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Low temperature behaviour of 3-D spin glasses in a magnetic field

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Résumé. — Nous présentons les résultats de deux ensembles de simulations numériques de verres de spins d’Ising tridimensionnels en présence d’un champ magnétique. Dans le premier ensemble nous calculons, entre autres quantités, la distribution de probabilité du recouvrement des configurations des spins \( P(q) \), la distribution de probabilité du recouvrement des configurations des liens \( P_e(q_e) \) et la susceptibilité verre de spin \( \chi_{SG} \) pour différents volumes et températures. Les résultats sont en bon accord avec la théorie du champ moyen : \( P(q) \) et \( P_e(q_e) \) sont non triviaux et non automoyennants et \( \chi_{SG} \) augmente avec la taille linéaire \( L \) du système comme \( \chi_{SG} \sim L^\omega \). Nous estimons \( \omega = 1,8 \pm 0,25 \) à \( T = 0,83 \). Dans le deuxième ensemble de simulations nous introduisons un petit couplage \( \epsilon \) entre deux copies du système et leur recouvrement \( Q(\epsilon) \) est calculé en fonction d’\( \epsilon \). La pente de \( Q(\epsilon) \) à l’origine augmente avec \( L \), en accord avec les autres simulations. Nos données ne sont pas compatibles avec les alternatives à la théorie du champ moyen proposées à ce jour.

Abstract. — We present the results of two sets of numerical simulations of 3-d Ising spin-glasses in the presence of an uniform magnetic field. In the first set, among other quantities, we compute the spin-spin overlap probability distribution \( P(q) \), the link-link overlap probability distribution \( P_e(q_e) \) and the spin-glass susceptibility \( \chi_{SG} \) for different volumes and temperatures. The results are in good agreement with mean-field behaviour : \( P(q) \) and \( P_e(q_e) \) are non trivial and non self-averaging and \( \chi_{SG} \) shows an increase with the linear size \( L \) of the system as \( \chi_{SG} \sim L^\omega \). Our estimate is \( \omega = 1,8 \pm 0,25 \) at \( T = 0,83 \). In the second set of simulations a small coupling \( \epsilon \) is introduced between two copies of the system and the copy overlap \( Q(\epsilon) \) is computed as a function of \( \epsilon \). \( Q(\epsilon) \) becomes steeper around \( \epsilon \sim 0 \) as \( L \) increases, in agreement with the previous set of simulations. Our data seem anyhow incompatible with the alternatives to mean-field theory proposed so far.
Introduction.

Spin glasses are well understood in the infinite range limit, where the mean field theory, based on the replica or on the cavity approach [1], should give the exact results. Quite likely the same behaviour is found in short range models in the limit of infinite dimensions. In this case, also at nonzero magnetic field, there are two phases: the usual paramagnetic high-temperature phase, and a low temperature, glassy phase, characterized by a large number (strictly speaking infinite) of pure equilibrium states. The dynamics of the system is quite complex. For intermediate times the system remains in a given pure state and the time correlation functions decay asymptotically (within this time range) with a power law; at much greater times the system hops between different pure equilibrium states. The hopping time diverges with the size of the system, and this feature makes numerical simulations of equilibrium properties quite awkward.

All these states have the same thermodynamical properties, in particular they have the same free energy density, but they differ in their local magnetizations; a quantity useful to compare different states is the overlap parameter $q^{\alpha\beta}$ defined as follows:

$$q^{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} m_i^\alpha m_i^\beta$$

(1)

where $m_i^\alpha$ is the local magnetization in the state $\alpha$ at the site $i$ and $N$ is the total number of sites. The self-overlap $q^{\alpha\alpha}$ turns out to be independent of the state $\alpha$ and is usually called the Edward-Anderson order parameter $q_{EA}$. Another useful quantity is the link-link overlap, defined as:

$$q_{e}^{\alpha\beta} = \frac{1}{N} \sum_{\langle ij \rangle} J_{ij} \langle \sigma_i \sigma_j \rangle_a J_{ij} \langle \sigma_i \sigma_j \rangle_\beta.$$  

(2)

Here $\langle \sigma_i \sigma_j \rangle_a$ is the value of the correlation between spins at sites $i$ and $j$ averaged in the pure state $\alpha$ and $J_{ij}$ is the coupling between these spins.

It is not completely understood whether the mean field picture remains correct also in a short range model at a given finite dimension. While this is possible for large dimensions, there must be a lower critical dimension below which this picture fails. In particular it is believed that in two dimensions there is no glassy phase. The behaviour in an external magnetic field is even more complex to foresee: as in finite dimension the amount of frustration is finite, there exists a critical field $h_c$ such that for $h > h_c$ no phase transition occurs. Is $h_c \neq 0$?

It is very difficult to understand the situation in three dimensions. Very long computer simulations [3, 4] at zero external magnetic field, hint at the existence of a phase transition, from the high temperature phase with zero $q_{EA}$, to a low temperature phase with non zero $q_{EA}$; numerical simulations of relatively few instances of the interactions at low enough temperatures (when the correlations length is larger than the size of the lattice) show a mean-field like behaviour both for the statics [5] and for the dynamics [6]. But it is not easy to extrapolate to the very large volume behaviour; moreover the experimental data are consistent with the occurrence of a phase transition although the possibility of a gradual freezing is difficult to exclude.

Most unfortunately there is even less information on the behaviour of the system at nonzero magnetic field: it would be extremely interesting to know if the glassy phase predicted by the mean field theory survives or not under these circumstances. Some qualitative scaling arguments [7, 8] predict that, in the infinite volume limit, any finite magnetic field would
destroy such a glassy phase and therefore no phase transition occurs in this case. The main assumption on which this simplified model rests, is that the excitations of the system at low temperature are due to the flipping of independent, localized regions (« droplets »); due to frustration, the interface energy of such an excitation would grow very weakly with the size of the droplet, whilst the gain in energy for any finite magnetic field to reverse all spins in a droplet in a given direction would always be favorable. Therefore any ordering other than the uniform one would be unstable (this is the so-called droplet model). So far this picture has not received a direct confirmation (e.g., via numerical simulation). An important quantity to study in this context is the probability distribution \( P_e(q_e) \) of the link-link overlaps \( q_e \) introduced in (Eq. (2)). When a domain of volume \( v \) and surface \( s \) is flipped, \( q \) changes by an amount proportional to \( v \), while \( q_e \) changes by an amount proportional to \( s \). Thus by comparing \( q_e \) and \( q \) it is possible to disentangle surface from volume effects.

In this paper we have investigated whether some of the predictions of the mean field theory for the low temperature, glassy phase are confirmed in three dimensions at nonzero magnetic field. Indeed, our numerical simulations seem to confirm many of the features proper to mean field theory. We have measured the spin glass susceptibility \( \chi_{SG} \) and we found that it exhibits a critical behaviour at low temperature. This may be expressed via an approximate scaling law of the form \( \chi_{SG} \sim L^\omega \), where \( L \) is the linear size of the system and \( \omega \) is a positive exponent. The probability distribution \( P(q) \) seems to be non trivial and non selfaveraging in the infinite volume limit. \( P_e(q_e) \) exhibits a similar behaviour.

In section 2 we introduce the model Hamiltonian and provide some technical details of the numerical simulations. In section 3 we present our numerical results. These results are discussed in section 4. A brief description of the results of the present simulations has already appeared elsewhere [9].

Simulation framework.

The question of the existence of many pure states and their overlaps may be studied considering two identical replicas of the same system, whose Hamiltonian is defined on the sites of a cubic lattice with periodic boundary conditions:

\[
-H_J = \sum_{\langle ij \rangle} J_{ij} (\sigma_i \sigma_j + \tau_i \tau_j) + \sum_i h (\sigma_i + \tau_i) + \varepsilon \sum_i \tau_i \sigma_i.
\] (3)

We indicate the two replicas of the system using the two sets of spins \( \sigma \) and \( \tau \). The notation \( \langle ij \rangle \) stands for the sum over pairs of nearest neighbour sites. The first two summations describe the standard Hamiltonian for a spin-glass in a uniform magnetic field (for two identical replicas). The coupling constants \( J_{ij} \) are statistically independent random variables, which take with equal probability the values \( \pm 1 \). There is also occasionally a very small coupling \( \varepsilon \) between the two replicas for reasons that will become clear later. Our analysis is based on a large set of Monte-Carlo simulations of the system described by the Hamiltonian (3). We used the Metropolis et al. algorithm. In all our simulations the magnetic field was kept fixed at the value \( h = 0.2 \). We did two kinds of numerical experiments. A first set (which in the following will be referred to as set A) concerns uncoupled copies (\( \varepsilon = 0 \) in formula (3)). Here measurements were performed at three different volumes, \( V = L^3 \), \( L = 6, 10, 14 \). To achieve statistical equilibrium, we started with random initial conditions at temperature \( T = 4 \) and then slowly cooled the system by increasing the inverse temperature \( \beta = 1/T \) by successive steps of \( \Delta \beta = 0.05 \). Measurements were performed at \( \beta = 0.65, 0.75, 0.85, 1, 1.2 \). For each volume a total of \( N_J \) different realizations of the couplings \( J_{ij} \) were randomly extracted, and for each of these realizations 128 copies of the system (differing in the initial
configurations of the spins) were simulated. For \( L = 6 \) \( N_J \) was set to 32, whereas for \( L = 10 \) and \( L = 14 \), \( N_J = 16 \).

The definitions of \( P(q) \) and \( P_e(q_e) \) given in equations (1) and (2) are not very useful for numerical purposes because they require the knowledge of the local magnetizations for every state \( \alpha \). It is well known [1] however that there exists an alternative definition, thermodynamically equivalent to the previous one, where this knowledge is not required. According to this definition it is enough to measure the probability distribution of the overlaps of \textit{individual configurations} of the copies provided that these configurations obey the Boltzmann distribution. So the \( P_J(q) \) probability distribution has been computed numerically as the probability distribution of the configuration overlap which for the copies \( \alpha \) and \( \beta \) is

\[
q^{\alpha \beta} = \frac{1}{V} \sum_{j=1}^{V} \sigma_j^\alpha \sigma_j^\beta .
\]  

(4)

Similarly we measure \( P_{e, J}(q_e) \), the probability distribution of the link-link overlaps \( q_e \):

\[
q_{e}^{\alpha \beta} = \frac{1}{3V} \sum_{\langle ij \rangle} J_{ij} \sigma_i^\alpha \sigma_j^\alpha \sigma_i^\beta \sigma_j^\beta = \frac{1}{3V} \sum_{\langle ij \rangle} \sigma_i^\alpha \sigma_i^\alpha \sigma_f^\beta \sigma_f^\beta .
\]  

(5)

Remember that in our simulations \( \delta_{ij} = 1 \). We did these measurements for several pairs of such copies for every one of the \( N_J \) Hamiltonians. We denote by \( P(q) \) and \( P_e(q) \) the average over the \( J \)'s. We also computed the spin glass susceptibility:

\[
\chi_{SG} = V \langle \langle q^2 \rangle \rangle - \langle q \rangle^2 \rangle_J
\]

(6)

where \( \langle \rangle_J \) means the average over the \( J \)'s.

In the second set of simulations (we will denote this as set B) we considered coupled replicas, i.e. the \( e \) term in (Eq. (3)) different from zero. The average overlap among two replicas is now a function of the coupling strength \( Q = Q(e) \). The reason for introducing this coupling between copies is the following. Consider the case of a ferromagnet. At the phase transition there is a spontaneous symmetry breaking with the appearance of a spontaneous magnetization. It is possible to study this symmetry breaking by measuring the response of the system to an external symmetry breaking field. One can study the magnetization \( m(h) \), the order parameter of this problem, as a function of an external magnetic field \( h \) (the variable conjugate to the order parameter). Below the critical temperature, \( m(h) \) becomes steeper and steeper around \( h \sim 0 \) as the volume increases and it develops a discontinuity at \( h = 0 \) in the infinite volume limit. The magnitude of this discontinuity is twice the spontaneous magnetization. In the spin-glass case the order parameter is the overlap \( q \). The variable conjugate to the order parameter is the coupling \( e \) between two copies. If there is a phase transition at a temperature \( T_c \) we expect that for \( T < T_c \), \( Q(e) \) will show a similar behaviour around \( e = 0 \), i.e. it will become a steeper function of \( e \) as the volume increases and develops a discontinuity if the transition in \( e \) is first order. \( Q(e) \) provides additional information which may be independent from that supplied by \( P(q) \) [10]. Remark that for \( \varepsilon = 0 \),

\[
\frac{d}{de} Q(e) = \chi_{SG} .
\]

(7)

The thermalization schedule for the set B of experiments was similar to the previous one. Simulations were performed for \( V = 4^3, 6^3, 8^3 \) and \( 10^3 \). The \( e \) term is chosen small compared with the other terms in the Hamiltonian, so that the landscape of energy is not altered. For
this purpose we chose \( \epsilon \) such that \( \epsilon Q(\epsilon) \approx \epsilon h m(h) \approx h^2 \). The values of \( \epsilon \) used in these simulations ranged from \( \epsilon = -0.0025 \) to \( \epsilon = 0.01 \). In this B set of runs for each \( \epsilon \) we had a single pair of copies for all the \( N_J = 128 \) different Hamiltonians we simulated.

It is not easy to ensure thermal equilibrium for spin-glasses. It is well known that very long relaxation times characterize these systems, and indeed no thermalization check is safe from criticism. If there exist several valleys one would like, for non self-averaging quantities, to disentangle thermalization within a valley from valley to valley transitions. To check thermalization we did the following. First we checked that the self-averaging quantities (namely the energy \( E \) and the magnetization \( m \)) did not show any drift during the measurements. This is illustrated in figures 1 and 2. Secondly in the case of the B runs (we recall that the thermalization schedule was the same for the set A and the set B run), we picked, at random, a few pairs of copies and looked at them separately. Figure 3 shows the recording of the overlap of one single pair versus simulation time and figure 4 and figure 5 show respectively its probability distribution during the first and the last quarter of the measuring time. What is characteristic in figure 3 is that the systems move by sudden jumps (it is tempting to interpret those as valley to valley transitions) and the overlap comes back to the original value at much later times. This strongly suggests, in our opinion, that the overlaps we measure correspond to equilibrium. We consider this as an evidence that the simulation times are of the order of the typical times to jump from one valley to another. It is interesting also to notice in figures 4 and 5 that the probability distribution of the overlap is very broad (we would like to say that several « states » are visited), and that this distribution is essentially the same for the first and the last quarter of the measuring time. This is another strong argument for equilibrium. For small sizes we see occasionally that \( q \to -q \), i.e. the system completely reverses itself, before coming back to the original position. For several \( 4^3 \) systems there are only two allowed values of the overlap \( q \) and \(-q\), which means that there is only one state, while for larger systems we find several different values of \( q \). This is in agreement with

![Fig. 1. — Internal energy, averaged over the different systems, as a function of Monte-Carlo time, at \( \beta = 1 \). The time scale is in arbitrary units.](image-url)
Fig. 2. — Magnetization, averaged over the different systems, as a function of Monte-Carlo time, at $\beta = 1$. The time scale is in arbitrary units.

Fig. 3. — Spin-spin overlap of one particular copy, as a function of Monte-Carlo time. The time scale is in arbitrary units.
previous simulations [5] which also show an increase of the number of states with volume. Note that the relative overlaps of these states are significantly different.

Finally we measured the time average of the local magnetizations of individual copies
\[ \mu_i^\alpha = \frac{1}{t} \sum_{\tau=1}^{t} \sigma_i^\alpha(\tau) \]
where \( \tau \) is the Monte-Carlo « time » and we required that

\[ \frac{1}{N_a} \sum_a \frac{1}{N} \sum_{i=1}^{N} \mu_i^\alpha^2 = \int dq \, qP(q) \]  

where \( N_a \) is the number of copies; i.e. we measure the average overlap in two completely independent ways. The first by time averaging a single copy and the second by using the overlap of different copies and we require them to coincide. If the Monte-Carlo time is too
short, the first determination is too large because a copy does not have time to thermalize and every spin remains strongly correlated with its initial position, while the other is too small, as the different copies start from different random configurations and would be almost orthogonal to each other. Equation (8) is a highly non trivial numerical constraint. Indeed, by looking to \( P(q) \) (see Figs. 8), one can estimate \( q_{EA} \), the maximum value of \( q \) for which \( P(q) \) is non zero and which corresponds to thermalization within a single valley. On the other hand \( \int dq \ q P(q) \sim 0.43 \), very different from \( q_{EA} \). As equation (8) is well verified by all our data, we conclude that what we are measuring are the equilibrium properties of our systems. This thermalization test is very similar to that of Bhatt and Young [4].

**Results.**

We start by presenting the results of the set A of runs, i.e. the case where there is no coupling between copies. Before discussing in detail the low temperature measurements, it is instructive to show the exchange energy (i.e. \( \langle J_{ij} \sigma_i \sigma_j \rangle \)) and the magnetization as a function of temperature. This is done in figures 6 and 7 respectively. We see that starting at a certain temperature which is quite high, the magnetization stops growing with \( \beta \) while the exchange energy continues to increase. This behaviour of the magnetization (which is reminiscent of mean-field theory), has already been observed experimentally [11].

![Fig. 6.](image1.png) ![Fig. 7.](image2.png)

Fig. 6. — Average magnetization as a function of the inverse temperature \( \beta \), for \( L = 14 \).

Fig. 7. — Average exchange energy as a function of the inverse temperature \( \beta \), for \( L = 14 \).

As the \( J = \pm 1 \) Hamiltonian we are simulating is only a theoretical abstraction of the more realistic Hamiltonians which describe the dynamics of real spin-glasses, we conclude that this behaviour of the magnetization is universal. It is not obvious to us how this can be accommodated within the framework of the droplet model.
Figures 8a and 8b show the (averaged over the J's) $P(q)$ at $\beta = 1.2$ and $\beta = 0.65$ respectively, for $L = 6, 10$ and 14. For $\beta = 0.65$ the behaviour of $P(q)$ depends strongly on the size of the system. For $L = 6$ $P(q)$ is non trivial, while it is like a $\delta$-function for $L = 14$. This indicates that at this temperature the correlation length is in between those two
sizes, in agreement with previous simulations [3]. For $\beta = 1.2$ the $P(q)$'s for the three sizes are non trivial and qualitatively similar to each other. Figure 9 shows the average link-link overlap $P_e(q_e)$ for $L = 10$ and for $\beta = 1$. We see that not only the configuration overlap but also the link-link overlap has a non trivial distribution. As we will see later, the two overlaps are in fact strongly correlated.

Another important observation is the absence of self-averaging of $P(q)$ (the same is true for $P_e(q_e)$, see later), as in mean-field theory [12, 13]. This can be seen by looking at different $P_J(q)$'s (three of them are shown in figure 10) or can be measured more quantitatively by

$$S = \int dq \left\{ \frac{1}{N_J} \sum \left( P_J(q) - P(q) \right)^2 \right\}^{1/2}.$$  \hfill (9)

At $\beta = 1$ we found that $S = 0.81, 0.82, 0.86$ for $L = 6, 10$ and 14 respectively: increasing the volume does not decrease the absence of self-averaging in $P(q)$.

One of the most striking results we observed was the apparent correlation between spin-spin and link-link overlaps. In order to clarify this important point, we did detailed measurements of the conditional probability $P(q_e; q)$, i.e. the probability for the link-link overlap to take the value $q_e$ when the spin-spin overlap equals $q$. We found that this probability is very peaked and self-averaging. To a very good approximation it is a delta function

$$P(q_e; q) = \delta(q_e - a - bq^2 - cq^4)$$  \hfill (10)

where $a$, $b$ and $c$ are constants depending on the temperature. The values of these constants are $a = 0.317 \pm 0.003$, $b = 0.27 \pm 0.01$ and $c = 0.41 \pm 0.02$ for $\beta = 0.65$ and $a = 0.44 \pm 0.01$, $b = 0.23 \pm 0.02$ and $c = 0.26 \pm 0.03$ for $\beta = 1$. To give an idea of the dispersion of our
data, we show \( P(q_e; q) \) averaged over the different coupling realizations in figure 11. As we will see later, in mean-field theory \( q_e \) is a quadratic function of \( q \).

When measuring \( P(q) \) we can simultaneously extract the spin-glass susceptibility

\[ \chi_{SG} = V \langle \langle q^2 \rangle - \langle q \rangle^2 \rangle_f. \]  

The results are given in figure 12 where we give the log-log plot of \( \chi_{SG} \) as a function of the linear size \( L \) of the systems. We plot the results for three values of the inverse temperature, \( \beta = 0.65 \) (the lower points) \( \beta = 1 \) and \( \beta = 1.2 \) (the higher points). For \( \beta = 1 \) and \( \beta = 1.2 \) the points seem to be aligned on a straight line, i.e. our results are compatible with the assumption of scaling for \( \chi_{SG} \), while this seems not to be the case for \( \beta = 0.65 \). The errors shown in the figure represent only the \( J_1 \) to \( J_2 \) fluctuations. Assuming naive scaling at \( \beta = 1.0 \), we get \( \chi_{SG} \sim L^\omega \) with \( \omega = 1.55 \pm 0.25 \) while at \( \beta = 1.2 \) we get \( \omega = 1.8 \pm 0.25 \).

We measured also the probability distribution \( P_l(e) \) of the average energy for a link. More precisely for every realization of the Hamiltonian and for every link \( \langle ij \rangle \) of the lattice we measured the average of the exchange energy

\[ e_{ij} = \frac{1}{N_c} \sum_a J_{ij} \langle \sigma_i \sigma_j \rangle_a \]  

where \( \langle \rangle \) is the time average, the sum is over the different copies of the same Hamiltonian and \( N_c \) is the number of copies. \( P_l(e) \) is the probability distribution of \( e_{ij} \) over the lattice links. We found that \( P_l(e) \) is self averaging. Our results are shown in figure 13. If the dynamics is driven by the successive flipping of the same domains on the lattice we expect to find a secondary peak in this distribution around \( e = 0 \). Clearly no such peak is found in our simulations. This again is an indication for a more complicated dynamics than the one suggested by the droplet picture.
Fig. 11. — $P(q_e ; q)$ (see text for its definition) averaged over the different realizations of the couplings at $\beta = 1.0$ and $L = 10$. The magnitude of $P(q_e ; q)$ is proportional to the size of the points.

Fig. 12. — Log-log plot of the spin-glass susceptibility versus the size of the system. The upper points correspond to $\beta = 1.2$, the middle points to $\beta = 1$ and the lower points to $\beta = 0.65$. 
Let us now discuss ultrametricity [12]. For every realization of the $J$'s we peaked three copies (in several different ways) and we calculated the corresponding three-configuration overlaps $q_1 \geq q_2 \geq q_3$. When $0.5 \leq q_1 \leq 0.6$, we measured the probability distribution $\mathcal{P}(\delta q)$ of $\delta q = q_2 - q_3$ as a function of the volume. This method of looking for ultrametricity is the same as in Bhatt and Young [14]. The results are shown in figure 14. There is a definite trend for $\mathcal{P}(\delta q)$ to become steeper as the volume increases. This is compatible with the space of states becoming ultrametric in the infinite volume limit, but one should be careful before jumping to conclusions, as we will discuss later.

In the set B of runs we measured the average configuration overlap $Q(\epsilon)$ as a function of the small coupling $\epsilon$ between two copies. The result is shown in figure 15 for the following values of the linear size of the system: $L = 4, 6, 8$ and $10$. $Q(\epsilon)$ becomes a steeper function of $\epsilon$ as the volume increases in agreement with the results on $\chi_{SG}$ of the runs with uncoupled copies.
Fig. 14. — $f(\delta q)$ for $L = 6$ (dashed line), $L = 10$ (dotted line) and $L = 14$ (continuous line) at $\beta = 1.2$.  

Fig. 15. — $\mathcal{Q}(\epsilon)$ as function of $\epsilon$ for $L = 4$, $6$, $8$, and $L = 10$ and $T = 1$. 
Discussion.

In this chapter we would like to discuss the following points.

a) The correspondence between configuration overlaps and link-link overlaps. — One of our most interesting results is the one-to-one correspondence between configuration overlaps \( q \) and link-link overlaps \( q_e \). This has already been observed in connection with the study of the robustness of ultrametricity both numerically [15] and in the framework of the Sherrington-Kirkpatrick (SK) model [15, 16]. In the latter case the correspondence can be made very precise. As is well known, when all the spins are coupled together, only the first two moments of the \( J \) distribution are relevant in the thermodynamic limit. So we can consider only the case of the \( J_{ij} = \pm 1 \) distribution. For two given configurations of the spins \( \sigma_i \) and \( \tau_i \), their link-link overlap is
\[
q_e = \frac{1}{N^2} \sum_{ij} \sigma_i \sigma_j \tau_i \tau_j
\]
where the sum over \( i \) and \( j \) runs over all the sites of the system. The right-hand expression is nothing but the square of the spin-spin overlap. So in the SK model we have \( q_e = q^2 \) for every spin configuration. One can also show on general grounds the following inequality: \( q_e \geq e^2 \), where \( e \) is the average energy of a link. This result is shown in the appendix. It seems to be a contradiction between this inequality and the SK model result \( q_e = q^2 \) for \( q = 0 \). In fact, because of the choice of normalization, \( e = 0 \) in the thermodynamic limit of the SK model and there is no contradiction. For two identical configurations \( q_e = q = 1 \). This relation provides a check to our numerical results.

Is there any relevance of the previous results for a droplet-like picture? When two configurations differ by the reversal of a compact domain of spins (a droplet), \( q = 1 - 2 v / V \) while \( q_e = 1 - 2 s / 3 V \) where \( v \) is the number of spins inside the domain, \( s \) the number of links at the interface between the domain and the rest of the system (the « surface » of the droplet) and \( V \) is the total volume of the system. In order for \( q \) and \( q_e \) to be substantially different from one, both the volume and the surface of the domains must have fractal dimension equal to three. For this reason this result together with the strong correlation between \( q \) and \( q_e \) are difficult to get in the framework of a simple droplet model.

b) Scaling and finite volume effects. — There are clearly several signs of finite volume effects in our simulations. The most obvious is in the volume dependence of \( P(q) \). There is a tail in \( P(q) \) for negative \( q \)’s and this tail strongly decreases with the volume of the system. There is also a volume dependence of \( q_{EA} \), the maximum value of \( q \). One would like to make a decomposition \( P(q, h) = P_{\infty}(q, h) + \Delta P(q, h, L) \) where \( P_{\infty}(q, h) \) is the infinite volume result and a scaling ansatz for the finite volume correction \( \Delta P(q, h, L) \). The positivity of \( P(q) \) for any volume and the lack of data for many different sizes and different values of the magnetic field did not allow us to do so.

The same finite volume effects were present in the B set of numerical experiments. We would like to make a scaling ansatz for the average overlap \( \langle q \rangle \) similar to the one valid in the ferromagnetic case. In that case it is well known that the magnetization as a function of an external magnetic field scales as \( m(h, L) = f(hL^\omega) \), \( \omega = 3 \). A similar ansatz in our case would be \( \langle q \rangle (h, L) = f(\epsilon L^\omega, hL^\delta) \). As we do not have data for different values of \( h \), we have, in a first approximation, ignored the possibility of dependence on \( hL^\delta \). In figure 16 we show the same data as in figure 15 plotted against the scaled variable \( \epsilon L^\omega \). We took \( \omega = 1.55 \) as determined by the volume dependence of the spin-glass susceptibility at \( \epsilon = 0 \). The data are less scattered, however there is still some volume dependence; indeed such an ansatz implies that for \( \epsilon = 0 \), \( \langle q \rangle \) is \( L \) independent. But we do find a volume dependence of \( \langle q \rangle (0) \) which means that for the volumes we study there are still corrections to simple scaling. Although the data are suggesting a discontinuity at \( \epsilon = 0 \) in \( \langle q \rangle \), the
difficulty of writing down a simple scaling law forbids us to reach a definite conclusion on this important point. Of course one should also consider the more radical possibility that spin-glasses have a more complicated behaviour than the systems without disorder we are familiar with (a multifractal behaviour, for example) and that naive finite size scaling is never valid.

c) Critical exponent for the spin-glass susceptibility. — As the discussion in the previous paragraph suggests, the best critical exponent we can measure is a kind of effective exponent. On the other hand the log-log plot of the spin-glass susceptibility versus the size, shown in figure 12, seems to give a straight line thus suggesting a simple scaling behaviour. We would like to be able to estimate the systematic error on $\omega$ due to corrections to naive scaling but lacking data for larger sizes makes it extremely difficult. Just to get an idea of their eventual importance, we made the assumption that the negative $q$ tail of $P(q)$ was due to the non leading finite volume effects only. We then computed $\chi_{SG}$ again by taking the moments of $P(q)$ for positive $q$ only (i.e. we imposed by hand $P(q) = 0$ for $q < 0$). The resulting log-log plot is shown in figure 17. Again the points seem to align on a straight line, but we get a quite different value for the exponent $\omega = 2.23 \pm 0.1$ at $\beta = 1$. This confirms the sensitivity of $\omega$ on the systematic uncertainties. The data for the energy overlap give a quite similar value.

We remind the reader that in mean-field theory $\omega = 3$. As $\chi_{SG}$ is simply related to the second cumulant of $P(q)$, one can view it as a measure of the width of $P(q)$, $\omega = 3$ meaning that the width is volume independent. We find smaller value of $\omega$ (but we saw that the systematic uncertainties are large) which hints to a shrinking of $P(q)$ as the volume increases. It would be very interesting to simulate larger systems to control the finite volume systematic errors. If the result that $\omega > 0$ is confirmed, the function $Q(\varepsilon)$ is singular at $\varepsilon = 0$. If $0 < \omega < 3$ the function $Q(\varepsilon)$ may or may not be continuous at $\varepsilon = 0$. In the latter case the replica symmetry is broken, while in the former one we face a situation similar to that of the Kosterlitz-Thouless phase in the two-dimensional xy-model where the correlation length is infinite at external magnetic field $h = 0$ for small temperature.
d) Ultrametricity. — Ultrametricity is very hard to test numerically. Our results for the volume dependence of \( \mathcal{f}(\delta q) \) seem to be a convincing evidence for ultrametricity, but we would like to mention two reasons for caution. One is the existence of the triangular inequalities. The other is the change of the shape of \( P(q) \) as we increase the volume. Because of the shrinking of the \( q < 0 \) tail of \( P(q) \) as the volume increases, \( \delta q = q_2 - q_3 \) is allowed to take larger values for smaller volumes. This « \( P(q) \) effect », combined with the triangular inequalities, could in principle explain some of the volume dependence of \( \mathcal{f}(\delta q) \).

Conclusions.

We presented the results of extensive simulations of three-dimensional Ising spin-glasses in the presence of an external magnetic field. All our results are compatible with a mean-field like behaviour. Both the configuration overlap \( q \) and the link-link overlap \( q_e \) have non trivial and non self-averaging probability distributions. There is numerical evidence for ultrametricity. Our results are compatible with the existence of a phase transition in the presence of an external magnetic field. We measured the critical exponent of the spin-glass susceptibility and we found that \( \chi_{SG} \sim L^\omega \) and that \( \omega = 1.8 \pm 0.25 \) at \( \beta = 1.2 \) but the systematic uncertainties on this exponent are large. Last but not least, we found that there is a very simple relation...
between \( q_e \) and \( q \), namely \( q_e = a + bq^2 + cq^4 \) and that the coefficients \( a \), \( b \) and \( c \) are self-averaging. There are limitations to the above results. Because of strong finite volume effects, we cannot produce a simple scaling picture for the transition.

The behaviour of the finite volume systems we simulated is in good agreement with the predictions of mean-field theory with broken replica symmetry. As already stated we cannot discriminate between a continuous or a discontinuous transition in \( \varepsilon \), although the properties we observed makes the latter more likely. Our data seem anyhow incompatible with the alternatives to mean-field theory proposed so far. We feel that a reasonable theoretical approach to finite dimensional spin-glass should use as a zeroth approximation the theory with broken replica symmetry, because it captures the behaviour of finite-volume systems. Indeed some very recent theoretical approaches \([17, 18]\) point in this direction.

Acknowledgments.

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Appendix.

In this appendix we prove the inequality \( q_e \geq \varepsilon^2 \) where \( q_e \) is the link-link overlap and \( \varepsilon \) is the average energy per link. We have

\[
q_e = \frac{1}{N_\ell} \sum_{ij} J_{ij}^2 \langle \sigma_i \sigma_j \rangle \langle \tau_i \tau_j \rangle
\]  

(13)

\[
\varepsilon^2 = \frac{1}{N_\ell} \sum_{ij} \sum_{kt} J_{ij} \langle \sigma_i \sigma_j \rangle J_{kt} \langle \tau_k \tau_t \rangle
\]  

(14)

where \( \sigma \) and \( \tau \) are the spins of the two configurations. The sums over \( \langle ij \rangle \) and \( \langle kt \rangle \) run over all the links of the lattice and \( N_\ell \) is the number of links. So

\[
q_e - \varepsilon^2 = \frac{1}{N_\ell} \sum_{ij} \sum_{kt} (\delta_{\langle ij \rangle \langle kt \rangle} - M_{\langle ij \rangle \langle kt \rangle}) \langle \sigma_i \sigma_j \rangle \langle \tau_k \tau_t \rangle
\]  

(15)

where

\[
M_{\langle ij \rangle \langle kt \rangle} = \frac{1}{N_\ell} J_{ij} J_{kt}
\]  

(16)

Remark that \( (M^2)_{\langle ij \rangle \langle kt \rangle} = M_{\langle ij \rangle \langle kt \rangle} \), i.e. \( M \) is a projector. Then \( II = 1 - M \) is the projector to the orthogonal space. It is easy then to show that the eigenvalues of \( II \) are all equal to one except for one of them which is equal to zero. In other words the matrix \( II \) is positive semi-definite. Averaging over long running times and over different copies of the system, ensures that

\[
\langle \sigma_i \sigma_j \rangle = \langle \tau_i \tau_j \rangle = \sum_a W_a \langle \sigma_i \sigma_j \rangle_a
\]  

(17)

where the sum is over all the pure states and \( W_a \) is their relative weight. Then the inequality \( q_e \geq \varepsilon^2 \) follows immediately.
References