}^2} \right) \quad (12)$$

In a magnetic field one could also define the curtosis by considering the cumulants of the $P(q)$ instead of its moments. But now one finds that due to the strong finite-size corrections and because of the asymmetry between the tail of $P(q)$ when $q < q_{\min}$ respect to the tail for $q > q_{\max}$ it is not possible to locate the transition point using data for not too very large sizes. The conclusion is that in a magnetic field the Binder function is not a good tool. Another technique in order to locate the transition point is to use the skewness of the distribution $P(q)$. This quantity is defined by

$$s = \frac{\overline{\langle q^3 \rangle_c}}{\overline{\langle q^2 \rangle_c}^{3/2}} \quad (13)$$

where the $\langle \dots \rangle_c$ mean the cumulants of the distribution $P(q)$. This quantity should be zero if the $P(q)$ function were symmetric. Only with a magnetic field and within the spin-glass phase it should be different from zero. As we will show in the next section, also studying the skewness it is difficult to locate the transition temperature with a magnetic field. Because of this, if a phase transition exists at finite magnetic field it is difficult to determine a function which could permit to see the transition temperature in an acceptable range of small sizes (i.e. L less than 10 for $d = 4$). This makes the determination of the phase transition more difficult because the transition point has to be searched more indirectly. A similar situation is present in the three-dimensional ising model at zero field. It is difficult to locate the phase transition

using the Binder function [22] and one searches for a divergence in the spin-glass susceptibility [23].

The non linear spin-glass susceptibility is defined by:

$$\chi_{nl} = N \left(\overline{\langle q^2 \rangle} - \overline{\langle q \rangle}^2 \right) \quad (14)$$

with $N = L^d$, d being the dimensionality of the system. These moments can be obtained from the probability distribution $P(q)$ which in the critical line and for short-ranged models is expected to scale like

$$P(q > q_0) \sim L^{d_q} f\left(\lambda_+ N (q - q_0)^{\frac{d}{d_q}}\right) \quad (15)$$

$$P(q < q_0) \sim L^{d_q} f\left(\lambda_- N (q_0 - q)^{\frac{d}{d_q}}\right) \quad (16)$$

The values λ_- and λ_+ have been computed in the mean-field case [20] and their values are related to the length of the left and right tails of the $P(q)$ distribution. In short-range models one finds that the region of negative overlaps of the left tail is slowly suppressed with the size. Also it is difficult to find the existence of a peak in the $P(q)$ distribution corresponding to the minimum overlap. Instead of, the right tail shows a prominent peak with a tail which progressively disappears when the size of the system increases. This features are also observed in the SK model and they suggest that in short-range models the relation $\lambda_- \ll \lambda_+$ is also expected. d_q are the dimensions of the operator Q_{ab} in units of the inverse correlation length.

$$\langle q \rangle = q_0 + O(L^{-d_q}) \quad (17)$$

Also, d_q is related to the critical exponents along the AT line:

$$d_q = \frac{d - 2 + \eta}{2} \quad (18)$$

where η is the Fisher exponent which governs the decay of the correlation function in the critical line:

$$G(i) = \langle q(0)q(i) \rangle_c \sim \frac{1}{r^{d-2+\eta}} \quad (19)$$

with $q(i) = \sigma_i \tau_i$ and the spins $\{\sigma, \tau\}$ belong to two different replicas of the system.

The non linear susceptibility is expected to diverge in the AT line

$$\chi_{nl} = \sum_i G(i) \sim L^{2-\eta} \quad (20)$$

and near the critical line we expect to find the scaling behaviour

$$\chi_{nl} \sim L^{2-\eta} f(\xi/L) \sim L^{2-\eta} f\left(L^{\frac{1}{\nu}} (T - T_c(h))\right) \quad (21)$$

Because of the fact $\lambda_- \ll \lambda_+$ we expect that the left tail of the $P(q)$ falls down very slowly reaching the side with negative overlaps. This finite-size effect is very strong and difficult to control. In mean-field theory ($d = 6$) we have $d_q = 2$ and $\eta = 0$. The non-linear susceptibility is expected to diverge like L^2 or (in case of the SK model) $N^{\frac{1}{3}}$. Figure 1 shows results for the SK model at the AT line (we have choose $T = 0.5$, $h = 0.569934$ far from the critical

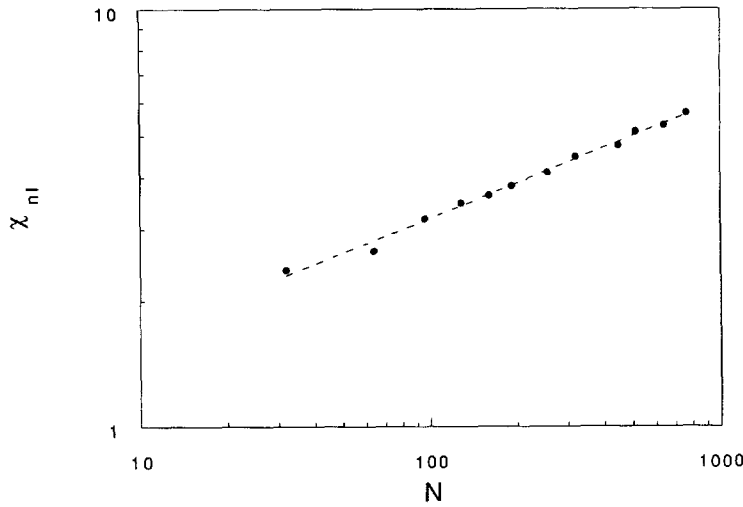


Fig. 1. — χ_{nl} versus the size N for the SK model in the AT line. It diverges like $N^{1/3}$

point $T_c = 1$, $h = 0$). This point in the $h - T$ plane has been determined solving the usual saddle-point equations [11]. The sizes range from $N = 32$ up to $N = 768$ with a number of samples which range from 6000 for the smallest sizes down to 2000 for the largest ones. We find a power law divergence $\chi_{nl} \sim N^{0.28}$ more or less consistent with the expected exponent $N^{1/3}$.

Below $d_u = 6$ we do not know the position of the AT line (if it exists). To determine it we use, as we commented previously, finite-size scaling techniques. In the spin-glass at four dimensions this has been already done in a previous work [12]. In that work, we found evidence of a divergence of χ_{nl} for $h = 0.6$ and $T \simeq 1.1$. Now we present results for smaller fields ($h = 0.3, 0.4$) and a similar range of sizes. In order to have more information on the transition line we have investigated also the behaviour of the link to link energy overlap. The energy overlap q^e is defined by

$$q^e = \frac{1}{8N} \sum_{(i,j)} \sigma_i \sigma_j J_{ij}^2 \tau_i \tau_j \quad (22)$$

with $J_{ij} = \pm 1$ and then $J_{ij}^2 = 1$.

This quantity was introduced in [24] in order to study the three dimensional Ising spin glass within a magnetic field. After that, it has been shown to be very useful to study the nature of the spin-glass phase at zero magnetic field in the four dimensional Ising spin glass [14, 15]. According to droplet models, the configurations of spins which have overlap q close to zero in the tail of the $P(q)$ (far from the maximum overlap $q_{\max}$ which is the true order parameter if there is a unique ground state) should correspond to excited states. These excited states are inversion of local compact domains of surface with fractal dimension $d_s \leq d$. In droplet models one naturally expects d_s not to be exactly equal to d . This implies that the probability distribution of q^e is peaked around a certain value. This discussion concerns short-range models (in the SK model all spins interact among them). At zero field [15] and $d = 4$ we found that this seems not to be the case and $P(q^e)$ develops two singularities reminiscent of the $P(q)$ of the SK model in a magnetic field. Then, even though $P(q)$ shows strong finite-size effects [25]

having a tail which extends down to $q = 0$ this should not to be the case for $P(q^e)$. It is true that d_s could be equal to d but we expect this result only when the surface is the volume (for example at infinite dimensionality). The difference between the fractal dimension d_s and d should increase as the dimensionality of the system decreases.

The fact is that $P(q^e)$ does not show so much large tails like $P(q)$ and it is not very much affected by the application of a magnetic field. Finite-size scaling techniques for the energy overlap q^e are also useful to determine the phase transition in a magnetic field. In the critical line we expect.

$$\langle q^e \rangle = q_0^e + O(L^{-d_e}) \quad (23)$$

and from equation (17) we expect the dimensions d_e of the operator energy to satisfy the inequality $d_e > d_q$ because $q_0 \neq 0$ ($d_e = d_q$ above six dimensions). This should be taken as a conjecture and we will see that our results are in agreement with it. At zero magnetic field the relation $d_e > 2d_q$ is satisfied as can be seen using renormalization group derivations near six dimensions [26]. The fact that $d_e = d_q = 2$ in mean-field theory is related to the nature of the finite-size corrections in the AT line. This was studied in a previous work [21]. It was found that finite-size corrections to the internal energy go like $N^{-2/3}$ in the AT line. The explanation why corrections behave like $N^{-2/3}$ instead of $N^{-1/3}$ is that the coefficient of the last one, even though it is the dominant for large sizes, is much smaller than the coefficient of the correction $N^{-2/3}$. A simple explanation of this fact comes when looking to the behaviour of $P(q)$ in the AT line. For a finite-size the $P(q)$ is not a delta function but a peaked one (with a finite variance) around a certain value $q_0(N)$. In mean-field theory $q_0(N)$ and the variance have in corrections $N^{-1/3}$ and $N^{-2/3}$ respectively. We can write

$$P(q) \sim N^{\frac{1}{3}} f\left(N(q - q_0(N))^3\right) \quad (24)$$

The function $f(x)$ behaves like $\exp(-|x|)$ for large values of the exponent x . From equation (24) we find that there are two finite-size corrections which affect all moments of $P(q)$. The first one is the motion of $q_0(N)$ with N and the other one is the progressive shrinking of the peak whose variance decreases like $N^{-2/3}$. The finite-size corrections to the internal energy can be computed if one takes into account the fact that (only valid in infinite dimensions) [27].

$$U = -\frac{\beta}{2} \left(1 - \int_0^1 q^2 P(q) dq\right) \quad (25)$$

Inserting equation (24) in equation (25) (which is exact for a finite size) we get for the internal energy two different finite-size corrections (one of order $N^{-1/3}$, the other of order $N^{-2/3}$). It can be shown that the effect of the shrinking of the peak has a coefficient neatly higher than that of the motion of $q_0(N)$ towards $q_0(\infty)$ (this can be analitically found in mean-field theory). This explains why finite-size corrections which go like $N^{-2/3}$ are found in the AT line for the energy. The coefficient of the $N^{-2/3}$ correction can also be analitically computed as was shown in [21].

A similar argument should be considered for short-ranged systems. This means that for the small sizes which can be studied using finite-size scaling one sees for the link to link energy a critical behaviour on the AT line which is mainly governed by a value of d_e approximately the twice of its real value (which should correspond to the next order finite-size correction). We expect

$$\chi_{nl}^e = N \left(\overline{\langle q_e^2 \rangle} - \overline{\langle q_e \rangle}^2 \right) \quad (26)$$

which should scale like

$$\chi_{nl}^e \sim L^{2-\eta_e} \bar{\chi} \left(L^{\frac{1}{\nu}} (T - T_c(h)) \right) \quad (27)$$

with

$$d_e = \frac{d - 2 + \eta_e}{2} \quad (28)$$

Even though we should expect (for very large sizes) both exponents η and η_e to be such that $d_q < d_e$ it could be that for the sizes one is able to study with numerical techniques, the exponent η_e obtained using the finite-size scaling equation (27) is different from the true exponent η_e derived from the main critical behaviour on the AT line for the parameter q_e . From these considerations about the critical behaviour on the AT line we expect the quotient d_e/d_q in the AT line to be approximately twice its true value. Also, for small sizes and not too much large fields the system could feel the effects of the critical point at zero field. In the critical point the value $d_e/d_q \simeq 2.7$ was obtained for $d = 4$ in a previous work [14]. In any case the value found for small sizes using finite-size scaling techniques should be intermediate between this ratio ($d_e/d_q \simeq 2.7$) and the correct one $d_e/d_q > 1$.

In the following section we are going to present our numerical results for small samples using finite-size scaling techniques. We remind the reader on the difficulty to extract a precise determination of the parameters describing the transition (critical temperature and critical exponents) and that our main derivations are obtained using the arguments presented in this section.

3. Finite-size scaling results.

In this section we show the numerical results we have obtained studying the four-dimensional ising spin glass with a magnetic field equation (11). We have done Monte Carlo numerical simulations using the heat bath method in a four-dimensional lattice with periodic boundary conditions. Two magnetic fields have been studied $h = 0.3, 0.4$ far from the $h = 0$ line. This is also smaller than the field $h = 0.6$ we studied in the previous work [12].

Firstly we present results for $h = 0.4$. In this case we have tried to determine the transition point studying the Binder function equation (12) and the skewness equation (13) of the order parameter q . To this end we have simulated three sizes $L = 3, 4, 5$ and a large number of samples (900,500,100 respectively). It is necessary to simulate a large number of samples because of the strong fluctuations of the curtosis and the skewness from sample to sample. A slow cooling procedure was done in order to thermalize the samples even though it was not too much difficult reach equilibrium because of the small sizes we simulated. Figures 2 and 3 show the Binder parameter and the skewness for these sizes in a wide range of temperatures (from $T = 2.5$ down to $T = 1.25$). In both cases (Binder parameter and skewness) all moments have been computed over the distribution $P(|q|)$. When the $P(q)$ has a tail extending down to negative overlaps the moments $\langle |q|^k \rangle$ are different from the moments $\langle q^k \rangle$. Anyway we expect that the crossing point can be determined using both types of moments because they should coincide for very large sizes.

There is no clear signature of a crossing point similar to that found at zero magnetic field. In fact, both parameters (curtosis and skewness) are highly irregular with the temperature and this could be a consequence of the strong-finite size effects in the tail of the $P(q)$ distribution. Also we have studied the curtosis and the skewness for the overlap q_e and in this case crossing point is seen. But these strong finite-size effects are more pronounced in the case of the overlap q than in case of the overlap q_e .

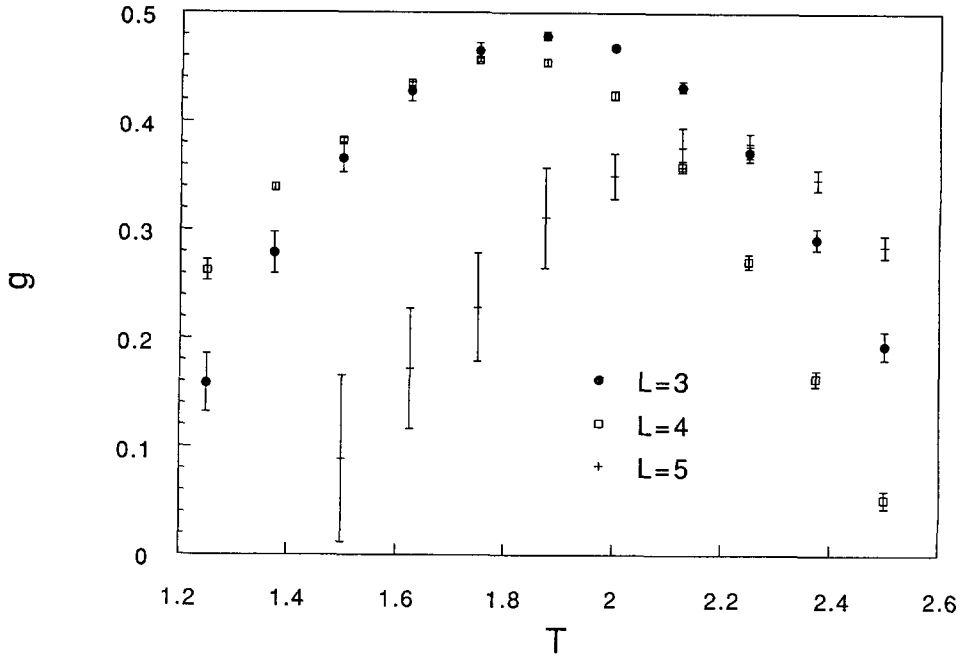


Fig. 2. — The binder parameter g as a function of the temperature for three different small sizes at $h = 0.4$. The error bars have been obtained using the jack-knife method.

It could be argued that this could be a sign of no phase transition. In fact, this possibility is not excluded but as we will see later, the clear evidence of this strong finite-size corrections (especially those which regard the left tail of the $P(q)$ distribution) give a direct explanation why is so difficult to locate the transition with a magnetic field.

As we commented in the second section we can try to determine indirectly the transition point using finite-size scaling (Eqs. (21 and 27)). Following the same procedure like in a previous [12] we have studied a smaller magnetic field $h = 0.3$ (in that case we studied a strong magnetic field $h = 0.6$ in order to be far from the critical point). We simulated six values of L from $L = 3$ up to $L = 8$ with 64 samples in each case. We computed the non linear susceptibilities χ_{nl} and χ_{nl}^e for q and q_e respectively. In order to suppress strong corrections because of the tail of the $P(q)$ extending down to negative overlaps (for q_e this effect is not present) we have calculated, instead of equation (14) the following non linear susceptibility

$$\chi_{nl} = N \left(\overline{\langle q^2 \rangle} - \overline{\langle |q| \rangle}^2 \right) \quad (29)$$

This expression tries to diminish the effect of the long tail of the $P(q)$ and it should give the same divergence for large sizes like equation (14). We used simulated annealing [28] in order to thermalize samples and a careful check was made in order to be sure that thermalization was achieved especially for the largest sizes. The temperature was decreased from $T = 2.5$ down to $T = 1.25$, the Monte Carlo time growing as a power of the k -th step in the annealing schedule. A power increase between three and four was enough to thermalize the samples. Typically for the largest sizes $L = 7, 8$ the system stayed 10000 Monte Carlo steps at $T = 2.5$

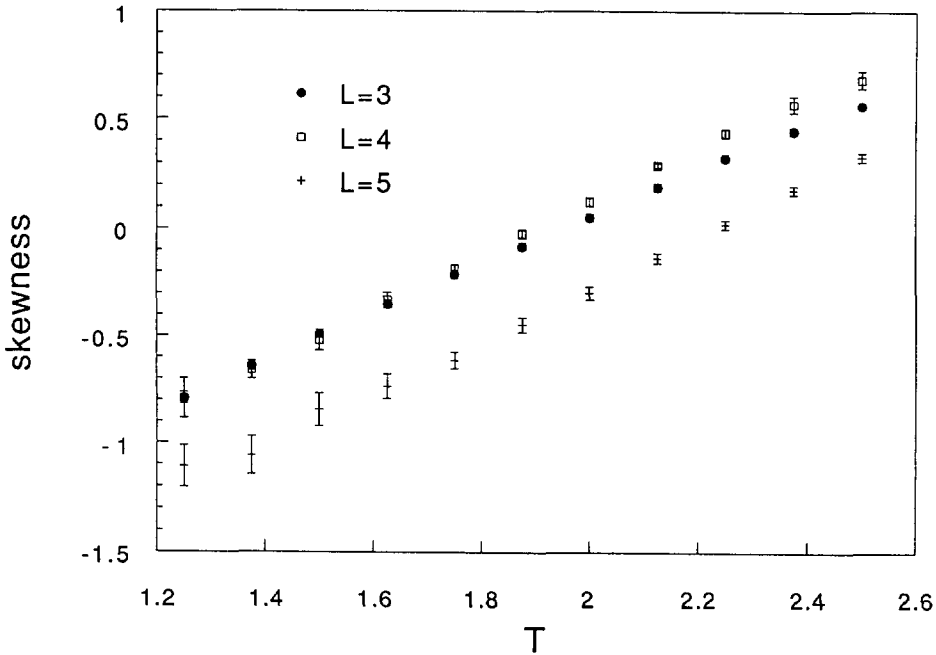


Fig. 3. — The skewness as a function of the temperature for three different small sizes at $h = 0.4$. The error bars have been obtained using the jack-knife method.

which were progressively increased up to 100000 at the lowest temperature $T = 1.25$ (in case $L = 8$ we simulated only down to $T = 1.5$). At each temperature statistics was collected over 20000 MCsteps. Also, 8 replicas were made to evolve in parallel increasing the statistics up to 160000 MCsteps.

Figures 4 and 5 show χ_{nl} and χ_{nl}^e respectively versus size in a logarithmic scale. Power law divergences set in close to $T = 1.7$. χ_{nl} seems to diverge like $L^{2.6}$ and χ_{nl}^e like $L^{1.0}$. In order to establish more accurately the transition point and the value of the critical exponents we have constructed a numerical algorithm which looks for the best fit. This algorithm uses the least squares method and looks for the three parameters (T_c , η and ν) which minimize the cost function (in data analysis it is usually called χ^2). The difficulty of finding the transition point is clearly seen when looking at the overlap q . In this case it is very difficult to find a good fit and this gives a critical temperature close to $T = 1.5$ which we judge not very fiable and too small because of the bad quality of the finite-size scaling (a similar feature was observed in our previous work for $h = 0.6$ and it could be that our estimate for the critical temperature close to $T = 1.1$ in that case were too small). The explanation why the overlap q is not useful to accurately determine the transition temperature and the critical exponents is because of the aforementioned strong finite-size effects. Figure 6 shows the symmetrized order parameter $P(|q|)$ for three sizes $L = 5, 6, 7$ for the field $h = 0.3$ at the lowest temperature $T = 1.25$. Even for $L = 7$ the $P(|q|)$ shows a long left tail extending to zero overlap. This means that $P(q)$ for $L = 7$ still reaches the region of negative overlaps.

Instead of, we can search for the best fit in case of the energy overlap q_e . Figure 7 shows $P(q_e)$ for the same sizes like figure 6. In this case the support of the distribution $P(q_e)$ is always in the region of positive values of the overlap q_e and finite-size effects are smaller.

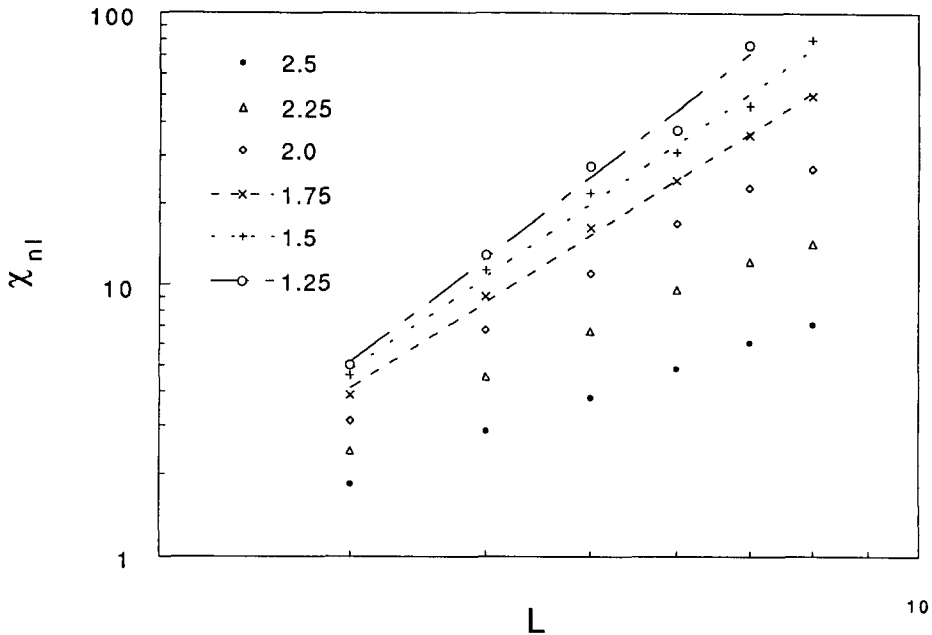


Fig. 4. — χ_{nl} versus size for a magnetic field $h = 0.3$ in a log-log scale. A divergence sets in close to $T = 1.7$ and $\chi_{nl} \sim L^{2-\eta}$ with $\eta \simeq -0.6$.

Using our numerical algorithm for the best finite-size scaling for the energy overlap q_e we find $T_c = 1.75 \pm 0.02$, $\nu = 0.9 \pm 0.1$ and $\eta_e \simeq 1.0 \pm 0.1$. The error bars delimit the region in which our numerical algorithm gives a good fit. These error bars should be taken with care and only like estimates. It is difficult to find the precise value of the error bars and they could be determined correctly only using a sophisticated jack-knife method. The best fit is of good quality to the naked eye and it is shown in figure 8. The value of $\eta_e \simeq 1.0$ for the critical temperature $T_c \simeq 1.75$ is consistent with the slope of the divergence shown in figure 5. Using the value of T_c found with the overlap q_e we can establish the value of η for the overlap q looking at figure 4. We obtain $\eta \simeq -0.6 \pm 0.1$ and using the previous values of T_c and ν for q_e we obtain the finite-size scaling plot shown in figure 9. The curves for different sizes do not seem to fall onto the same universal curve but this has not to be a surprise because, as we commented previously, also does not the best fit (let us remember that the parameters T_c , η and ν we have used in figure 9 are not the ones we obtain looking at the best fit for the overlap q using our numerical algorithm).

Using equations (18 and 28) we obtain $d_q \simeq 0.7$ and $d_e \simeq 1.5$ giving the ratio $\frac{d_e}{d_q} \sim 2.2$. This ratio should be intermediate between the value found at zero field ($\simeq 2.7$) [14] and its real value ($d_e/d_q > 1$). This gives support to the fact that the energy overlap shows the critical behavior of the codominant finite-size correction (which is the dominant one at zero magnetic field). In fact, we can estimate the true ratio $\frac{d_e}{d_q}$. Because d_e shows the codominant finite-size correction which should be the second order one we can estimate d_e to be the half one $d_e \simeq 0.75$. As commented in the previous section, this also happens in mean-field theory in the AT line. Using numerical simulations one finds $d_e = 4$ but the correct value is the half one $d_e = d_q = 2$.

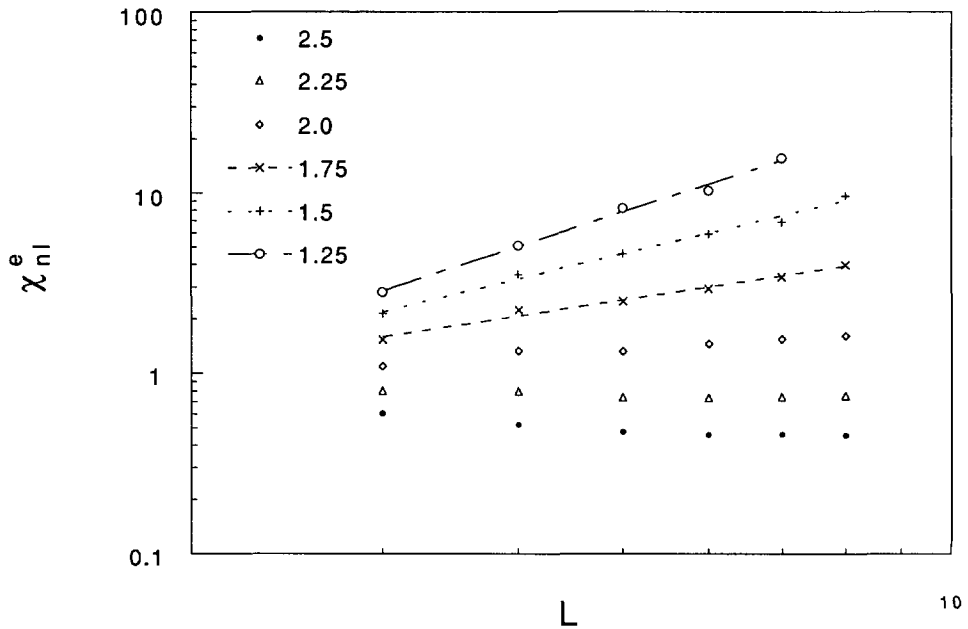


Fig. 5. — χ_{nl}^e versus size for a magnetic field $h = 0.3$ in a log-log scale. A divergence sets in close to $T = 1.7$ and $\chi_{nl} \sim L^{2-\eta_e}$ with $\eta_e \simeq 0.6$.

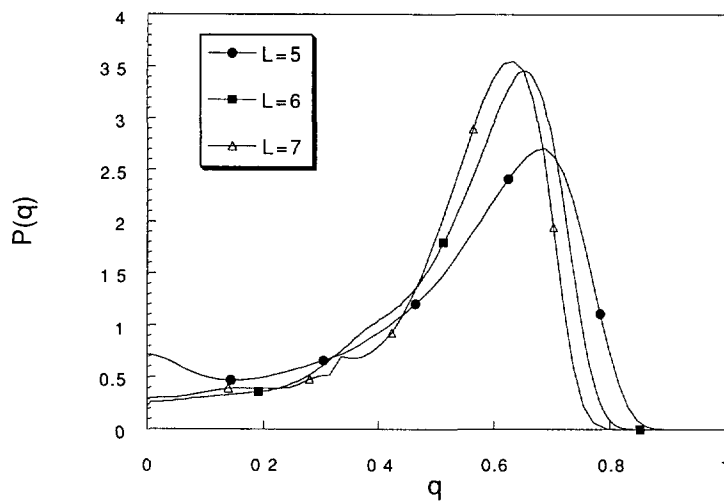


Fig. 6. — $P(|q|)$ for three different sizes at $h = 0.3$ and $T = 1.25$. There is a long tail that reaches the region of negative overlaps q .

In the four-dimensional case with applied magnetic field we obtain the ratio $\frac{d_e}{d_q} \simeq 1.1$.

Our results for $h = 0.3$ (altogether with those previously found at $h = 0.6$ [12]) are compat-

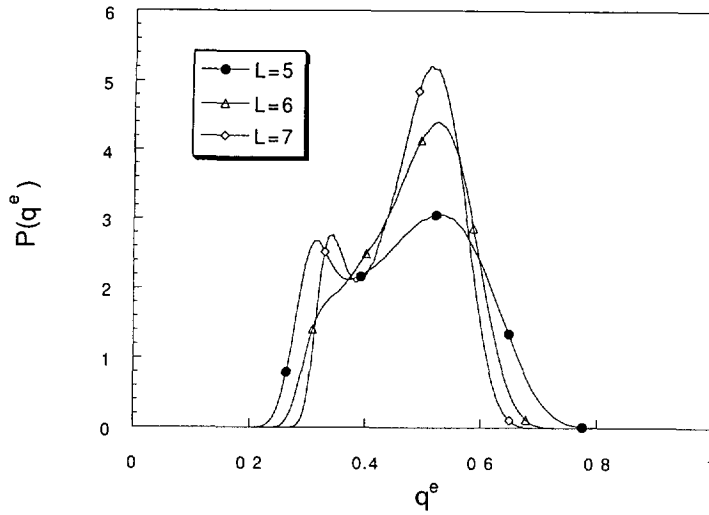


Fig. 7. — $P(q^e)$ for three different sizes at $h = 0.3$ and $T = 1.25$. It has two peaks and there are not so large tails like in case of $P(q)$.

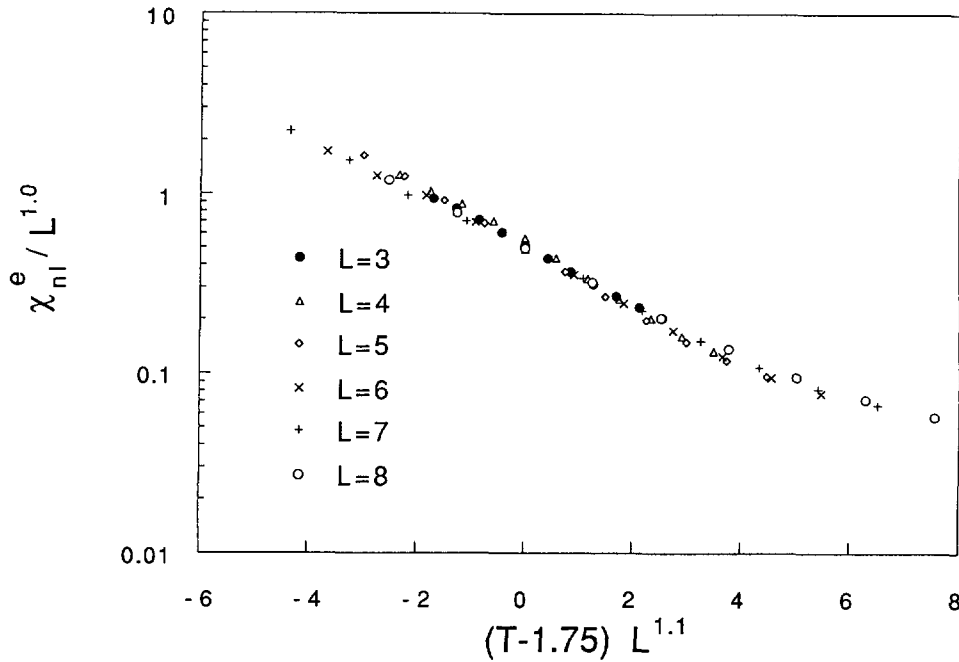


Fig. 8. — Finite-size scaling for χ_n^e at $h = 0.3$.

ible with the existence of a transition line in finite magnetic field with a similar form to that of mean-field theory and (obviously) with different critical exponents. The Fisher exponent $\eta \sim -0.6(\pm 0.1)$ differs from that found at zero field $\eta \sim -0.25(\pm 0.1)$. Also the exponent ν

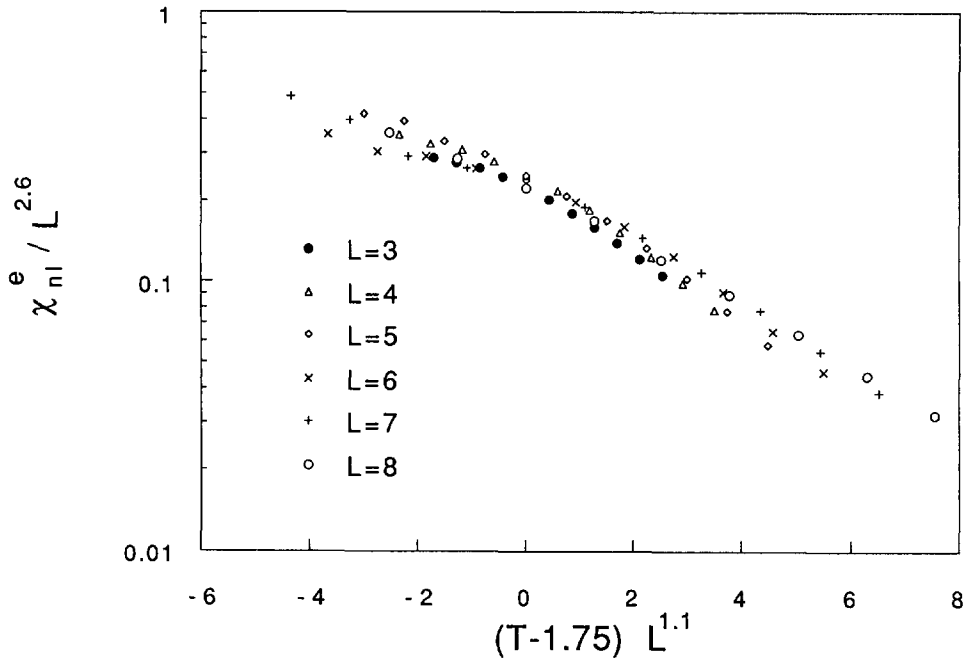


Fig. 9. — Finite-size scaling for χ_{nl} at $h = 0.3$.

seems to be sensibly different ($\nu \sim 0.9 \pm 0.1$ versus $\nu \simeq 0.7 \pm 0.2$ at zero field) within our numerical precision. Then the AT line seems to be in a different universality class in respect to the transition at zero magnetic field.

We stress that it is very difficult to locate the transition point using the overlap q for the small sizes we have investigated. It is affected of very strong finite-size corrections (the always commented effect of the left tail of the $P(q)$). In our previous determination of the AT line with a higher field $h = 0.6$ these effects were smaller in respect to the results we now present at field $h = 0.3$ because in a higher field we expect that the left tail of the $P(q)$ is suppressed faster. In fact, in that case the finite-size scaling for the overlap q (our Fig. 9) was better to the naked eye. It is difficult to quantify how many this higher-order corrections can perturb the results and a precise determination of the critical temperature and of the critical exponents along the AT line seems to be very difficult using finite-size scaling methods for small sizes.

In the following sections we present different approaches in order to discover the existence of a transition line in a magnetic field but using larger sizes.

4. Replica symmetry breaking for large sizes.

As was explained in the second section one of the very features of a replica symmetry broken phase with magnetic field is the existence of an infinity of equilibrium states which can be described using the $P(q)$ function. If the spin-glass phase in a magnetic field in short range models were similar to the phase predicted by the mean-field theory we expect that the $P(q)$ should have two singularities as described in equation (8).

Let us now couple two replicas with a field ϵ :

$$H_2[\sigma, \tau] = H_1[\sigma] + H_1[\tau] + \epsilon \sum_i \sigma_i \tau_i \quad (30)$$

and the single replica Hamiltonian H_1 is given in equation (11).

For a very large size and a finite coupling ϵ the overlap q among two replicas σ and τ can vary with ϵ in two different ways according to the sign of ϵ . Generally, within the spin-glass phase, we can expect [14]:

$$q(\epsilon) = q_{\max} + E^+ \epsilon^{\xi_{qq}} \quad \epsilon > 0 \quad (31)$$

$$q(\epsilon) = q_{\min} - E^- (-\epsilon)^{\xi_{qq}} \quad \epsilon < 0 \quad (32)$$

In mean-field theory $\xi_{qq} = 1/2$ and in four dimensions at zero magnetic field its value seems to be close to $1/3$ [14]. Because of the large tail of the $P(q)$ which extends down to negative overlaps we expect E^- to be much smaller than E^+ and the equation for $q(\epsilon)$ with $\epsilon < 0$ to be much affected by higher-order corrections.

At zero magnetic field this quantity $q(\epsilon)$ is very useful because it thermalizes relatively quickly and it can be also easily measured using the Monte Carlo method. Physically speaking it corresponds to the intra-valley overlap or overlap among two identical pure states with an extra added perturbation proportional to the field ϵ . It can be also shown that it gives equivalent information to the tails of the $P(q)$ functions (see [14, 15]). With a magnetic field is more difficult to extract information about the behaviour of $q(\epsilon)$ with ϵ especially when $\epsilon < 0$. This is because the region of interest in which the equations (31 and 32) are valid is when $\epsilon < h^2$. When $\epsilon < 0$ the behaviour of $q(\epsilon)$ for $\epsilon < h^2$ differs from its behaviour for $\epsilon > h^2$ because the effect of the magnetic field conflicts with the effect of the negative coupling ϵ which tends to make the spins of each of the two replicas to point in different directions. This effect is not important when $\epsilon > 0$. This means that only for very small values of ϵ one can use the equations (32) to extrapolate to $\epsilon \rightarrow 0$. Then the problem is that for such small values of ϵ is very difficult to thermalize and one encounters serious difficulties in order to find the values of $q_{\min}$.

Anyway we have tried to discover indications of a finite discontinuity in $q(\epsilon)$ for $\epsilon = 0$. The existence of a discontinuity in the quantity $q(\epsilon)$ in the limit $\epsilon \rightarrow 0$ is a signature of a replica broken phase. Figure 10 shows $q(\epsilon)$ for a very large size $L = 17$ at finite magnetic field $h = 0.2$ and temperature $T = 1.5$. According to our finite-size scaling results we expect this point in the $h - T$ plane to be within the spin-glass phase. The function $q(\epsilon)$ is far from being symmetric under the interchange $\epsilon \rightarrow -\epsilon$ as expected (symmetry is expected only in the region $|\epsilon| \gg h^2$ where the effect of the field is negligible).

Fitting our data to equation (31) for different positive values of ϵ (from $\epsilon = 0.5$ down to $\epsilon \sim 6 \times 10^{-3}$) we obtain $q_{\max} \simeq 0.41$ and ξ_{qq} close to 0.4. This value 0.41 is very similar to the value of $q_{\max}$ found at zero magnetic field at the same temperature. This very small dependence of $q_{\max}$ with the magnetic field is a peculiar feature also in mean-field theory.

For ϵ negative we see that the overlap remains negative in a wide range of values of ϵ . The extrapolation using equation (32) does not work well. Using only values of ϵ smaller than 0.01 (in order to be in the region $\epsilon < h^2$) one sees that next order corrections for ϵ in equation (32) when ϵ is negative are important. This conclusion which is clearly seen for this very large size is equivalent to the fact already commented in previous sections regarding the long left tails of the $P(q)$ function for small sizes. It is really difficult to obtain a fiable extrapolation of $q_{\min}$ and we are not able to precisely determine the discontinuity in q for $\epsilon \rightarrow 0$. What can be concluded from looking at figure 10 is that there is a strong asymmetry between the behaviour

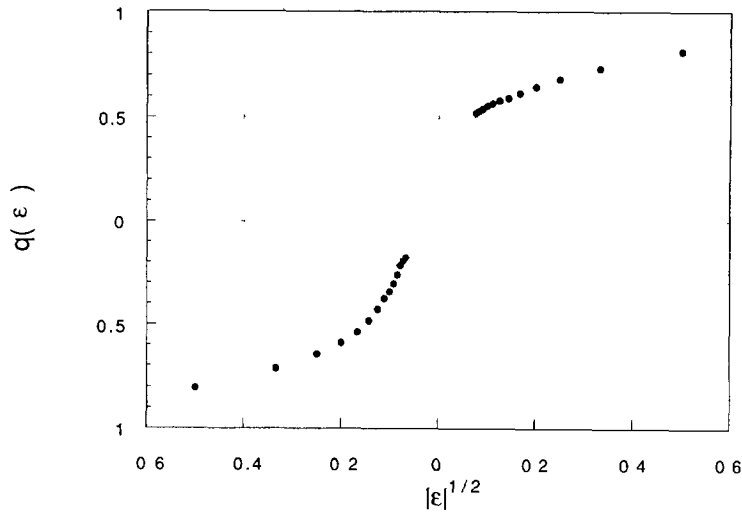


Fig. 10. — $q(\epsilon)$ for a very large size $L = 17$ at $h = 0.2$, $T = 1.5$. For $\epsilon > 0$ and fitting to equation (31) it converges to $q_{\max} \simeq 0.41 \pm 0.02$. For $\epsilon < 0$ it is very difficult to determine $q_{\min}$. The grid helps to see the asymmetry of the two branches of $q(\epsilon)$.

of $q(\epsilon)$ when $\epsilon > 0$ from its behavior for $\epsilon < 0$. This is compatible with the existence of a finite discontinuity of $q(\epsilon)$ for $\epsilon = 0$.

5. Dynamical studies.

Dynamical effects are very interesting within the spin-glass phase because of the existence of several thermodynamic states. We have studied the dynamics of a very large size $L = 18$ at $h = 0.3$ in order to see the effects of the dynamics when the temperature is above or below the critical one (from the previous section we estimated $T_c \simeq 1.75$). One very interesting way to see replica symmetry breaking effects is to study the evolution of the overlaps q and q_e in function of the time but with different initial conditions. The same procedure was used at zero field (see [15]).

We have made to evolve 2 replicas in parallel during a number of t_0 Monte Carlo steps. During this time the system thermalizes over all energy barriers of height smaller than $\Delta E_{\max} \sim T \log(t_0)$. The system is in local equilibrium over length scales $R \sim t^{\frac{1}{z}}$ (or $(\log(t))^{\lambda}$ according to the droplet model) where z is a dynamical exponent. At this time we make both replicas one equal to the other and we study the evolution of q and q_e over scales of time $t < t_0$ (more precisely one should collect data over time scales such that $\log(t) < \log(t_0)$). During this time the system is in local equilibrium and all overlaps evolve as if they were at equilibrium. This is a true characteristic of aging phenomena (see [29] for interesting results on this issue for the three dimensional ising spin glass). Both overlaps $q_{\max}$ and $q_{\max}^e$ should evolve towards their maximum values $q_{\max}$ and $q_{\max}^e$ respectively.

On the other hand, we can study the time evolution of q and q^e starting from random initial configurations. They are expected to evolve towards its corresponding minimum values $q_{\min}$ and $q_{\min}^e$ respectively.

In the spin-glass phase we expect $q_{\max} \neq q_{\min}$ and $q_{\max}^e \neq q_{\min}^e$. The existence of disconti-

nities

$$\delta q = q_{\max} - q_{\min} \quad \delta q_e = q_{\max}^e - q_{\min}^e \quad (33)$$

is, at least, a sign of metastability. If this discontinuities survive for very large times (less than $\exp(N^\lambda)$ with λ close to $1/3$ according to [30] which is the characteristic time of crossing energy barriers among pure states) this could be naturally explained in terms of a phase with replica symmetry breaking features.

But we can do more. We can study the time evolution of the overlaps for the same realization of disorder but different initial conditions (i.e. different pairs of replicas). Within the spin-glass phase we expect that starting from different pairs of thermalized (over a time t_0) initial configurations, the overlaps q and q_e will evolve identically over time scales t such that $\log(t) < \log(t_0)$. After that, the different pairs of replicas will begin to surmount energy barriers (higher than those of size $T \log(t_0)$ over which the replicas were initially at thermal equilibrium). And overlaps will follow different trajectories in phase space. This first regime is well known in mean-field theory [31]. Instead of, starting from random initial configurations we expect diverging trajectories in phase space as soon as the time evolution takes place.

This is observed in our results. We have simulated a very large size $L = 18$ for one realization of the disorder. Figures 11 and 12 show the time evolution of q and q_e in the paramagnetic phase $T = 2.0$, $h = 0.3$ well above the AT line. The upper curves correspond to the case of thermalized initial configurations over a time $t_0 = 10000$. The lower curves correspond to the evolution starting from random initial configurations. Upper and lower curves show the time evolution of four pairs of replicas. No sign of discontinuities (Eq. (33)) δq and δq_e are observed. Also there is no sign of diverging trajectories. Even though there is metastability (note that the time evolution of the overlaps is noticeable only on large time scales) no sign of replica symmetry breaking is observed.

The picture is very different in figures 13 and 14. They correspond to dynamics below the AT line, $T = 1.25$, $h = 0.3$ and the parameters are the same like figures 11 and 12. Firstly we find evidence of a finite discontinuity for δq and δq_e . Also, the upper curves (corresponding to 4 pairs of replicas) follow the same time evolution up to a time t close to t_0 . After that time, they begin to depart one from the other. The lower curves (corresponding to random initial configurations) began to depart very soon.

This results are in agreement with a phase transition at $h = 0.3$ between $T = 1.25$ and $T = 2.0$ from a paramagnetic phase to a spin-glass phase with replica symmetry breaking features as we know in mean-field theory.

6. Conclusions.

One of the open questions in spin glasses regards the existence of a finite temperature phase transition with an applied magnetic field. This question is of maximum interest in case of short-range ising spin glasses in which mean-field theory and droplet models give substantially different predictions.

We have adressed this question studying the four dimensional Ising spin glass. The technique we have used is finite-size scaling. Our results are consistent with the existence of an AT line similar to that found in mean-field theory (even though our numerical precision is not enough in order to predict its precise form). This phase transition seems to be in a different universality class to that found at zero field. We find $\eta \simeq -0.6 \pm 0.1$ and $\nu \simeq 0.9 \pm 0.1$ along the AT line. The first exponent differs clearly from that found at zero field ($\eta \simeq -0.25 \pm 0.1$) but the second one is only sensibly different ($\nu \simeq 0.7 + 0.2$). These results have been obtained studying both

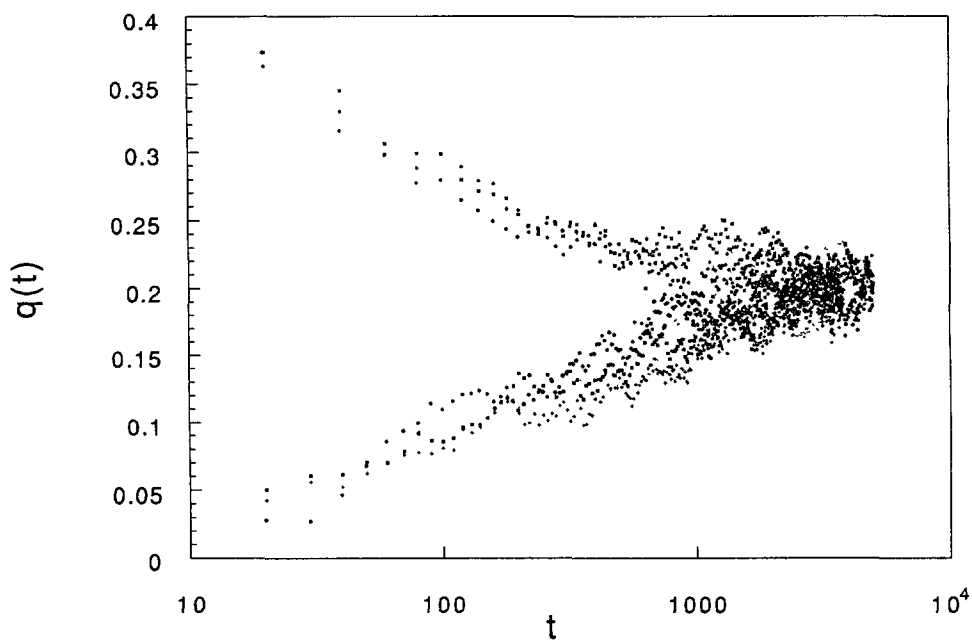


Fig. 11. — Time evolution of the overlaps of four different pairs of replicas starting from different initial conditions within the paramagnetic phase ($T = 2.0$, $h = 0.3$).

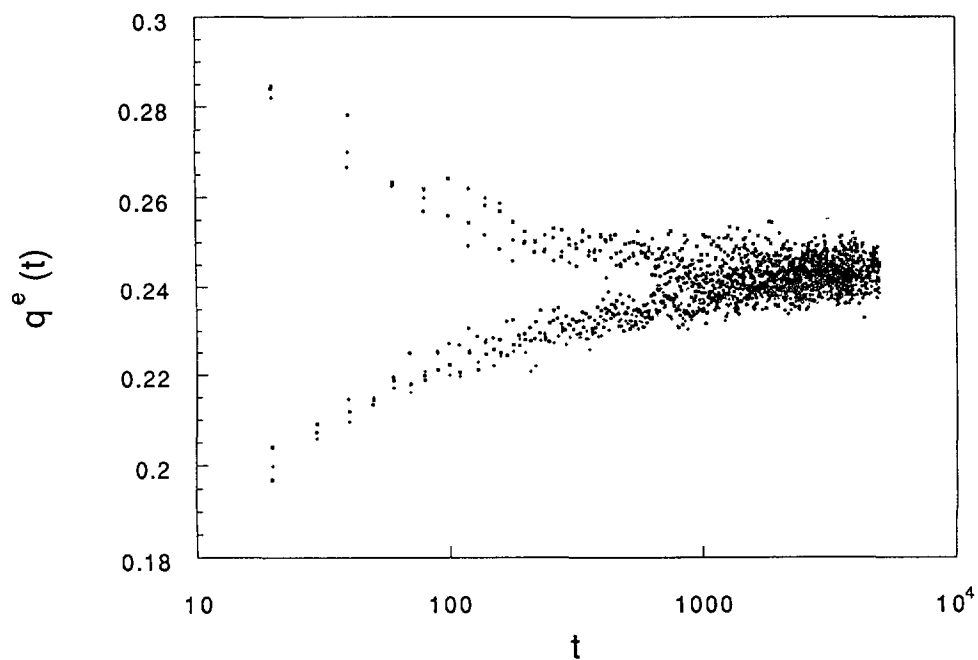


Fig. 12. — Time evolution of the energy overlaps of four different pairs of replicas starting from different initial conditions at $T = 2.0$, $h = 0.3$.

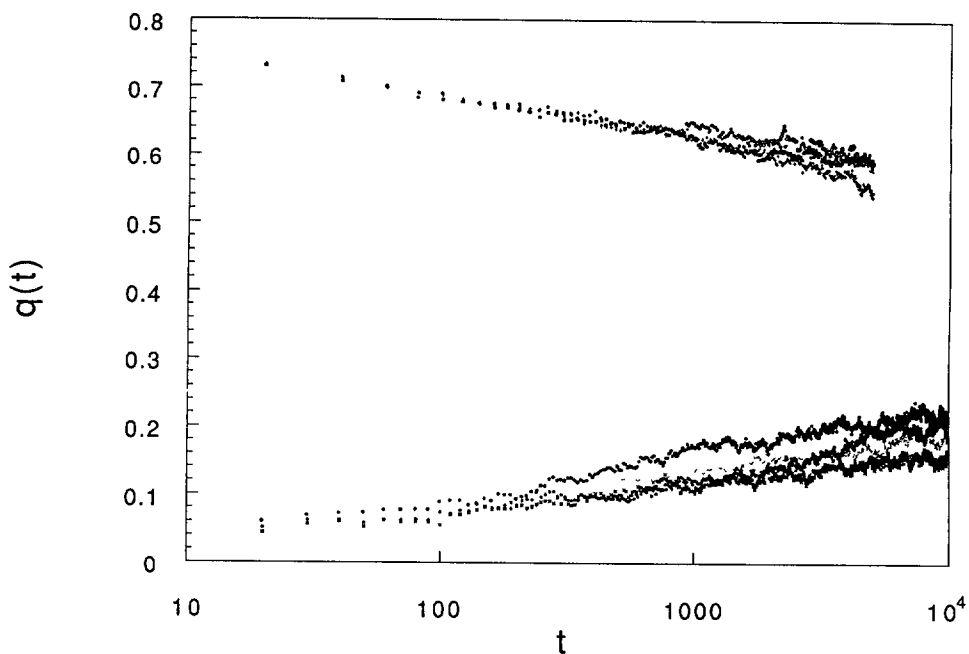


Fig. 13. — Time evolution of the overlaps of four different pairs of replicas starting from different initial conditions within the spin-glass phase ($T = 1.25$, $h = 0.3$).

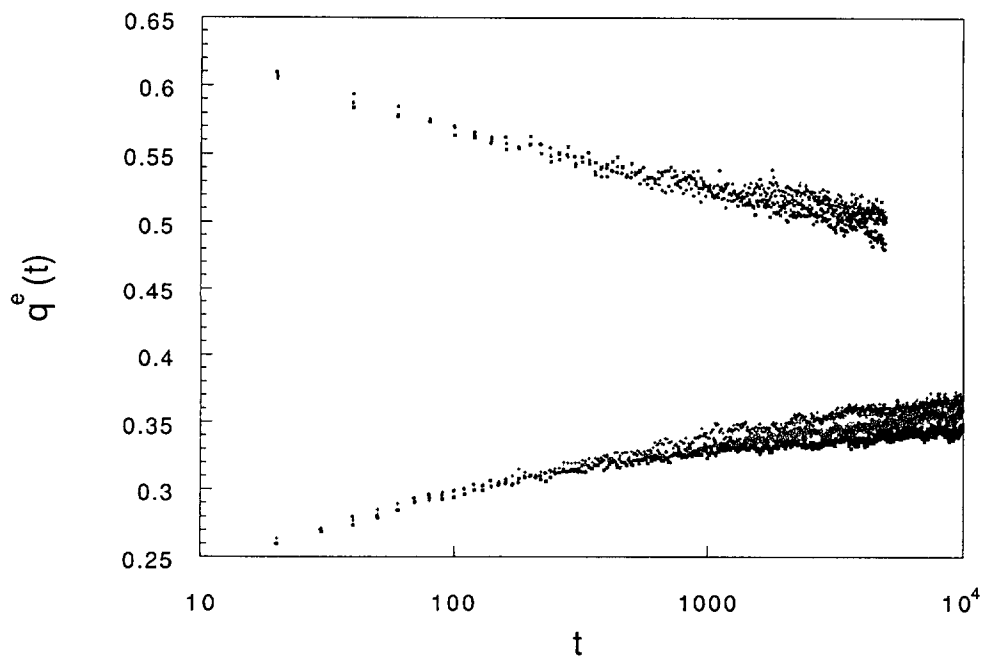


Fig. 14. — Time evolution of the energy overlaps of four different pairs of replicas starting from different initial conditions at $T = 1.25$, $h = 0.3$.

the order parameter q and the energy overlap q^e and they reveal the same kind of features like in mean-field theory. Two main comments are in order.

The first one regards the limitation of finite-size techniques. As we said in the second section we are not able to see the dominant critical behaviour for the energy overlap q^e and it is very difficult to obtain a best finite-size scaling for the non linear-susceptibility corresponding to the overlap q . In fact, for the largest sizes we have been able to simulate ($L = 8$), the probability distribution $P(q)$ for a finite magnetic field still has a long tail reaches a wide zone of negative overlaps. The consequences of this strong effect is that the Binder parameter and the skewness are not useful in order to locate the transition and this has to be searched more indirectly. It is clear then that if the effects of the tail of the $P(q)$ are very strong, we cannot exclude the possibility of a crossover to a different regime for larger sizes. As a consequence (and we have concentrated our numerical study on the field $h = 0.3$) we have been able to extract critical exponents looking for the best finite-size scaling for the energy overlap q^e . After that, we have been able to determine the critical exponent η for the overlap q . Our results for the critical exponents are compatible with those found in a previous work at a higher field $h = 0.6$ and they suggest that the AT line is in a different universality class.

A different approach but for much larger sizes (in which there is not a long tail for $P(q)$ which reaches down to negative values of the overlap) is mandatory. To this end, we have investigated the prediction of mean-field theory regarding the existence of two singularities in the $P(q)$ distribution (this was done for a size $L = 17$). Also we have studied the dynamics of a large sample ($L = 18$) within and out of the spin-glass phase. Our results obtained by coupling two replicas suggest that the left tail of the $P(q)$ has very strong next order corrections and that there is a slight indication of a discontinuity in the overlap $q(\epsilon)$ in the limit $\epsilon \rightarrow 0$. This is in agreement with the mean-field prediction on the existence of two singularities for the $P(q)$ located at two different values of the overlap q . Also, we have studied the dynamics of the system with a magnetic field. Our results are consistent with the picture of a spin-glass phase with many valleys similar to what happens in mean-field theory.

The second comment refers to the order of the phase transition in a magnetic field. This problem was studied long time ago by A.J. Bray and S.A. Roberts [32] using the ϵ expansion near six dimensions. They did not found a non-gaussian fixed point below six dimensions suggesting that there is not a usual phase transition with magnetic field. From our results we have seen it seems to be of the usual second order type (for the largest size $L = 8$ we have seen that there is no latent heat) even though we cannot exclude the possibility of a different kind of phase transition with some features of first order ones. This is a very interesting open problem.

In order to complement more all our results it would be necessary to perform a large scale simulation for a very large size in order to confirm all our predictions for the critical exponents. This is a very interesting open numerical task.

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References

- [1] Mezard M., Parisi G., Virasoro M.A. "Spin Glass Theory and Beyond" (World Scientific, 1987).
- [2] Binder K., Young A.P., *Rev. Mod. Phys.* **58** (1986) 801.
- [3] Parisi G. "Field Theory, Disorder and Simulations" (World Scientific, Singapore 1992).
- [4] Sherrington D., Kirkpatrick S., *Phys. Rev. B* **17** (1978) 4384.
- [5] De Dominicis C., Kondor I., *Physica A* **163** (1990) 265.
- [6] McMillan W.L., *J. Phys. C* **17** (1984) 3179.
- [7] Fisher D.S., Huse D.A., *Phys. Rev. Lett.* **56** (1986) 1601.
- [8] Fisher D.S., Huse D.A., *Phys. Rev. B* **38** (1988) 386.
- [9] Recent Progress in Random magnets, D.H. Ryan Ed. (McGill, University of Montreal October 1991).
- [10] Hamman J., Ledermann M., Ocio M., Orbach R., Vincent E., *Physica A* **185** (1992) 278.
- [11] de Almeida J.R., Thouless D.J., *J. Phys. A* **11** (1978) 983.
- [12] Badoni D., Ciria J.C., Parisi G., Pech J., Ritort F., Ruiz J.J. *Europhys. Lett.* **21** (1993) 495.
- [13] Grannan E.R., Hetzel R.E., *Phys. Rev. Lett.* **67** (1992) 907.
- [14] Parisi G., Ritort F., to appear in *J. Phys. A*.
- [15] Ciria J.C., Parisi G., Ritort F., to appear in *J. Phys. A*.
- [16] Mézard M., Parisi G., Sourlas N., Toulouse G., Virasoro M., *J. Phys. France* **45** (1984) 843.
- [17] Parisi G., *J. Phys. A* **13** (1980) 1101.
- [18] Young A.P., *Phys. Rev. Lett.* **51** (1983) 1206.
- [19] Parisi G., *J. Phys. A* **13** (1980) 1887.
- [20] Franz S., Parisi G., Virasoro M.A., *J. Phys. I France* **2** (1992) 1869.
- [21] Parisi G., Ritort F., Slanina F., *J. Phys. A* **26** (1993) 3775.
- [22] Bhatt R.N., Young A.P., *Phys. Rev. B* **37** (1988) 5606.
- [23] Ogielsky A.T., *Phys. Rev. B* **32** (1985) 7384.
- [24] Caracciolo S., Parisi G., Patarnello S., Sourlas N., *Europhys. Lett.* **11** (1990) 783.
- [25] Reger J.D., Bhatt R.N., Young A.P., *Phys. Rev. Lett.* **16** (1990) 1859.
- [26] Green J.E., *J. Phys. A* **18** (1985) L43.
- [27] Bray A.J., Moore M.A., *J. Phys. C* **13** (1980) 419.
- [28] Kirkpatrick S., Gelatt C.D. Jr., Vecchi M.P., *Science* **220** (1983) 671.
- [29] Rieger H., *J. Phys. A* **26** (1993) L615.
- [30] Colborne S.G.W., *J. Phys. A* **23** (1990) 4013.
- [31] Sompolinsky H., Zippelius A., *Phys. Rev. B* **25** (1982) 6860.
- [32] Bray A.J., Roberts S.A., *J. Phys. C* **13** (1980) 5405.
- [33] RTN collaboration. Experience on RTN. Proceedings of the International Conference on Computing in High Energy Physics '92 Annecy. CERN.