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Replica symmetry breaking in four-dimensional spin glasses

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Abstract. In this paper we present a new numerical method to test mean-field ideas in the Ising spin glass at finite dimensions. Very large sizes can be studied and numerical results are presented in the case of the four-dimensional Ising spin glass. New exponents are introduced within the spin-glass phase and we find evidence of a phase with replica broken features.

1. Introduction

Replica symmetry breaking [1–3] apparently correctly describes the behaviour of spin glasses in the infinite range limit [4]. It would also be very interesting to understand whether it is also a correct description of short-ranged spin glasses in finite dimensions.

It has been shown that in sufficiently high dimensions the pertubative corrections to the mean-field approach based on replica symmetry breaking are finite, so that it is reasonable to assume that the replica approach is correct above a lower critical dimension, which has not yet been identified [5]. Of course it is very difficult to dismiss theoretically the possibility that there are non-perturbative effects which destroy replica symmetry at finite dimensions.

In order to clear the theoretical situation, we have studied numerically short-ranged spin glasses in four dimensions in order to see whether their behaviour is the one suggested by replica symmetry breaking. We have decided to study this question in four dimensions for several reasons:

(i) We hope that dimension four is sufficiently above the lower critical dimension so that corrections to the mean-field approximation are not too large.

(ii) In dimensions greater that four it is time consuming (and memory demanding) to study lattices of large linear size.

(iii) It is known that in dimension four the dynamics is sufficiently fast so that the phase transition and the behaviour can be studied within a reasonable amount of time on commercial computers.

There are already numerical studies in four dimensions which confirm some of the predictions of the mean-field approach, i.e. the existence in the non-zero magnetic field of the de Almeida–Thouless line [6, 7], where the correlation length (and consequently the spin-glass susceptibility) diverges, the non-vanishing of the function $P(q)$ at $q = 0$ [8] and the scaling of the approach to equilibrium in terms of the variable $T \ln(t)$ [9]. Unfortunately

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these studies (apart from the last one) have been done on relatively small lattices (up to a linear size $L = 6$–7) and they are quite difficult to extend to high values of L.

In this paper we follow a different strategy which allows us to verify some of the crucial predictions of replica theory for much larger sizes (i.e. up to $L = 18$). Results for small sizes regarding the investigation of finite-size scaling laws within the spin-glass phase, ultrametricity and questions concerning the dynamics are presented in a forthcoming paper [10].

This paper is divided as follows. In section 2 we introduce some general ideas regarding the nature of the spin-glass phase according to mean-field theory and we recall the energy overlap which has proved to be very useful. Section 3 introduces the definitions of the critical exponents and sections 4 and 5 present numerical results for the critical point and below it respectively. Section 6 presents some conclusions.

2. General theoretical predictions

In this section we will present some of the results of broken replica theory for spin glasses (in the mean-field approximation), which can probably be extended *mutatis mutandis* to other systems.

In the replica approach it is crucial to consider the behaviour of a system composed of two identical replicas. More precisely we have two spins systems (the spin variables being σ_i and τ_i) with total Hamiltonian

$$H^{(2)} = H_J[\sigma] + H_J[\tau] \tag{1}$$

where H_J is the usual Hamiltonian which depends on the random variables J.

Broken replica theory predicts the existence of many possible equilibrium states for each of the two replicas [11]. These states have similar macroscopic properties (like internal energy, magnetization). In order to point out the existence of these equilibrium states it is convenient to define the overlap q between the two replicas as

$$q = \frac{1}{N}\sum_i \sigma_i \tau_i . \tag{2}$$

For each finite system of size L we can define a function $P_J(q)$, which depends on the variables J's. We can also define the function

$$P(q) \equiv \overline{P_J(q)} \tag{3}$$

where the bar denotes (as usual) the average over the J's.

In the limit when the volume ($N \equiv L^D$) goes to infinity the function $P(q)$ has its support in the interval q_m–q_M, with two delta functions at the end of the interval. This is the generic situation in non-zero magnetic field [12]. In the limit where the magnetic field goes to zero, q_m goes to 0 and the corresponding delta function disappears. When the magnetic field is strictly zero, the function $P(q)$ is symmetric (under the exchange of q with $-q$) and often one shows only $P(q)$ for positive q.

It is interesting to note that the function $P(q)$ strongly fluctuates from system to system inside the interval q_m–q_M, indeed one finds that

$$\overline{P_J(q_1)P_J(q_2)} = \tfrac{1}{2}P(q_1)\delta(q_1 - q_2) + \tfrac{1}{2}P_J(q_1)P_J(q_2). \tag{4}$$

These predictions are quite clear and, in principle, could be easily tested. Unfortunately, in doing Monte Carlo simulations we can measure the function $P_J(q)$ only if we wait a time which is sufficiently large to allow for the system to have explored all possible states and have done a non-negligible number of transitions among the lower-lying states. The equilibrium states are separated by barriers, whose height should go to infinity as a power of N, and for large volumes such a time becomes so large that it is impossible to do such a long numerical simulation. We would also reach similar conclusions if we consider real experiments (supposing that the measurement of individual spins would be possible). In other words, the function $P_J(q)$ cannot be measured for large systems.

The difficulty in obtaining the correct $P_J(q)$ from experiments (real or numerical) is connected to the fact that $\ln(P_J(q))$ is not an intensive quantity [13]. Fortunately, the replica symmetry breaking approach also gives predictions for other quantities, which are intensive and can be measured much more easily.

Let us consider a system with two replicas which are now coupled one to the other:

$$H^{(2)} = H_J[\sigma] + H_J[\tau] - \epsilon N q = H_J[\sigma] + H_J[\tau] - \epsilon \sum_i \sigma_i \tau_i. \tag{5}$$

It is interesting to study the function $q(\epsilon)$, i.e. the expectation value of the overlap as a function of ϵ. An explicit computation shows that [14]

$$\lim_{\epsilon\to 0^+} = q_M \qquad \lim_{\epsilon\to 0^-} = q_m \tag{6}$$

A first-order phase transition is present at $\epsilon = 0$. Such a phase transition should be detectable in times which are not exponentially large.

The quantity q_M has the physical meaning of the overlap inside the same state and is also called the Edwards–Anderson order parameter (q_{EA}). In principle we could measure q_M by considering the time dependence of the overlap of two replicas (using any local form of dynamics) in the case in which we have imposed the same initial (equilibrium) condition at time zero. In the case of very large volume the two replicas would remain in the same state (for a long but not exponentially long time) and their mutual overlap would be q_M. Indeed we expect that the jump from one to another equilibrium state takes a time which is exponentially large compared with the size of the system [15].

By the same token, if for the two replicas we set uncorrelated initial conditions at time 0, their overlap should be in the same time region q_m. Indeed the two replicas will evolve toward two different equilibrium states and the two generic states will have overlap q_m. A similar effect is present if we consider two replicas at slightly different magnetic fields. In this case the overlap between the two replicas will also be q_m.

It is quite interesting that the mean-field approximation predicts quite peculiar behaviour for the function $q(\epsilon)$ [16]. Indeed one finds that, for small ϵ,

$$\begin{aligned} q(\epsilon) &= q_M + C^+\epsilon^{1/2} \qquad && \epsilon > 0 \\ q(\epsilon) &= q_m - C^+(-\epsilon)^{1/2} \qquad && \epsilon < 0. \end{aligned} \tag{7}$$

The susceptibility $\chi_q \equiv \partial q/\partial\epsilon$ diverges in the limit $\epsilon \to 0$. In this limit it is interesting to study the connected correlation function

$$G_q(i) = \langle q_i q_0 \rangle_c \tag{8}$$

where

$$q_i \equiv \sigma_i \tau_i. \tag{9}$$

At large distances we naively expect an exponential decay

$$G_q(i) \simeq \exp(-i/\xi_q) \tag{10}$$

where ξ_q is the relevant correlation length.

As far as

$$\chi_q = \beta \sum_i G_q(i) \tag{11}$$

the correlation length ξ_q must diverge at the transition point.

From the thermodynamic point of view such behaviour is characteristic of a spontaneous breaking of a continuous symmetry: the point $\epsilon = 0$ is a first-order transition point, because of the discontinuity of q and it is also a second-order transition point at which the correlation length diverges. This property is probably at the root of many of the peculiar properties of spin glasses and it is the physical manifestation of the breaking of the replica symmetry in a hierarchical way [17]. This result of the infinite-range model is in agreement with direct analytic computations done in the spin-glass phase. Indeed it has been found that the correlation functions decay as a power law of the distance in the spin-glass phase [18]. Different exponents are expected to be present according to the correlation function one is considering.

As usual it is useful to consider the free energy per site as function of q, which is equal to

$$F(q) = -\frac{1}{N\beta} \lim_{N\to\infty} \sum_{\{\sigma,\tau\}} \delta\left(\frac{1}{N}\sum_i \sigma_i\tau_i - q\right) \exp(-\beta(H_J[\sigma] + H_J[\tau])). \tag{12}$$

In other words we constrain the two non-interacting replica systems to have a fixed overlap q. Standard thermodynamical arguments imply that

$$\partial F/\partial q|_{q=q(\epsilon)} = \epsilon. \tag{13}$$

The function $F(q)$ does not depend on q in the whole interval q_m–q_M, while, for q slightly outside this interval,

$$\begin{aligned} \delta F(q) &= A^+(q - q_M)^3 \qquad & q > q_M \\ \delta F(q) &= -A^-(q_m - q)^3 \qquad & q < q_m \end{aligned} \tag{14}$$

where δF is the variation in the free energy for configurations $\{\sigma, \tau\}$ with overlap outside the interval $[q_M$–$q_m]$ with respect to the free energy of those configurations in which q lies inside the same interval.

The A's are related to the C's according to

$$3A^+(C^+)^2 = 3A^-(C^-)^2 = 1. \tag{15}$$

This behaviour of the free energy is related to the behaviour of the function $P(q)$ in the tail, i.e. outside its support in the infinite volume limit (the interval q_m–q_M). Indeed in the region where q is slightly outside this interval we expect that the function $P(q)$ will behave as [19]

$$
\begin{aligned}
P(q) &\propto \exp(-NA^{+}(q-q_M)^3) \qquad q > q_M \\
P(q) &\propto \exp(-NA^{-}(q_m-q)^3) \qquad q < q_m.
\end{aligned} \tag{16}
$$

Such a result is correct for fixed q and N going to infinity, however we also expect that it will remain essentially correct in the region where $N(q-q_M)^3$ is large.

More precisely, we can assume that the function $P(q)$ is a homogeneous function of N and $q-q_M$. If the function $P(q)$ behaves as a delta function at $q=q_M$ in the infinite volume limit, simple scaling arguments imply the following behaviour in the whole region of small $q-q_M$

$$P(q) = N^{1/3} f(N(q-q_M)^3) \tag{17}$$

where the function $f(z)$ should behave as $\exp(-A^{+}z)$ for large values of z. Similar considerations could be done for $q < q_m$. The exponent $\frac{1}{3}$ is related to the existence of a delta-type singularity in $P(q)$ and it should be modified if such a singularity is absent. The same arguments imply that there are finite-size corrections to equation (17), which are present as soon as the quantity $N\epsilon^{3/2}$ is not very large.

Direct study of the function $P(q)$, which can be done on small samples, gives similar information and complements the information obtained by introducing a coupling among replicas in the Hamiltonian [10]. It should be stressed that, if we work at fixed ϵ and send N to infinity, we introduce a perturbation proportional to N, so that all equilibrium states will be relevant, together with those which give a contribution to $P(q)$ which vanishes as $\exp(-aN^{\alpha})$, with $\alpha < 1$ (this is because we are adding a perturbation which is of order N).

The existence of different values for q_m and q_M is a clear signal for the existence of at least two different equilibrium states. We can ask how much these states differ from each other. Let us consider the case with zero magnetic field. It is possible that the τ variables have opposite magnetization to the σ variables and consequently the overlap is equal to $-q_M$. We can reject this trivial possibility by considering only the case where q is positive.

However in spin glasses (and also in ferromagnetic systems) we can construct domain states, in which the τ variables have opposite magnetization to the σ variables in a domain $\mathcal{D}$ and the two magnetizations are equal in the complement of $\mathcal{D}$. If $\mathcal{D}$ is compact, these configurations have the same free energy density as those in which the τ variables have the same magnetization as the σ variables everywhere. A very relevant question is whether all the different equilibrium states of the system can be obtained from each other in this way or whether there are pairs of states which cannot be so trivially related to each other.

This question may be addressed by considering the overlap in energy introduced in [20] to study the three-dimensional Ising spin glass in a magnetic field. In that work it was shown that the spin-glass phase can be understood within the framework of the droplet theory only if droplets had fractal dimesion equal to three (the dimension of the lattice). Two domain states have the same energy density nearly everywhere, the energy density differs only on the boundary of the domain; if we consider only their energy density, not the magnetization density, these two states will differ by a negligible amount in the infinite-volume limit. Indeed the difference in energy density will be concentrated only on the boundary of $\mathcal{D}$ and it becomes irrelevant in the infinite volume limit.

In order to be more quantitative it is convenient to introduce the energy density for the σ variables (which we suppose to be localized on the bonds among spins), defined as

$$E^{\sigma}_{i,k} = J_{i,k}\sigma_i\sigma_k. \tag{18}$$

The energy overlap is thus given by

$$q^e \equiv \frac{1}{cN}\sum_{i,k} E^\sigma_{i,k}E^\tau_{i,k} = \frac{1}{cN}\sum_{i,k} J^2_{i,k}q_i q_k$$

where the constant $c = (1/N)\sum_{i,k} J^2_{i,k}$ has been inserted in order to impose the useful normalization condition $q^e = 1$ for $\tau = \sigma$.

The analysis we have done for q can be repeated for q^e. If the coordination number is infinite, as in the SK model, one finds that

$$q^e = q^2 \tag{19}$$

so that no extra information can be extracted from q^e. This is quite reasonable, because domain states are forbidden in the infinite-range model. Domain states may exist only because the surface grows slower than the volume so that surface effects may be neglected with respect to bulk effects. However, the surface-to-volume ratio in dimensions D scales as $N^{-1/D}$ so that this ratio is volume independent when $D \to \infty$. It should not be a surprise that domain states are suppressed in the infinite-range limit which is quite similar to the infinite-dimension limit.

We can thus consider the following coupled replica system with Hamiltonian

$$H^{(2)} = H_J[\sigma] + H_J[\tau] - \epsilon_e N q^e = H_J[\sigma] + H_J[\tau] - \frac{\epsilon_e}{c}\sum_{i,k} J^2_{i,k}q_i q_k. \tag{20}$$

In a similar way we find in the mean-field approximation in non-zero magnetic field that

$$\begin{aligned} q^e(\epsilon) &= q^e_M + E^+\epsilon_e^{1/2} \qquad && \epsilon_e > 0 \\ q^e(\epsilon) &= q^e_m - E^+(-\epsilon_e)^{1/2} \qquad && \epsilon_e < 0. \end{aligned} \tag{21}$$

In the SK *model the quantities appearing in the previous equation can be simple related to* those of equation (7) using the relation (19). At zero magnetic field q^e_m goes to zero, but this is an artefact due the infinite coordination number.

We can consider equations (7) and (21) as the key predictions of a naive replica approach in which all effects due to finite dimensions and the short-range nature of the forces are neglected. (It is quite possible that the exponent $\frac{1}{2}$ is modified at sufficient low dimensions.) Summarizing we have seen that

(i) $\delta q = q_M - q_m \neq 0$ implies the existence of different pure states;

(ii) $\delta q^e = q^e_M - q^e_m \neq 0$ implies that the different pure states are not domain states, i.e. they are not locally the reverse of the others; and

(iii) the dependence of the overlaps as a non-integer power of the perturbation (ϵ) implies the divergence of the correlation length in the absence of an external perturbation.

We will see later how these three properties can be verified to hold in the four-dimensional short-range spin-glass model.

3. Critical exponents

If we study spin glass in the high-temperature phase the renormalization group approach does not reveal any strange behaviour, at least at zero magnetic field. Critical exponents are those predicted by mean-field theory in dimensions greater than six.

In less than six dimensions non-trivial exponents appear. Only two independent exponents (η and ν) control the critical behaviour of most quantities. One finds that

$$\xi_q \propto \tau^{-\nu} \qquad \chi_q \propto \tau^{-\gamma} \tag{22}$$

where $\tau = |T - T_c/T_c|$, T_c being the critical temperature and

$$\gamma = (2-\eta)\nu. \tag{23}$$

Theoretically there are no signs of violation in less than six dimensions of the hyperscaling relations

$$\alpha = 2 - D\nu \tag{24}$$

which relates the exponent for the specific heat ($C \propto \tau^{-\alpha}$), to the exponent ν. The relation is satisfied in dimensions not greater than six (the mean-field value for α is -1).

In the field-theoretical approach only two operators have dimensions less than D: the overlap $Q_{a,b}(x)$ and the energy density, which is proportional to $\sum_{a,b} Q^2_{a,b}(x)$. The energy overlap density is given by $Q^2_{a,b}(x)$, so in the continuum limit it scales in the same way as the energy. The crucial quantities are the dimensions of these operators, which (in inverse-of-length units) are given by

$$\begin{aligned} d_q &= \tfrac{1}{2}(D-2+\eta) \\ d_e &= D - 1/\nu = (1-\alpha)/\nu. \end{aligned} \tag{25}$$

In high dimensions, where mean-field exponents are exact, $d_e = 2d_q$. This relation does not hold in less than six dimensions, where $d_e > 2d_q$.

If we stay at the critical point and we add a term proportional to ϵq, we find that

$$q(\epsilon) \propto \epsilon^{d_q/(D-d_q)} \equiv \epsilon^{\omega_{qq}}. \tag{26}$$

In a similar way if we add a term proportional to $\epsilon_e q^e$ in the Hamiltonian we would find an irregular term given by

$$q^e(\epsilon_e) - q^e(0) \propto \epsilon_e^{d_e/(D-d_e)} \equiv \epsilon_e^{\omega_{ee}}. \tag{27}$$

However there is also a regular term $q^e(\epsilon_e) - q^e(0) \propto \epsilon_e$ which dominates for small values of ϵ_e so that the dependence of q_e on is smooth (we recall that $d_e/(D-d_e) = -\alpha + 1$, which is two in six dimensions and it is likely higher than two in dimensions less than six. In this case we should get that $\omega_{ee} = 1$.

On the other side we should have (adding a term $\epsilon_e q^e$ to the Hamiltonian like in equation (20) and computing the overlap $\sigma\sigma$ or $\tau\tau$ which is $q(\epsilon_e)$)

$$q(\epsilon_e) \propto \epsilon_e^{d_q/(D-d_e)} \equiv \epsilon^{\omega_{qe}} \tag{28}$$

where $\omega_{qe} = \beta$, which in this context it is the exponent for the order parameter ($\Delta q \propto \tau^\beta$). In this first case (coupling a term ϵq to the Hamiltonian as in equation (5)) the scaling laws imply that

$$q^e(\epsilon) - q^e(0) \propto \epsilon^{[d_q/(D-d_q)](d_e/d_q)} \equiv \epsilon^{\omega_{eq}}. \tag{29}$$

Here one finds the following relation among the overlaps:

$$q^e(\epsilon) - q^e(0) \propto q(\epsilon)^{(d_e/d_q)}. \tag{30}$$

Summarizing there are four exponents which can be measured (ω_{qq}, ω_{qe}, ω_{eq}, ω_{ee}), the last being identically one ($\omega_{ee} = 1$). The three non-trivial exponents depend on only two standard critical exponents, so that we can extract them with some confidence.

Below the critical temperature it is possible that the relations (7) and (21) are not modified.

A similar phenomenon happens for Heisenberg ferromagnets, where the longitudinal susceptibility (χ_L) diverges as h^{-1}, h being the magnetic field. It is also possible that the exponent $\frac{1}{2}$ is modified at finite dimensions.

In this case one should introduce new critical exponents (e.g. ζ_{qq} and ζ_{ee}) such that

$$\begin{aligned} q(\epsilon) &= q + E^+ \epsilon^{\zeta_{qq}} \qquad && \epsilon > 0 \\ q^e(\epsilon_e) &= q^e - E^+ (\epsilon_e)^{\zeta_{ee}} \qquad && \epsilon_e > 0. \end{aligned} \tag{31}$$

The value of the exponents ζ's should be equal to $\frac{1}{2}$ in the mean-field approximation but is quite possible that they become different from $\frac{1}{2}$ in dimensions less than six. A detailed analytic computation is needed to clarify this important issue.

In any case the scaling laws imply that the discontinuity in the overlap in the low-temperature region scales as

$$\Delta q(\tau) \propto \tau^{d_q \nu} \qquad \Delta q^e(\tau) \propto \tau^{d_e \nu}. \tag{32}$$

In this article we will mainly concentrate our efforts in proving the non-vanishing of the discontinuities and of the divergence of the spin-glass susceptibility. We will not pay too much attention to the precise determination of the exponents.

4. Simulations at the critical temperature

Here we will study the four-dimensional nearest-neighbour interaction model with discrete couplings (± 1). The single replica Hamiltonian is given by

$$H = \sum_{i,k} J_{i,k} \sigma_i \sigma_k \tag{33}$$

where the sum runs over all the pairs of nearest-neighbour points of a four-dimensional cubic lattice (the coordination number is 8). The couplings Js are randomly chosen with equal probability ± 1. The lattices we study will contain $N = L^4$ spins, with periodic boundary conditions.

For this model the energy overlap q^e simply becomes

$$q^e = \frac{1}{8N} \sum_{i,k} q_i q_k = \frac{1}{8N} \sum_{i,k} \langle \sigma_i \sigma_k \rangle \langle \tau_i \tau_k \rangle \tag{34}$$

where the sum runs over nearest-neighbour points.

A finite-size analysis of the susceptibility χ_q on lattices of size from 3 to 7 [7] and high-temperature expansions [21] shows that there is a transition at $T_c = 2.02 \pm 0.04$, which is characterized by a divergence of the spin-glass susceptibility. The reported values of the exponents are $\eta = -0.25 \pm 0.1$ and $\nu = 0.70 \pm 0.2$ [7], in good agreement with the results obtained for the four-dimensional model on the same lattice with couplings which have a Gaussian distribution [22].

We tentatively assume that the critical tenperature has been correctly determined and we study the dependence of q and q^e on ϵ and ϵ_e at $T = T_c$.

To this end we consider a two replica system and we add a coupling between the replicas of the form ϵq, as discussed in section 2. We slowly cool the system from high temperature to the critical temperature in the presence of a field ϵ. Subsequent measurements are done at decreasing values of ϵ (we have chosen to decrease ϵ by a factor 2 each time). At each value of ϵ the first 20% of the simulation is disregarded, because we fear the system may not have reached equilibrium. The dependence of the overlaps on the Monte Carlo time is monitored in order to find out the existence of unwanted systematic drifts in the remaining 80% of the simulation, which is used for the measurements.

The simulations we present now are done on a 18^4 system. The number of Monte Carlo steps at each value of ϵ is $10^3\epsilon^{-1/2}$. The number of steps increases when ϵ goes to zero in order to fight against critical slowing down, the exponent $\frac{1}{2}$ being an arbitrary choice. The quantities that we are considering should not fluctuate in the infinite-volume limit, so that the sample-to-sample fluctuations should be relatively small and this is confirmed by doing simulations on other systems.

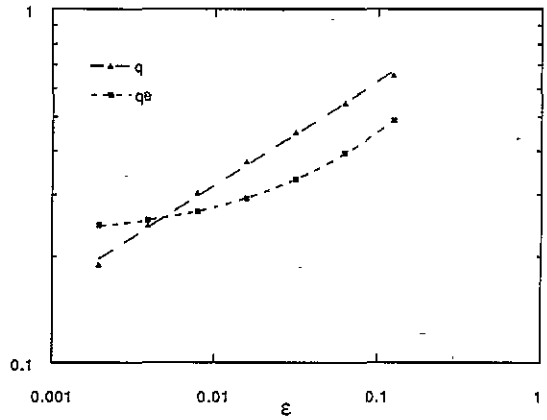

Figure 1. The value of the overlaps q and q_e as function of ϵ at the critical point ($T_c = 2.02$) on a lattice of size $L = 18$. The fits are done according to equations (26) and (29) and give $\omega_{qq} = 0.29$, $\omega_{eq} = 0.67$. The symbols are: triangles (q), squares (q^e).

In figure 1 we see the overlaps as function of ϵ for ϵ in the range 2^{-3}–2^{-10}. We display the fits done according to the equations in the previous section. The corresponding values of the ω's are

$$\omega_{qq} = 0.29 \qquad \omega_{eq} = 0.67. \tag{35}$$

In figure 2 we show the same results in which we plot q^e against q. The results in both cases are quite similar. The fits gives for the ratio of the dimensions d_e/d_q the value

$$\frac{d_e}{d_q} = \frac{\omega_{eq}}{\omega_{qq}} = 2.67. \tag{36}$$

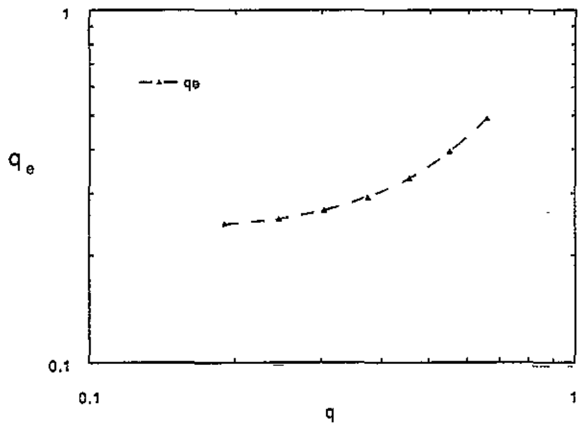

Figure 2. The overlap q_e against q, the fit done according to equation (30) gives $d_E/d_q = 2.63$.

It is difficult to attach a meanful error to those numbers. The statistical errors can be obviously computed, but its value would be unreasonable small. The real uncertitude comes from the fact that the scaling law are valid in the limit $\epsilon \to 0$ and for finite ϵ there are corrections to the scaling law which we do not control. Some estimates on the error may be obtained by changing the procedure we use to fit the data.

To this end we have found it useful to slightly modify the definition of overlap. In order to have simple fits which work better and to decrease the saturation effects for q close to 1, we find it slightly more convenient to consider plotting the quantity

$$h_q \equiv \tanh^{-1}(q) \tag{37}$$

instead of q. The physical meaning of h_q is clear: if we consider two replicas with a single spin on each replica, the expectation value of the overlap will be equal to q if the Hamiltonian (multiplied by β) is equal to $h_q\sigma\tau$.

For the same reason we introduce the quantity

$$h_e \equiv \tanh^{-1}(q^e). \tag{38}$$

In figure 3(a) we show the same data as in figure 2 but using these new variables. There is a small impovement; the fits agree slightly better with the data, although this is hard to see with the naked eye. From the fits one finds the ω's are

$$\omega_{qq} = 0.33 \qquad \omega_{eq} = 0.68 \tag{39}$$

Fom this data one could estimate $\omega_{qq} = 0.31 \pm 0.02$, however a similar estimate (e.g. 0.67 ± 0.01) for ω_{eq} is not safe. Indeed the internal energy should scale exactly as q_e at the critical point. If we plot the internal energy as a function of ϵ (see figure 3(b)) one finds that the corresponding value of the exponent is

$$\omega_{eq} = 0.75. \tag{40}$$

This discrepancy is not so strange because if ω_{eq} is near to 1, one should take into account the regular term and fit the data as

$$q^e(\epsilon) = A + B\epsilon^{\omega_{eq}} + D\epsilon. \tag{41}$$

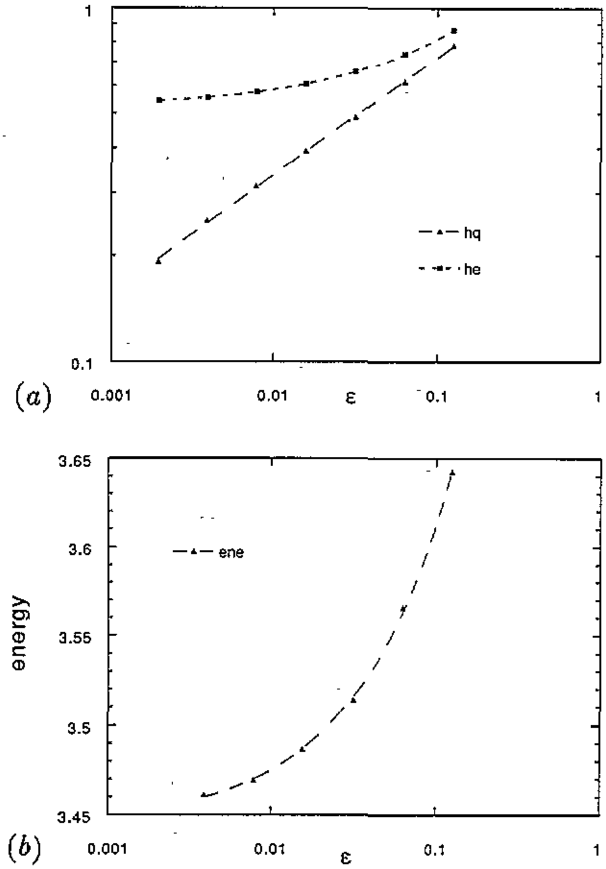

Figure 3. (*a*) The same data as figure 1 with h_q and h_e instead of q and q_e. The fits give $\omega_{qq} = 0.33$, $\omega_{eq} = 0.68$, (*b*) the internal energy as a function of ϵ_q, the fit gives $\omega_{eq} = 0.75$.

Such a four-parameter fit can be done and it gives in both cases (energy and energy overlap) a value of ω_{eq} in the range 0.8–0.9, but such a result may only be indicative. In any case the need to add an extra term (linear in ϵ), which is not universal, may explain the difference in the estimate of ω_{eq} when we change the observable.

In the limit in which $\omega_{eq} = 1$ one obtains $\epsilon \ln(\epsilon)$ dependence. In order to see whether this possibility can be dismissed, we have plotted the data for q_e against $-\epsilon \ln(\epsilon)$ in figure 4. A linear fit can be accepted.

At this stage we can only say that

$$0.66 < \omega_{eq} < 1. \qquad (42)$$

These values implies that $d_q = 0.95 \pm 0.05$ and correspondingly $\eta = -0.1 \pm 0.1$. In a similar way we find that d_e falls in the interval 2.2–3, corresponding to ν in the interval 0.55–1. The result for ν is probably correct but it does not carry too much information.

We have also done simulations in which we add a coupling between the replica of the form $\epsilon_e q^e$. In this case symmetry arguments imply that the expectation value of q is identically zero. Here we substitute $\langle q \rangle^{1/2}$ or $\langle |q| \rangle$ for it. A similar substitution in the previous case would not make too much difference and it would be negligible in the infinite-volume limit. In the following we will not pay too much attention to the difference between

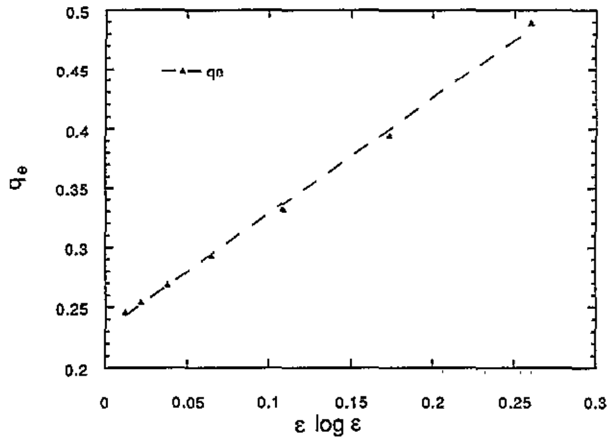

Figure 4. The data for q_e as a function of $-\epsilon\ln(\epsilon)$. A linear dependence is very compatible with the data and corresponds to $\omega_{eq} = 1$ with logarithmic corrections.

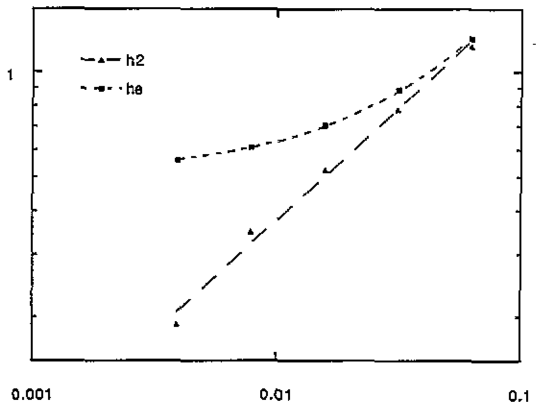

Figure 5. *The value of the overlaps h_q and h_ϵ as a function of ϵ_e. The fits give $\omega_{qe} = 0.64$,* while $\omega_{\epsilon e} = 1$ has been imposed.

these quantities and they will be denoted by q. The results are shown in figure 5 for ϵ_e in the range 2^{-4}–2^{-8}. The values of the exponent β from the fit is

$$\omega_{qe} = \beta = 0.64. \tag{43}$$

Using the scaling law $\beta = d_q\nu$ one finds that $\nu = 0.67$, which is a rather reasonable value.

These results are well compatible with those obtained from other methods (such as expansions near infinite-temperature or finite-size scaling) although the determination of ν is not very precise.

As the reader can see, a relatively small value of ϵ also produces relatively large effects, however it might not be wise to go to too small an ϵ, where finite-volume effect and thermalization problems lurk.

Summarizing, the method we have introduced for studying the overlaps as a function of the parameter ϵ can be used to compute successfully the dimensions of the relevant operators and there are no unwanted surprises.

We have also done numerical simulations at the critical temperature for smaller systems and they will reported elsewhere [10].

5. Numerical results for large systems below T_c

We have first studied the behaviour of q against ϵ below the critical temperature, mainly at $T = 1.5 \simeq 0.74 T_c$.

Simulations have been done for different systems with sizes that range from 8 to 18 for ϵ in the range 2^{-2}–2^{-6}. We have obtained the data by cooling the system with the largest value of ϵ, which has been slightly removed. The data for q are shown in figure 6 for several sizes. One does not see any systematic drift with the size.

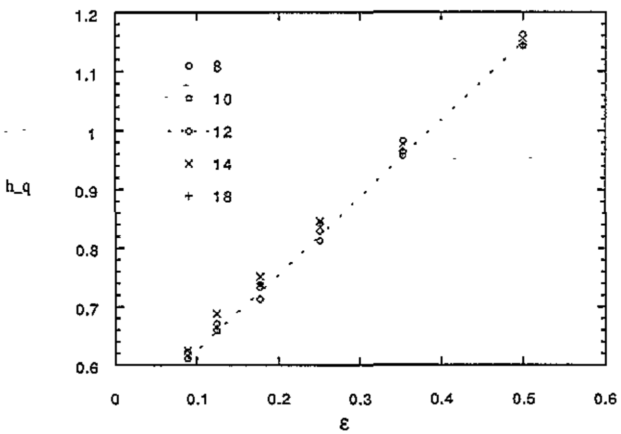

Figure 6. The dependence of q on ϵ at $T = 1.5$ for $L = 8, 10, 12, 14, 18$. The broken line is a linear fit to the data at $L = 14$.

The approximate linearity of the data against $\epsilon^{1/2}$ implies the presence of a non-trivial power dependence of q on ϵ and of a divergent susceptibility in the limit $\epsilon \to 0$. This conclusion is reinforced by studying the behaviour of the correlation length among the overlaps. A tentative extimate of the correlation length as function of ϵ has been obtained for the $L = 18^4$ system and it is shown in figure 7. We clearly see a sign of a divergence of the correlation lengh when ϵ goes to zero.

In order to better investigate the exponents which characterize the divergence of the overlap susceptibily we have performed longer simulations at smaller values of ϵ. The data are shown in figures 8 and 9. One sees that a fit of the form

$$q(\epsilon) = q(0^+) + A\epsilon^{1/2} + B\epsilon \tag{44}$$

fits the data reasonably well, the coefficient B being smaller if we substitute q by h_q.

It is possible to fit the data using a different exponent

$$q(\epsilon) = q(0^+) + A\epsilon^{\zeta_{qq}} \tag{45}$$

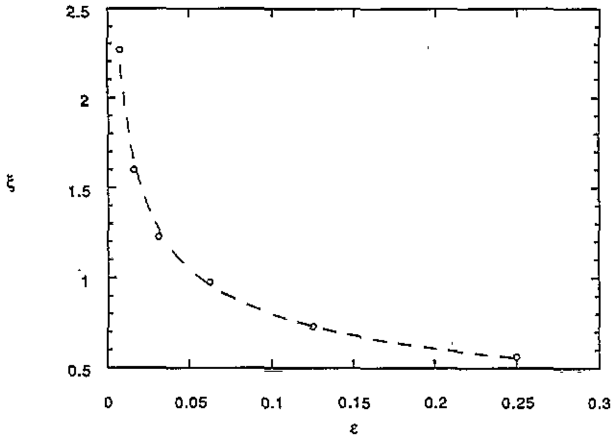

Figure 7. The dependence of ξ_q on ϵ at $T = 1.5$ for $L = 18$. The fit is a power law of the form $\epsilon^{-0.4}$.

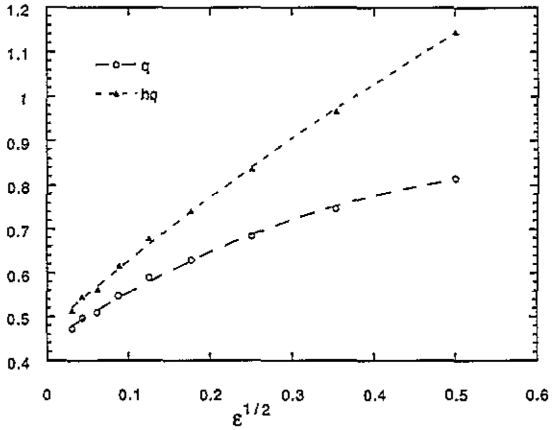

Figure 8. The dependence of q and h_q on ϵ at $T = 1.5$ for $L = 18$; the fits are of the form $q(\epsilon) = q(0) + A\epsilon^{1/2} + B\epsilon$.

with $\zeta_{qq} = 0.33$ if we fit q and $\zeta_{qq} = 0.39$ if we fit h_q.

For the quantity q_e as a function of q^2, data have been obtained for various values of ϵ at $T = 1.5$. These data show the existence of a non-vanishing $q_{\rm EA}$ order parameter with a power dependence on ϵ, with a power in the range 0.35–0.5.

In figure 10 one shows the energy overlap q^e† as function of q^2. Approximatively linear behaviour is observed. We recall again that in the infinite-range model the energy overlap is an exactly linear function of q^2.

The next issue is the verification of a discontinuity in q and q_e at $\epsilon_e = 0$, as predicted by replica theory. To this end we add a term equal to $\epsilon_e q_e$ to the Hamiltonian density. As before we cool a system of size 18^4 for a positive ϵ_e at $T = 1$ and later we remove ϵ_e at

† We remark for the careful reader that for this case only the energy overlap is defined in a slightly different way from the rest of the paper (i.e. assuming that the energy is concentrated on the sites and not on the bonds): $1/N \sum_i (\sum_k J_{i,k}\sigma_i\sigma_k)(\sum_k J_{i,k}\tau_i\tau_k)$.

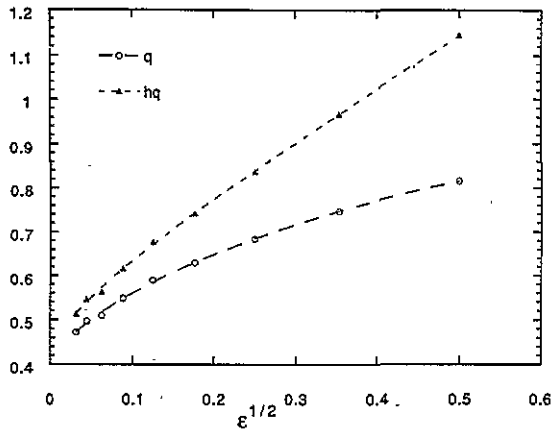

Figure 9. The dependence of q on ϵ at $T = 1.5$ for $L = 18$; the fits are of the form $q(\epsilon) = q(0) + A\epsilon^{\zeta_{qq}}$, with $\zeta_{qq} = 0.32, q(0) = 0.39$ if we fit q, $\zeta_{qq} = 0.34, q(0) = 0.40$ if we fit h_q.

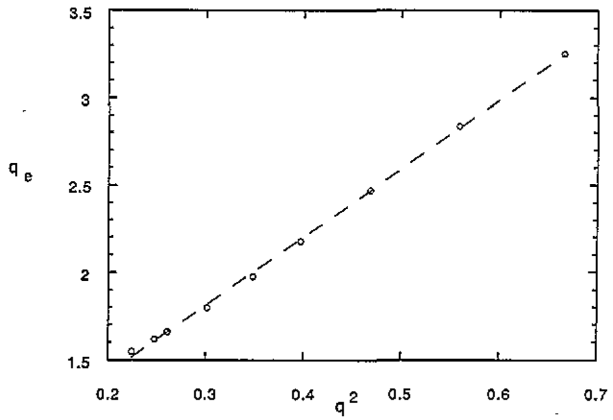

Figure 10. The quantity q_e as function of q^2, data have been obtained for various values of ϵ at $T = 1.5$.

fixed temperature. The data for the energy overlap (defined in the usual way) can be very well fitted with a simple formula of broken replica theory:

$$q_e(\epsilon_e) = q_e(0^+) + A\epsilon_e^{1/2} + B\epsilon_e \tag{46}$$

as can be seen in figure 11†.

In the same simulations we have measured the dependence of q on ϵ_e, which we display in figure 12. Here the data are also compatible with the prediction

$$q(\epsilon_e) = q(0^+) + A\epsilon_e^{1/2} + B\epsilon_e. \tag{47}$$

One should notice that in this case $q(0^+)$ is not the maximum overlap as found in equation (44). The presence of a power of ϵ_e smaller than 1 implies a divergence of the

† In this case h_e is defined as $h_e = \text{arth}(q_e^{1/2})$.

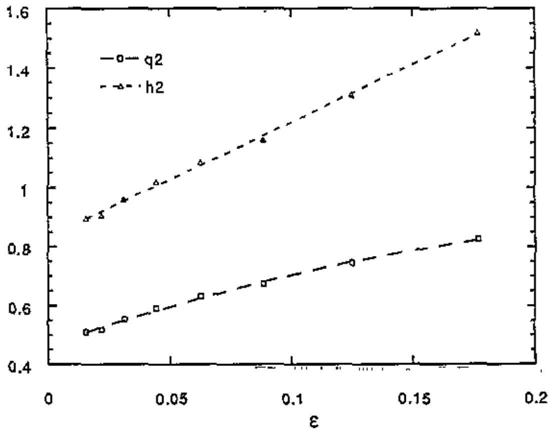

Figure 11. The quantity q_e and h_e as a function of ϵ_e on an 18^4 lattice at $T = 1$. The fits give $q_e(0^+) = 0.47$ in both cases.

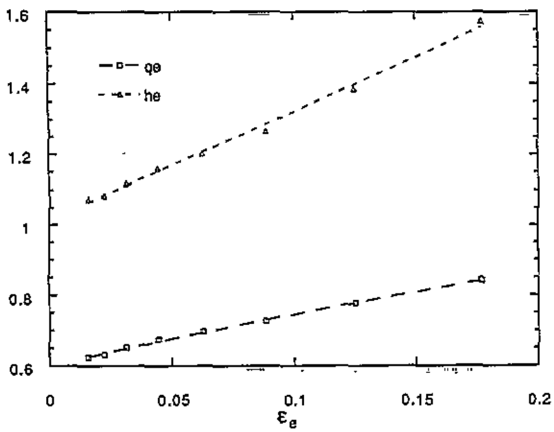

Figure 12. The quantity q^2 and h_q as a function of ϵ_e on an 18^4 lattice at $T = 1$. The fits are both compatible with $q(0^+) = 0.6$.

spin-glass susceptibilies e.g. $\partial q/\partial\epsilon_e$. This is possible if the correlation length diverges when ϵ_e goes to zero. In order to check this prediction we have measured the two-point correlation function of the q variable. The data are not very precise, especially at distances larger than 4, which would be crucial to obtain a careful measurement of the correlation functions. It seems that much longer simulations should be done in order to obtain precise data.

Anyway, the data seem to be compatible with a power-law divergence at $\epsilon_e = 0$.

In order to measure the discontinuities at $\epsilon_e = 0$ of the order parameters we have cooled the system in presence of a fixed field ϵ_e†.

The data for q^2 as function of of the temperature at different ϵ_e on a 10^4 lattice are

† In order to minimize the temperature dependence of the order parameters, we have kept ϵ_e fixed when cooling the system for negative ϵ_e, while we kept $\beta\epsilon_e$ fixed at positive ϵ_e.

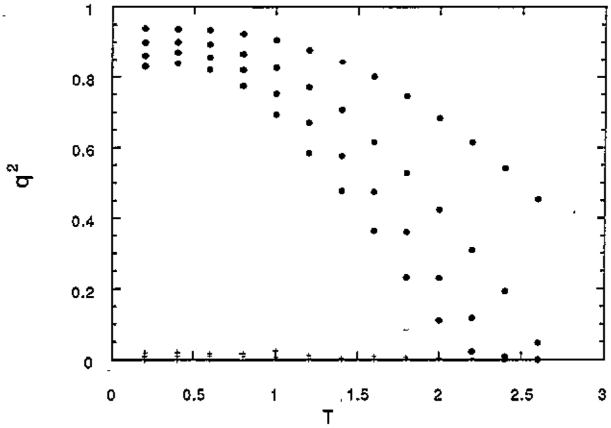

Figure 13. The quantity q^2 as a function of the temperature T for different values of ϵ_e. The data for negative ϵ_e are the triangles near the $q^2 = 0$ axis.

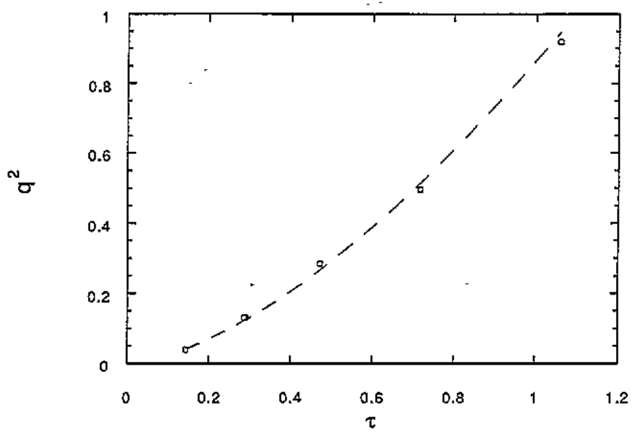

Figure 14. The value of q^2 extrapolated at $\epsilon_e = 0$. The broken curve is a fit of the form $q^2 \propto (T/T_c - 1)^{2\beta}$, with $\beta = 0.6$.

shown in figure 13. As expected q^2 is identically zero at high temperatures and for positive ϵ_e it becomes different from zero at a transition temperature which is ϵ_e dependent. Naively one would expect that this transition temperature $T_c(\epsilon_e)$ would be a linear function of ϵ_e for small ϵ_e. We have not checked whether this naive prediction is compatible with the results obtained from the renormalization group near six dimensions. Linear behaviour is not incompatible with the data, but we have not carefully investigated this point. The transition at $T_c(\epsilon_e)$ definitely belongs to a different universality class from the usual spin-glass transition. Simple arguments using the effective Hamiltonian for two coupled replicas suggest that this transition is in the same universality class as the disordered ferromagnetic Ising model in the value of the coupling. For such a transition one expects that the exponent β would be equal to its mean-field value $\frac{1}{2}$, apart from logarithmic corrections, so that q^2 should vanish approximatively linearly as a function of the temperature. This behaviour is not in disagreement with the data, although this point should be investigated more carefully.

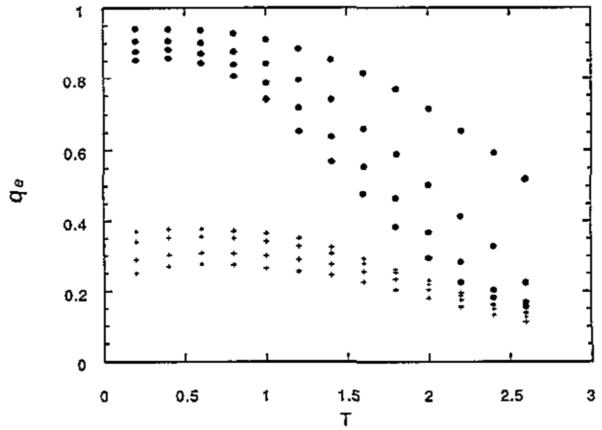

Figure 15. The quantity q_e as a function of the temperature T for different values of ϵ_e. The data for negative ϵ_e are the triangles near the $q = 0$ axis.

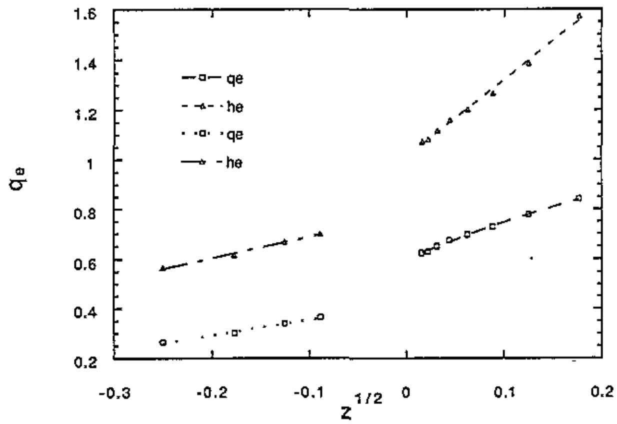

Figure 16. The quantity q_e at $T = 1.$ as a function of $\epsilon_e^{1/2}$ where, for simplicity, we use the notation $z^{1/2}$ at the place of $\text{sign}(z)z^{1/2}$ with $z = \epsilon_e$.

The extrapolation at $\epsilon_e = 0$ can be done assuming the correctness of the previous equation: one finds the results shown in figure 14. A power-law fit to the data, assuming a critical temperature of 2.02 gives an exponent β close to 0.6. On the other hand, the data at ϵ_e negative (shown in figure 13) are compatible with zero, apart from finite-volume corrections (ϵ_e is in the range 2^{-4}–2^{-7}). The expected discontinuity of q^2 at $\epsilon_e = 0$ is quite evident.

In a similar way we show the data for q_e as a function of ϵ_e in figure 15. As can be seen by the naked eye the extrapolation at $\epsilon_e = 0$ shows a discontinuity starting at a temperature about 1.5. A section of these data at $T = 1$ is shown in figure 16, as function of $\epsilon_e^{1/2}$, where for simplicity we use the notation $z^{1/2}$ instead of $\text{sign}(z)z^{1/2}$ (with $z = \epsilon_e$). Fitting q_e we obtain $q^e_{\text{max}} = 0.6$, $q^e_{\text{min}} = 0.42$ and $q^e_{\text{max}} = 0.59$, $q^e_{\text{min}} = 0.42$ fitting h_e.

The data for $q_e(0^+)$ and $q_e(0^-)$ are shown in figure 17 as function of the temperature. The extrapolation at $\epsilon_e = 0$ is done assuming the presence of a term proportional to $\epsilon_e^{1/2}$.

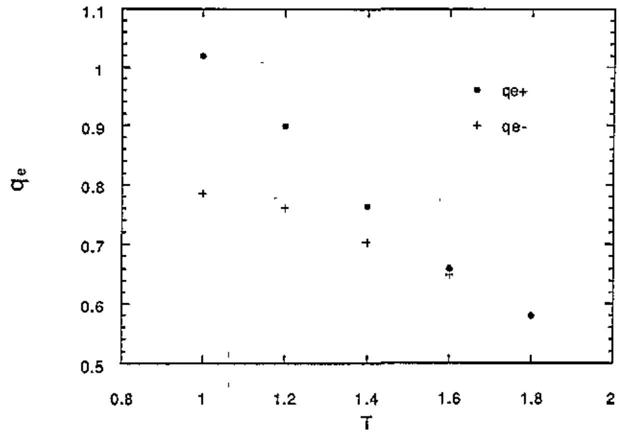

Figure 17. The extrapolated values for $q_e(0^+)$ and $q_e(0^-)$ as a function of temperature.

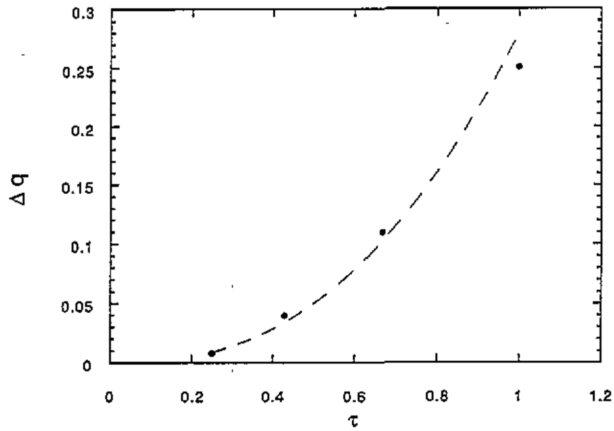

Figure 18. Δq_e as a function of temperature. The fit is a power of $(T/T_c - 1)$ and gives an exponent 2.2.

Only at temperatures around 1.5 or less do these two functions become different in a sensible way .

In figure 18 we show the value of Δq_e as function of the temperature. Δq_e is compatible with zero at temperature greater than 1.6. An indicative fit as a power of $(T/T_c - 1)$ gives an exponent 2.2. The fit is not reliable, because we do not have data close to the critical point, however this behaviour is compatible with the one expected from the renormalization group (we recall that the theoretical predictions are that the exponent should be equal to $1 - \alpha$). The apparent vanishing of the discontinity near the critical point is just what is expected from the known values of the critical exponents.

6. Conclusions

In this work we have shown a numerical method which allows large systems in finite-dimensional spin glasses to be studied, testing explicit predictions within replica broken theory. By coupling two replicas we can avoid the problem of the enormous computational time needed to thermalize large samples. In fact, with a finite coupling ϵ we are able to restore self-averaging and to avoid the problem of thermalization within a very complex landscape with many minima.

We have introduced the energy overlap which gives information about the nature of different states which equally contribute to the partition function. The existence of at least two states not differing by inversion of local compact domains gives support to the common mean-field picture of several states which are far one from each other in phase space by a finite distance.

We have used some new critical exponents ζ which we hope could be estimated in future within spin-glass field theory. Its precise determination within the spin-glass phase would be important for a precise understanding of short-range spin glasses. The ideas we have introduced in this work can be tested for small systems by means of finite-size scaling of the tails. These results are presented in a forthcoming work [10].

All our results give support to a complex landscape in the case of four-dimensional Ising spin glasses reminiscent of what we know in mean-field theory. This method can also be applied to study other short-range models and we hope it will give very interesting results in the three-dimensional case.

Acknowledgment

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