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Replica Symmetry Breaking in Short-Range Spin Glasses: Theoretical Foundations and Numerical Evidences

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We discuss replica symmetry breaking (RSB) in spin glasses. We update work in this area, from both the analytical and numerical points of view. We give particular attention to the difficulties stressed by Newman and Stein concerning the problem of constructing pure states in spin glass systems. We mainly discuss what happens in finite-dimensional, realistic spin glasses. Together with a detailed review of some of the most important features, facts, data, and phenomena, we present some new theoretical ideas and numerical results. We discuss among others the basic idea of the RSB theory, correlation functions, interfaces, overlaps, pure states, random field, and the dynamical approach. We present new numerical results for the behaviors of coupled replicas and about the numerical verification of sum rules, and we review some of the available numerical results that we consider of larger importance (for example, the determination of the phase transition point, the correlation functions, the window overlaps, and the dynamical behavior of the system).

KEY WORDS: Disorder; state; finite volume; spin glass; interface; replicas; symmetry breaking.

1. INTRODUCTION

The concept of replica symmetry breaking (RSB) as a crucial tool in the study of spin glass systems has been introduced close to twenty years ago,

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and a successful Ansatz for the breaking pattern has been proposed.[1–3] Nowadays there are no doubts that it describes correctly what happens in infinite range models.[4–6] On the contrary its correctness in the case of short range models has remained controversial. For short range models we cannot exhibit a solution in closed form, and things are made more difficult from the fact that the picture that emerges from the RSB is substantially different from the usual scenario valid for normal ferromagnets, with which we are familiar.

Moreover we have to deal with rather complex theoretical predictions, that can be interpreted in a simpler way by recasting them as the claim of the existence of an extremely large number of pure states (or phases) for very large systems. However this notion of many equilibrium states (not related by a trivial symmetry) is rather counterintuitive in the case of spin glasses (since it is difficult to visualize the situation in a fruitful way) while it would be quite natural in other contexts. For example the picture is clear in the case of protein folding, where a different equilibrium state corresponds to a different folding (tertiary structure) of the protein. Such intrinsic novelty and unusual character of the RSB formalism (and maybe some lack of precision in the mathematical definitions of some of the relevant literature)[4] has led to some degree of controversy on the precise definition and meaning of RSB and on its range of validity[7–12] (for the possible application of the Migdal–Kadanoff approximation, MKA, to spin glass systems, see refs. 13–16, it is interesting to notice that Gardner[17] has shown that it fails already at the mean field level).

In this paper we try to bring a positive contribution to the discussion by stating in the most clear and complete way which are the predictions implied by a RSB scenario, and summarizing; the quite ample numerical evidence for its validity in finite dimensional systems. This paper integrates and supplements the review[18] (for relevant books and reviews see refs. 4, 19–21). In order not to mix different conceptual issues we will first state the RSB predictions without using the concept of finite volume pure state. However this concept will be used later, when discussing the physical interpretation of the Ansatz. We will also discuss the relation among the finite volume pure states and the infinite volume ones.

We will analyze the two cases of the infinite range model and of short range one. We will discuss the problem of the number of *phases* for a finite system in the infinite volume limit and for an actual infinite system (these are two related but *different* problems). In doing that one should distinguish clearly the predictions coming from RSB from their consequences on the equilibrium states of the system. We will also discuss in detail the available numerical evidence. We will present new data which should help in clarifying the situation further.

2. THE REPLICA METHOD

2.1. The Basic Results

The first steps are quite simple. We consider a system of N spins whose Hamiltonian depends on some quenched random couplings J. In order to avoid all the complications present in the definition of the Boltzmann–Gibbs distribution for an actual infinite volume system (see Section 7) we follow the traditional approach of defining a probability distribution of the configuration C as $P(C) \propto \exp(-\beta H)$ for a finite volume system. It is evident that as it stands this definition cannot be used naively for an actual infinite system, since the exponent would be always infinite. A more careful treatment is needed.

For definiteness we shall consider two different models:

- A long range model, i.e., the SK model[22] with Hamiltonian

$$\mathscr{H}_J = \sum_{i,k} \sigma_i J_{i,k} \sigma_k - \sum_i h_i \sigma_i \tag{1}$$

where $\sigma_i = \pm 1$, the first sum is over all couples of sites of the lattice and the second one over all sites. The couplings J are quenched random variables with zero expectation value and for a system with N sites $\overline{J^2} = N^{-1}$ (we denote by brackets the thermal average and by an upper bar the averages over the quenched disorder).

- A short range model, i.e., the EA model[23] with Hamiltonian:

$$\mathscr{H}_J = \sum_{i,k}{}' \sigma_i J_{i,k} \sigma_k - \sum_i h_i \sigma_i \tag{2}$$

where now the primed sum runs over couples of first neighboring sites, and $\overline{J^2} = 1$.

In order to study the average over the couplings J of the free energy and of the correlation functions it is useful to consider a system where the spin configurations are replicated n times (in the same realization of the random interaction), with Hamiltonian

$$\mathscr{H}^{(n)} = \sum_{a=1}^{n} \mathscr{H}_J(\{\sigma^{(a)}\}) \tag{3}$$

After integration over the J one arrives to a new Hamiltonian in which different replicas are coupled. In order to study the model it is convenient to introduce the quantity

$$q_{a,b} \equiv \frac{1}{N} \sum_i \sigma_i^{(a)} \sigma_i^{(b)} \tag{4}$$

where a and b characterize two of the different replicas that we have introduced, and N is the number of spins per configuration.

We follow here a standard procedure (used in Statistical Mechanics and Field Theory in the last 75 years[24]): we first derive a mean field approximation, in which some kind of fluctuations are neglected (for a ferromagnet we would get the equation $m = \tanh(\beta zJm)$, where m is the magnetization, z is the coordination number of the lattice and J does not depend on the site).

At a second stage we deduce the correlation from the mean field approximation, obtaining the equivalent of the Ornstein–Zernike (OZ) expression for the correlation functions. In a third stage, which even for ferromagnets is relatively recent, we compute systematically the corrections to the mean field approximation and (when this is possible) we use the renormalization group to sum them up. In the case of spin glasses this last stage is still lacking, so that we are going to discuss only the mean field predictions with the computation of OZ correlations.

In the mean field approximation (i.e., when we neglect fluctuations) we find a free energy $F[Q]$, where $Q_{a,b} \equiv \langle q_{a,b} \rangle$. It is usually assumed (and it can be proved for $n > 1$) that the value of Q can be found by solving the equation

$$\frac{\partial F}{\partial Q_{a,b}} = 0 \tag{5}$$

under the condition that all the eigenvalues of the Hessian

$$(\mathrm{Hess})_{ab,cd} \equiv \frac{\partial^2 F}{\partial Q_{a,b}\, \partial Q_{c,d}} \tag{6}$$

are non negative.

The real problem arises when the saddle point equations admit more than one solution, and these solutions are related by a symmetry. This phenomenon is well known (it was discovered by Archimedes a long time ago), and in the context of Statistical Mechanics it goes under the name of *symmetry breaking*. In this particular case the obvious symmetry[4] is the permutation of different replicas. This symmetry is broken as soon as the non-diagonal elements of $Q_{a,b}$ depend on a and b. In this case the usual prescription is too average over all the different solutions of the saddle point equations in replica space (which being related by a symmetry have exactly the same free energy). Therefore if the value of an observable A depends on Q we find that

$$\overline{\langle A \rangle} = \frac{1}{n!} \sum_{\Pi} A(Q_{\Pi(a),\, \Pi(b)}) \tag{7}$$

where the sum runs over the $n!$ permutations (Π) of n elements.

If we apply this procedure to the correlation functions we find that[3, 25]

$$\overline{\frac{1}{N^2} \left\langle \sum_{i,k} \sigma_i \sigma_k \right\rangle^{2s}} = \lim_{n \to 0} \frac{1}{n(n-1)} \sum_{a,\, b;\, a \neq b} Q^s_{a,\, b} \tag{8}$$

The previous equation can also be written as

$$\int dq\, P(q)\, q^s = \lim_{n \to 0} \frac{1}{n(n-1)} \sum_{a,\, b;\, a \neq b} Q^s_{a,\, b} \tag{9}$$

where

$$P(q) = \overline{P_J(q)} \tag{10}$$

and $P_J(q)$ is the probability that two configurations selected according to the Boltzmann–Gibbs (B–G) distribution are such that their overlap (4) is equal to q.

The properties of the systems are related to those of the matrix $Q_{a,b}$. At first view the introduction of this matrix could appear a strange step. It has been shown however that it represents a compact way to encode the probability distribution of the overlaps among an arbitrary number of equilibrium configurations, and to describe how this probability changes when we change the couplings J.

The form of the matrix Q is crucial. In the replica approach we are forced by stability considerations (see Section 6 on stochastic stability) to consider matrices in which every line is a permutation of the other lines. The consequences of this form of the matrix Q, or equivalently of *stochastic stability*, will be discussed in the rest of this paper. There are some extra

[4] Exactly at zero magnetic field more symmetries would appear, but we do not deal with this case and we do not take them into account.

predictions which come from more specific assumptions about the form of the matrix Q. For example if we also assume ultrametricity we will refer to them as the *Mean Field predictions*. Indeed in the mean field approximation one finds that the matrix Q which makes the mean field free energy stationary is ultrametric. When we will meet a prediction which depends on the specific form of the matrix Q we will note it explicitly.

If the function $P_J(q)$ is trivial, i.e., if

$$P_J(q) = \delta(q - q_{EA}) \tag{11}$$

independently on the coupling J (as it happens in ferromagnets), the use of the replica method would be not interesting.[5] If the function $P(q)$ is non-trivial we say that *replica symmetry is broken.*

It is convenient to introduce the function $x(q)$

$$x(q) = \int_0^q dq\, P(q) \tag{12}$$

where we assume the function $P(q)$ has support for positive values of q. We define a function $q(x)$ as the inverse of $x(q)$. Of course $q(x)$ is defined only in the interval $0 \leqslant x \leqslant 1$. We thus have

$$P(q) = \frac{dx}{dq} \tag{13}$$

It is clear that the correlation functions are not clustering unless the function $q(x)$ is constant, i.e., (see (45)) $q(x) = q_{EA}$ (this is needed so that in a translational invariant system intensive quantities do not fluctuate in the infinite volume limit and to make all connected correlation functions vanishing at large distance): for clustering systems the function $P(q)$ must be equal[6] to $\delta(q - q_{EA})$.

The replica formalism also allows to study the dependence of the function $P_J(q)$ over the overlap q. Under general assumptions one finds[(26)] that universal relations like

$$\overline{P_J(q_1)\, P_J(q_2)} = \tfrac{2}{3} P(q_1)\, P(q_2) + \tfrac{1}{3} P(q_1)\, \delta(q_1 - q_2) \tag{14}$$

[5] For simplifying the discussion we assume that a non-zero, albeit small, magnetic field is turned on, so that the symmetry $\sigma \to -\sigma$ is broken. If this is not true the function $P(q)$ is be symmetric under the transformation $q \to -q$. Usually, even in a ferromagnet, in the cold phase the function $P(q)$ is not continuous at $h = 0$: its value at $h = 0$ is different from the limits $h \to 0^{\pm}$.

[6] We remind the reader that we are in finite volume and that the delta functions are slightly smoothed. It is implicit that all our statements become valid (obviously in distribution sense) without corrections only when the volume of the system goes to infinity.

hold (q_1 and q_2 are two given values of q). A set of relations of this type has been proven under general hypothesis (i.e., stochastic stability) in refs. 5 and in 6.

In the most popular scheme for replica symmetry breaking,[2, 3] which is supposed to be correct for the infinite range Sherrington–Kirkpatrick (SK) model, given any function function $q(x)$ (where x goes from 0 to 1) in the limit $n \to 0$ we can find a matrix $Q_{a,b}$ such that the previous equations are satisfied.

In the infinite volume limit the typical form of the function $q(x)$ is such that (at least in the mean field approximation)

$$P(q) = a\delta(q - q_m) + b\delta(q - q_M) + r(q) \tag{15}$$

where the function $r(q)$ is smooth.[7]

Some further relations which are not necessarily valid on general grounds turn out to hold in the RSB Ansatz, that is verified in the solution of the mean field theory of spin glasses: the most popular one is the ultrametric relation,[26] which states that the overlap distribution of three overlaps $(q_{1,2}, q_{2,3}, q_{3,1})$ among three replicas (1, 2, and 3) in the same realization of the quenched disorder is zero as soon as the ultrametricity inequality

$$\min(q_{1,2}, q_{2,3}) \geqslant q_{3,1} \tag{16}$$

(or one of the two other permutations of the former relation) is violated. It can be shown[88] that these inequalities (plus the general conditions which come from stochastic stability) imply that the average probability distribution of three overlaps is given by:

$$\begin{aligned}
&\overline{P_J(q_{1,2})\, P_J(q_{2,3})\, P_J(q_{3,1})} \\
&\quad = \tfrac{1}{2} P(q_{1,2})\, x(q_{1,2})\, \delta(q_{1,2} - q_{2,3})\, \delta(q_{2,3} - q_{3,1}) \\
&\qquad + \tfrac{1}{2} [P(q_{1,2})\, P(q_{2,3})\, \theta(q_{1,2} - q_{2,3})\, \delta(q_{2,3} - q_{3,1}) \\
&\qquad + \text{two permutations}]
\end{aligned} \tag{17}$$

As we discuss many times in this paper relations like 14 and 17 are also valid in the case of a trivial $P_J(q)$, but we want to stress that will show in detail that this is not the case in finite dimensional EA spin glasses (see for example Fig. 8 and the related discussion).

Moreover all the probability distributions of more that three overlaps and their variation from system to system are completely determined by the

[7] The form of the function $P(q)$ is discontinuous in the limit of zero magnetic field.

function $P(q)$, or equivalently by the function $q(x)$. In other words the usual replica symmetry breaking of mean field theory is the only possible pattern of replica symmetry breaking that is ultrametric.

In principle it is possible that ultrametricity is valid in the infinite range model and it is violated in finite dimensional short range models, the function $P(q)$ remaining non-trivial and consequently replica symmetry being still broken. In this case one would have to consider, in the short range models, more complex forms of the matrix Q. Indications that this does not happen and that ultrametricity will hold in finite dimensional models will be discussed later.

Summarizing we are considering three possibilities

- The function $P(q)$ is a single delta function at $q = q_{EA}$, and q_{EA} is nonzero below the critical temperature. This situation, with no breaking of the replica symmetry, is realized in the Migdal Kadanoff approximation or equivalently in the droplet model, and in the *chaotic pairs* scenario of refs. 7, 11, and 12.
- The $P(q)$ is a not a single delta function: in this case replica symmetry is broken. The condition of replica equivalence strongly constrains the behavior of the system.
- The ultrametricity condition is satisfied. This is the mean field case, where many more detailed predictions can be obtained.

2.2. The Correlation Functions

We have already commented on the fact that a non trivial form of the function $P(q)$ implies that the correlation functions are non-clustering. In this case the study of the correlation functions can be involved, since we can select different values of the overlap. In all generality we can try to determine correlations of Θ operators at different fixed overlap q_θ. Here we will focus only on the simplest kind of such correlation functions.

As before we consider two copies of the system in the same realization of the disorder, and we denote their spin variables by σ and τ. We define the local overlap on the site i by

$$q_i \equiv \sigma_i \tau_i \tag{18}$$

which can take the values ± 1. We define the average $\langle \cdot \rangle_{\hat{q}}$, restricted to the configurations of the system such that

$$\frac{1}{N} \sum_i q_i = \hat{q} \tag{19}$$

We define now a (non-connected) correlation function

$$G_{\hat{q}}^{N}(i) \equiv \overline{\langle q_i q_0 \rangle_{\hat{q}}} \tag{20}$$

where we are considering systems with N spins. These $\hat{q}$ dependent correlation functions can be computed in the replica formalism by using the analogue of the OZ formulae. We consider the case, relevant for spin glasses, where the function r of (15) is non-zero and $q_m \leqslant \hat{q} \leqslant q_M$ (i.e., $\hat{q}$ is in the support of $P(q)$). In the usual Ansatz for replica symmetry one finds that[27–30]

$$\lim_{i \to \infty} \lim_{N \to \infty} G_{\hat{q}}^{N}(i) \equiv \lim_{i \to \infty} G_{\hat{q}}^{\infty}(i) = \hat{q}^2 \tag{21}$$

Therefore for all $q_m \leqslant \hat{q} \leqslant q_M q - q$ connected correlation functions at fixed q value satisfy the usual cluster decomposition.

The total free energy of the constrained system (with fixed $\hat{q}$) is (apart from corrections of order one) equal to the unconstrained free energy because $P(\hat{q}) \neq 0$.

A behavior of this type is unusual, and we will discuss it in better detail in the next sections. One can think about a similar construction in a ferromagnet: in that case when forcing a value of the magnetization smaller than the spontaneous magnetization one would create a situation where the correlation function of the magnetization would not be clustering (there would be at least an interface).

What is happening here is that for each value of the overlap $\hat{q}$ that we can select we find a different asymptotic limit for the value of the correlation functions. The approach of these correlation functions to their large distance asymptotic value is very interesting: in mean field using the OZ approximation one finds that for large i

$$\lim_{N \to \infty} G_{\hat{q}}^{N}(i) \approx \hat{q}^2 + A(\hat{q})\, i^{-\theta(\hat{q})} \tag{22}$$

The exponent (which is a non trivial function of $\hat{q}$) is known only at zero loops in the mean field approximation.[29, 27] It is an extremely important and open question to verify if its value is correct beyond tree level. We can distinguish three cases:

- $\theta(q_M) = D - 2$. There is a feeling that this result may be exact, and that it corresponds to some kind of Goldstone theorem (see ref. 27 and references therein, and ref. 31).

• $\theta(q) = D-3$ for $q_M > q \geqslant q_m$ (where the last equivalence holds only for q_m different from 0). There is a feeling that this result may be modified by corrections to the mean field approximation,[27] although there is no final evidence of this effect. On the contrary, if the exponent would be exact even in three dimensions, one should conclude that replica symmetry breaking disappears in $D=3$, and 3 should be identified as the lower critical dimension (but for the existence of a phase transition in $3D$ see refs. 32, 33, 18, 34, and 35).

• $\theta(q_m) = D-4$ for $q = q_m = 0$ (i.e., only in zero magnetic field). This result does not apply in $D < 6$. The following formula has been conjectured (see ref. 27 and references therein):

$$\theta(q=0) = \frac{(D-2+\eta_c)}{2} \tag{23}$$

where η_c is the exponent η for the $q-q$ correlations at the critical point.

A phenomenon which is related to this behavior of the correlation functions is the non-triviality of the window overlap distributions. Let us consider the case of 3 dimensions. We select a cubic region B of B^3 spins in the center of our system (of N spins) and we define the *window overlap*

$$q_B \equiv \frac{1}{B^3} \sum_{i \in B} q_i \tag{24}$$

We can define the probability distribution

$$P_B(q) \equiv \lim_{N \to \infty} P_B^N(q) \tag{25}$$

where $P_B^N(q)$ is the probability distribution of q_B in a system with N spins. The prediction of the replica approach is then that $P_B(q)$ is non trivial. One finds that

$$\lim_{B \to \infty} P_B(q) = P(q) \tag{26}$$

If we define the restricted probability distributions $P_B(q \mid \hat{q})$, i.e., we consider only those pairs of configurations with a fixed value of the overlap $\hat{q}$, we find that

$$\lim_{B \to \infty} P_B(q \mid \hat{q}) = \delta(\hat{q} - q) \tag{27}$$

where the rate of the approach to the asymptotic limit is controlled by the appropriate exponent $\theta(\hat{q})$ that we have just discussed.

In other words if we fix the value of the total overlap we expect that the average overlap in each large region will become equal to the global overlap. This mean that without paying any price in free energy density we can change the average value of the overlap in each region of the space. This in sharp contrast with what would happen in a ferromagnet, where locally the system would remain in the phase of positive or negative magnetization.

2.3. No Disguised Interfaces

The results shown in the previous sections are the main predictions of the RSB Ansatz. Broken Replica Theory predicts that for realistic spin glasses the function $P(q)$ is non trivial not because of the presence of interfaces among two different phases, which are located in random position. In order to stress this point and to clarify the implications of these predictions we will discuss now a negative example: we will examine a very simple physical system with a non-trivial $P(q)$ which **does not** satisfy these predictions, and we will show how RSB theory is adamant in differentiating this case.

The system is simple: we consider a three dimensional ferromagnet that in the infinite volume limit, develops a non-zero spontaneous magnetization m (i.e., with $T<T_c$). For sake of simplicity we also suppose that the temperature is sufficiently small that the interface among the positive and negative magnetized phases is not rough. We also consider a finite volume realization of the system in a cubic box of N spins with periodic boundary conditions in the y and z direction and antiperiodic boundary conditions in the x direction. At a sufficiently low temperature the antiperiodic boundary conditions force the formation of a domain wall. For very large volumes N we can classify the equilibrium configurations by the magnetization profile

$$m(i_x) \equiv \frac{1}{N_y N_z} \sum_{i_y=1,\, N_y;\, i_z=1,\, N_z} \sigma(i_x, i_y, i_z) \tag{28}$$

that will be of the form

$$m(i_x) = f(i_x - I) \tag{29}$$

where I is the position of the interface, and the function f characterizes the profile. If i_x takes integer values from 1 to N_x, f is or $+m$ for $i_x \to 0$ and $-m$ for $i_x \to N_x$ or it is $-m$ for $i_x \to 0$ and $+m$ for $i_x \to N_x$ and it satisfies $f(\pm\infty) = \pm m$. This will be true for almost all equilibrium configurations, with exceptional configurations whose probability goes to zero when N goes to infinity. If we now consider two generic equilibrium configurations a trivial computation shows that in the limit $N \to \infty$ $P(q) = 1/2m^2$ for $-m^2 \leqslant q \leqslant m^2$.

Apart from the absence of fluctuation of $P_J(q)$ with J (this system is not a random system) the results for the correlation are different from the prediction of the RSB Ansatz. The fact that in teach configuration there is a single domain wall implies that

$$\lim_{B \to \infty} P_B(q) = \tfrac{1}{2}\delta(q - m^2) + \tfrac{1}{2}\delta(q + m^2) \tag{30}$$

because if we look to a local observable we have zero probability of hitting an interface. In this example the window overlaps are insensitive to the boundary conditions.

With the same token we get that here

$$\lim_{i \to \infty} G^{\infty}_{\hat{q}}(i) = m^4 \tag{31}$$

In other words in this case the system may exist in two different phases separated by an interface. The arbitrariness in the position of the interface implies a non trivial form of the function $P(q)$. However local quantities are insensitive to the presence of an interface and the replica predictions are not valid. This situation is not described by replica symmetry breaking, and a study of the relevant quantities makes it clear.

If we add a random term to the Hamiltonian, for example a random dilution, it is possible to create a situation where the interface will be pinned in one single position. In this case the function $P(q)$ will become a single trivial delta function. If we allow to the interface two or more positions we will obtain again a non trivial function $P(q)$. The local overlaps are insensitive to all these variations. In the two cases that we have described where the function $P(q)$ is non-trivial (an infinite number of positions or few positions allowed to the interface) the relation (14) is not satisfied (unless some magic coincidence happens in the last case, where the interface may be located in a few selected positions).

2.4. The Energy Overlap

An alternative way to understand how much the predictions of the RSB Ansatz differ from the situation described in the previous section (i.e., where there are two or more different phases related by a symmetry separated by an interface) is considering different kinds of overlaps among spin configurations, in particular the energy overlap.

Generally speaking, given a local quantity[8] $A_i[\sigma]$ which depends only over the spins of the configuration σ that are close to the site i, we can define the A-overlap of two configurations as

$$Q_A[\sigma, \tau] \equiv \frac{1}{N} \sum_i A_i[\sigma]\, A_i[\tau] \tag{32}$$

A very interesting case is taking as local operator the energy E, i.e., writing

$$\mathscr{H}[\sigma] = \sum_i E_i[\sigma] \tag{33}$$

and using E_i to compute what we call the *energy overlap* (q_E).

The crucial point is that in the infinite volume limit the interfaces have vanishing weight. If the bulk of the system is in two or more different phases related by a symmetry, away from the interface the contribution to the energy overlap is constant. In this way one sees that in this case in the infinite volume limit the probability distribution of q_E becomes a delta function.

On the contrary when replica symmetry is broken the probability distribution of q_E remains non trivial also in the infinite volume limit. In the SK model one has that $q_E[\sigma, \tau]$ is a linear function of $q[\sigma, \tau]^2$: it is clear that here the two probability distributions $P(q)$ and $P_E(q_E)$ are strongly related, and they must become simultaneously different from a delta function.[9] This linear relation may approximately hold also in finite dimensional systems, but there are no reasons why it should remain exact. At least in the mean field approximation all possible types of overlaps are functions of the basic overlap q, so that their probability distribution can be computed by evaluating the function $P(q)$ and the relation among the generalized overlap and the basic overlap q.

An other relevant quantity is the *link overlap*

$$q_{\text{link}}[\sigma, \tau] \equiv \frac{2}{zN} \sum_{i,k} \sigma_i \sigma_k \tau_i \tau_k \tag{34}$$

where the sum is taken over all nearest neighbor pairs, and z is the coordination number of the lattice. In the case of a model with $J = \pm 1$ it

[8] In the infinite volume limit $A_i[\sigma]$ is a continuous function of σ in the usual product topology.

[9] By using some imagination we could say that the breaking of the replica symmetry corresponds to a situation where we have an interface which occupies a finite fraction of the volume. On the other hand in this situation we could not speak anymore of an interface in a proper sense.

coincides with an energy overlap where the sum is done over the sites and not over the links. The link overlap is clearly sensitive to differences in the correlation functions of the two configurations. It is also equal to the $q-q$ correlation at distance one. The fact that the link overlap has a non trivial distribution is related to the dependence of the correlation function $G_{\hat{q}}^{\infty}(i)$ on $\hat{q}$ at $i=1$.

3. FINITE VOLUME STATES AND RSB RESULTS

3.1. The Definition of States of a Finite System

In order to develop a formalism useful to discuss the physical meaning of the results contained in the previous section it is convenient to introduce the concept of *pure states in a finite volume*. This concept is crystal clear from a physical point of view. However it can be difficult to state it in a rigorous way (i.e., to prove existence theorems) mostly because the notion of finite volume pure states (or phases) is deeply conditioned by the physical properties of the system under consideration. In order to prove theorems on finite volume pure states one needs a very strong rigorous command of the physical properties of finite, large statistical system.

Most of the research in mathematical physics has been devoted to the study of the pure states of an infinite system. Unfortunately the concept of pure states of an infinite system is too rigid to capture all the statistical properties of a finite system and it is not relevant for the physical interpretation of the replica predictions: here we needs, as we will see later, more sophisticated tools, that are exactly finite volume pure states.

Readers who are not interested to enter the details of this interpretation of the physical picture of RSB may skip this section and base their considerations on the results discussed in the previous chapter. Those who decide to read this section should be aware that the finite volume pure states we introduce here are mathematically different from the pure states for an infinite system which are normally used in the literature.

We must admit that there has been some confusion on this point in the literature on RSB. In the first paper where the interpretation of replica symmetry breaking was presented[(36)] the words *pure states*, *clustering decomposition*... were used, strongly suggesting that the states one was speaking about were the infinite volume states which are normally used in the literature. Only later on, after some reflections, it became clear from the cavity approach[(37)] and from the presence of a chaotic dependence on the volume,[(38)] that the there were some problems in identifying the states that were needed in the replica approach with the infinite volume states.

A first attempt in describing directly what happens in finite volume was done in ref. 39. For a while the problem was not investigated further and the words *pure states* continued to be used in the literature: no explicit discussion appeared about why finite volume states should be used, as opposed to the infinite volume pure states. One of the reasons of this lack of precision was that the decomposition into states is a theoretical tool mainly needed to reach a better understanding of the theoretical framework, and that no ambiguity was present for predictions about numerical simulations and about experimental results.

Let us see how approximate pure states or phases in a large but *finite* system can be defined, introducing a definition of state that is different, but maybe more physical than the usual one. We will at first give a rough definition. Our strategy is to mimic the definition of pure states of an infinite system and to apply it to the physical relevant situation (which is the only one accessible by numerical simulations and by experiments) of a finite (and large) system.

We consider a system in a box of linear size L, containing a total of N spins. We partition the configuration space in regions, labeled by α, and we define averages restricted to these regions:[39, 40] *these regions will correspond to our finite volume pure states or phases*. It is clear that in order to produce something useful we have to impose sensible constraints on the form of these partitions. We require that the restricted averages on these regions are such that connected correlation functions are small[10] at large distance x.

In the case of a ferromagnet the two regions are defined by considering the sign of the total magnetization. One includes configurations with a positive total magnetization, the second selects negative total magnetization. There are ambiguities for those configurations which have exactly zero total magnetization, but the probability that such a configuration can occur is exponentially small at low temperature.

Physical intuition tells us that this decomposition exists (at least for familiar systems), otherwise it would make no sense to speak about the spontaneous magnetization of a ferromagnetic sample, or to declare that a finite amount of water (at the melting point) is in the solid or liquid state.

[10] The precise definition of *small at large distance* in a finite volume system can be phrased in many different ways. For example we can introduce a function $g(x)$ which goes to zero when x goes to infinity and require that the connected correlation functions evaluated in a given phase are smaller than $g(x)$. Of course the function $g(x)$ should be carefully chosen such not to give trivial results; one should also prove the independence of the results from the choice of g in a given class of functions. The choice of the class of functions to which g belongs would be the first step towards a rigorous proof of the existence of this construction.

Moreover all numerical simulations gather data that are based on these kinds of notions, since the systems that we can store in a computer are always finite. The concept of finite volume states is preeminent from the physical point of view: infinite volume states are mainly an attempt to capture their properties in an amenable mathematical setting. We strongly believe that this decomposition of a finite but large system into phases does make sense, although its translation in a rigorous mathematical setting has not been done (also because it is much simpler, and in most cases informative enough, to work directly in the infinite volume setting).

In order to present an interpretation of these results we assume that such decomposition exists also for spin glasses (the contrary would be very surprising for any system with a short range Hamiltonian). Therefore the *finite* volume Boltzmann–Gibbs measure can be decomposed in a sum of such finite volume pure states. The states of the system are labeled by α: we can write

$$\langle \cdot \rangle = \sum_{\alpha} w_\alpha \langle \cdot \rangle_\alpha \tag{35}$$

with the normalization condition

$$\sum_{\alpha} w_\alpha = 1 \tag{36}$$

The function $P_J(q)$ for a particular sample is given by

$$P_J(q) = \sum_{\alpha, \beta} w_\alpha w_\beta \, \delta(q_{\alpha, \beta} - q) \tag{37}$$

where $q_{\alpha, \beta}$ is the overlap among two generic configurations in the states α and β.

We want to stress that in our construction (mainly based, at this point, on the analysis of results from numerical simulations) the definition of finite volume pure states that we have introduced here is only used in order to present an interpretation of the results. The predictions of the mean field theory concern correlation functions computed in the appropriate ensemble,[(2)] and computer simulations measure directly these correlation functions. The decomposition into finite volume states (which is never used by the actual computer simulations) is an interpretative tool which translates to a simple and intuitive framework the complex phenomenology displayed by the correlation functions. We stress again that the analysis of the overlap probability distribution $P(q)$ can be based on the definition given in Eqs. (8, 9) that is more direct but has, in our opinion, much less appeal and intuitive meaning than the previous one.

3.2. More on the Finite Volume State Classification

We will try now to give a few more details about the definition of equilibrium pure states for a finite volume system that we have just discussed. As we have already pointed out our statements will be relevant for configurations which appear with a non negligible probability in the low temperature region. In the following we will consider again a system with N spins σ_i, which can take the values ± 1, and we will not need to specify the details of the Hamiltonian of the system. We assume however that there are no continuous symmetries that are spontaneously broken, otherwise the states would be labeled by a continuous parameter: the discussion of this case would need more details, without bringing anything substantially new.

Given two spin configurations (σ and τ) from the overlap definition (4) one can introduce a natural concept of distance by

$$d^2(\sigma, \tau) \equiv \frac{1}{N} \sum_{i=1}^{N} (\sigma_i - \tau_i)^2 \tag{38}$$

that belongs to the interval [0–1], and is zero only if the two configurations are equal. In analogy with our discussion of section (2.4) and with the definition (32), we can define more general distances based on the local operator $A_i(\sigma)$, which is a function of the spins at a finite distance from the site i. In this way we have

$$d_A^2(\sigma, \tau) \equiv \frac{1}{N} \sum_{i=1}^{N} (A_i(\sigma) - A_i(\tau))^2 \tag{39}$$

In the thermodynamical limit, i.e., for $N \to \infty$, the distance of two configurations is zero if the number of different spins remains finite. The percentage of different σ's, not the absolute number, is relevant in this definition of the distance. It is also important to notice that at a given temperature β^{-1}, when N goes to infinity the number of relevant configurations is extremely large: it is proportional to $\exp(N\mathscr{S}(\beta))$, where $\mathscr{S}(\beta)$ is the entropy density of the system).

Finite volume pure states will enjoy a set of properties that we will discuss now: these conditions will be satisfied by the finite volume states we have defined above, as well as by any other reasonable definitions of finite volume states, and are by themselves a strong characterization of the state.

• When $N \to \infty$ each state belonging to the decomposition (taken for a given N value) includes an exponentially large number of configurations.[11]

• The distance of two different generic configurations C_α and C_β belonging one to state α and the other to state β does not depend on the C_α and C_β, but only on α and β. In this way we can define a distance $d_{\alpha,\beta}$ among the states α and β, as the distance among two generic configurations in these two states. The reader should notice that with this definition the distance of a state with itself is not zero. We could define a distance

$$D_{\alpha,\beta} \equiv d_{\alpha,\beta} - \tfrac{1}{2}(d_{\alpha,\alpha} + d_{\beta,\beta}) \tag{40}$$

in such a way that the distance of a state with itself is zero ($D^A_{\alpha,\alpha} = 0$). In the rest of this paper we prefer to stick to the previous definition.

• The distance between two configurations belonging to the same state α is strictly smaller than the distance between one configuration belonging to state α and a second configuration belonging to a different state β. This last property can be written as

$$d_{\alpha,\alpha} < d_{\alpha,\beta} \tag{41}$$

where $d_{\alpha,\beta}$ is the distance between the states α and β, i.e., the distance between two generic configurations belonging to the states α and β. This property forbids to have different states such that $D_{\alpha,\beta} = 0$, and it is crucial in avoiding the possibility of introducing arbitrary states, doing a too fine classification. For example if in a ferromagnet at high temperature we would classify the configurations into two states which we denote by e and o, depending on if the total number of positive spins is even or odd, we would have that $d_{e,e} = d_{e,o} = d_{o,o}$.

• The classification into states is the finest one which satisfies the three former properties.

The first three conditions forbid a classification too fine, while the last condition forbids a classification too coarse.

For a given system the classification into states depends on the temperature of the system. In some case it can be rigorously proven that the classification into states is possible and unique[(41–43)] (in these cases all the

[11] We warn the reader that we will *never* consider $N \to \infty$ limit of a given finite volume pure state. In order to address such a question one should compare the properties of systems with different values of N. There are some difficulties in doing this comparison, due the chaotic dependence of the statistical expectation values on the size of the system (see Section 4).

procedures we will discuss lead to the same result). We want to note that the definition of state is reminiscent of the definition of species which is familiar to biologists.

States can also be discussed from a slightly different point of view, that we analyze now. One starts by considering a generic quantity B, and by studying its fluctuations

$$\langle B^2 \rangle_c \equiv \langle B^2 \rangle - \langle B \rangle^2 = \langle (B - \langle B \rangle)^2 \rangle \tag{42}$$

Intensive quantities are defined as

$$b = \frac{1}{N} \sum_{i=1}^{N} B_i(\sigma_i) \tag{43}$$

where the site functions B_i depend only on the value of σ_i. We then ask ourselves if intensive quantities fluctuate in the infinite volume limit. In general we would expect a negative answer, since intensive quantities are averages over the whole system. This is not the case at a first order transition point, where different phases coexist.

As we have discussed before in the usual case of a ferromagnet (in the broken phase) spin configurations are classified according to the sign of the majority of the spins: on averages restricted to one type of these configurations the density of spin with a given sign does not fluctuate.

The argument is simple. If the Hamiltonian $\mathscr{H}$ is symmetric under the global transformation where $\sigma_i \to -\sigma_i$ in all sites i, than $\langle \sigma_i \rangle = 0$. In this situation intensive quantities do fluctuate. If we call Σ the intensive quantity corresponding to the spins (i.e., $\Sigma \equiv N^{-1} \sum_{i=1}^{N} \sigma_i$), the expectation value of Σ is zero ($\langle \Sigma \rangle = 0$), while the expectation value of its square is non zero ($\langle \Sigma^2 \rangle = m^2 \neq 0$).

By classifying the configurations in two sets, we can define restricted averages $\langle (\cdots) \rangle_+$ and $\langle (\cdots) \rangle_-$, such that

$$\langle \Sigma \rangle = \tfrac{1}{2}(\langle \Sigma \rangle_+ + \langle \Sigma \rangle_-), \qquad \langle \Sigma \rangle_+ = +m, \qquad \langle \Sigma \rangle_- = -m \tag{44}$$

In normal ferromagnetic systems it is possible to prove[41–43] that intensive quantities do no fluctuate in $\langle \ \rangle_+$ and in $\langle \ \rangle_-$. The decomposition of a probability distribution under which intensive quantities fluctuate into the linear combination of restricted probability distributions where the intensive quantities do not fluctuate works in many physical situations. The restricted probability distributions correspond to different states, that are identified by the expectation value of intensive quantities. Equations (35) and (36) give the decomposition of the expectation value.

If we consider the classification into states for a finite system we must face the fact the probability distribution is not the Boltzmann–Gibbs one, since some configurations are excluded. This amounts to say that the DLR relations which tell us that the distribution probability is locally a Boltzmann–Gibbs distribution will be violated, but the violation will go to zero in the large volume limit.

It is interesting to note that in usual situations in Statistical Mechanics the classification in phases is not very rich. For usual materials, in the generic case, there is only one phase: such a classification is not very interesting. In slightly more interesting cases (usual symmetry breaking) there may be two states. For example, if we consider the configurations of a large number of water molecules at zero degrees, we can classify them as water or ice: here there are two states. In slightly more complex cases, if we tune carefully a few external parameters like the pressure or the magnetic field, we may have coexistence of three or more phases (a tricritical or multicritical point).

In all these cases the classification is simple and the number of states is small. On the contrary in the mean field theory of spin glasses the number of states is very large (it goes to infinity with N), and a very interesting nested classification of states is possible. We note "en passant" that this behavior implies that the Gibbs rule is not valid for spin glasses. The Gibbs rule states that in order to have coexistence of n phases (n-critical point), we must tune n parameters. Here no parameters are tuned and the number of coexisting phases is infinite! This point will be further elaborated in Section 6.

3.3. The RSB Predictions and Finite Volume States

Now we are ready to rephrase the predictions of the RSB Ansatz under the hypothesis that the finite volume Boltzmann–Gibbs state may be decomposed into finite volume pure states. For finite N the decomposition (35) holds, together with the normalization condition (36).

Let us stress once again how crucial it is that this decomposition is done for finite large volume. We are not assuming that quantities like $\langle \cdot \rangle_\alpha$ have a limit when the volume goes to infinity: that would not be wise because of the chaotic dependence of the states on the volume (as we discuss better in (4)). The set of the weights w_α also changes with the volume, and we only assume that the probability distribution of this decomposition has a limit when the volume goes to infinity. The potential and not appropriate use of Eq. (35) to describe an infinite system, which is ironically called the *standard mean field or SK picture* in refs. 9, 11, and 12, is completely foreign to the RSB Ansatz (see also our discussion about this issue in Section 3.1).

We can rephrase the predictions of the RSB Ansatz as follows:

• State equivalence. States cannot be distinguished by looking to the expectation value of intensive quantities like the energy, the magnetization, the Edward–Anderson parameter, i.e,

$$q_{EA} \equiv \frac{1}{N} \sum_i (\langle \sigma_i \rangle_\alpha)^2 \tag{45}$$

correlation functions or any other quantity which depends in a simple way on the couplings J (for example quantities like $\sum_{i,k,l,m} \sigma_i J_{i,k} J_{k,l} J_{l,m} \sigma_m$).

• If we compare two or more states all expectation values depend only on the set of overlap among these states. For example given two states we can define the three different correlation functions

$$\begin{aligned} C_2(k) &= \frac{1}{N} \sum_i \langle \sigma_i \sigma_{i+k} \rangle_\alpha \langle \sigma_i \sigma_{i+k} \rangle_\beta \\ C_3(k) &= \frac{1}{N} \sum_i \langle \sigma_i \rangle_\alpha \langle \sigma_{i+k} \rangle_\alpha \langle \sigma_i \sigma_{i+k} \rangle_\beta \\ C_4(k) &= \frac{1}{N} \sum_i \langle \sigma_i \rangle_\alpha \langle \sigma_{i+k} \rangle_\alpha \langle \sigma_i \rangle_\beta \langle \sigma_{i+k} \rangle_\beta \end{aligned} \tag{46}$$

All these correlation functions depend on the overlap $q_{\alpha,\beta}$ and do not fluctuate in the infinite volume limit at fixed $q_{\alpha,\beta}$. More precisely for N fixed we can consider the values of the correlations in the right hand side of the previous equations when we change α and β at fixed overlap $q_{\alpha,\beta}$: the variance of these values goes to zero when the volume goes to infinity.

• As we have remarked for each realization of the couplings J one finds a different set of weights w and allowed overlaps q. The probability distribution of the couplings J induces a probability distribution over the set of the w and the q. This probability distribution $\mathscr{P}_N[w, q]$ has a limit when N goes to infinity. This statement does not imply that the dependence on N of the w and q is smooth. Only their probability distribution (or equivalently the average over the J) has a smooth dependence (see the discussion of the quenched state in ref. 6). The detailed form of $\mathscr{P}[w, q]$ depends on the exact pattern of the replica symmetry breaking.

• If we order the weights w in a decreasing sequence (from the largest weight to the smallest one) we find that,[26]

$$\sum_{\alpha=1}^{K} \langle w_\alpha \rangle_{\mathscr{P}} \to 1 \tag{47}$$

when $K \to \infty$ (K still being much smaller than N). Here the expectation value $\langle \cdot \rangle_{\mathscr{P}}$ is taken over $\mathscr{P}$. This last property implies that practically all the weight is carried by a finite number of finite volume pure states.

There are some extra predictions which are characteristic of the RSB Ansatz of 2 which describes the mean field approximation.

- If we order the weights as before

$$\sum_{\alpha=1}^{K} \langle w_\alpha \rangle_{\mathscr{P}} = 1 - O(K^{-\chi}) \tag{48}$$

where the expectation value $\langle \cdot \rangle_{\mathscr{P}}$ is taken over $\mathscr{P}$, and the exponent χ is given by

$$\chi = \frac{1}{x(q_{EA})} \tag{49}$$

We expect a power law decay to hold in general. The exponent may depend on the form of the RSB Ansatz. Numerical simulations[34] confirm this behavior.

- The different definitions of the distance, depending on the choice of the local operator A, are equivalent. Neglecting terms which go to zero when N goes to infinity one must have

$$d^A_{\alpha,\beta} = f^A(q_{\alpha,\beta}) \tag{50}$$

In other words any type of distance can be computed in terms of the overlap. For given N we can consider the values of the correlations in the r.h.s. of the previous equations when we change α and β at fixed overlap $q_{\alpha,\beta}$: the variance of these numbers goes to zero when the volume goes to infinity.

- The overlaps satisfy the *ultrametricity condition*

$$q_{\alpha,\beta} \geqslant \min(q_{\alpha,\gamma}, q_{\beta,\gamma}) \qquad \forall \alpha, \beta \text{ and } \gamma \tag{51}$$

The presence of an ultrametric structure strongly simplifies the theoretical analysis: for each realization of the couplings J we can construct the tree of the states, where the states are the leaves of the tree and the probability distribution $\mathscr{P}[w, q]$ reduces to a probability distribution over the hierarchical tree (which has been studied in detail by Ruelle).[44]

Of course we can restate the ultrametricity property without using the concept of finite volume states. It amounts to say that three generic equilibrium configurations σ^1, σ^3 and σ^3 satisfy the equivalent inequality

$$d(\sigma^1, \sigma^2) \leqslant \max(d(\sigma^1, \sigma^3), d(\sigma^2, \sigma^3)) \tag{52}$$

with probability one when the volume goes to infinity. In other words it says that the joint probability distribution of the overlaps among three different equilibrium configurations for finite N, averaged over the couplings J, goes to a limit which is zero in the region of overlaps where the previous inequality (52) is not satisfied.

Ultrametricity is quite likely correct in the SK model and what happens in short range models will be discussed later.

This picture based on finite volume states has a clear and direct meaning. It has the advantage to be potentially applicable also in different contests, as for example when discussing protein foldings. Here the concept of finite volume state is clear: a given tertiary structure is the equivalent of a state in our spin model. In this case theoretical instruments to discuss the behavior of finite systems are badly needed, also since the limit of a protein of infinite length is not very interesting from the biological point of view.

4. THE CAVITY APPROACH AND CHAOS

The original derivation of the properties of the infinite range model of spin glasses[(2)] was based on the replica method, which involves an analytic continuation from integer to non integer values of n (the number of replicas). An alternative approach is the so called cavity approach.[(4)] Here one starts by assuming that in a finite volume the decomposition in pure states is possible and has the properties that we have described in the previous section. Then one compares a system containing N spins to a system with $N+1$ spins: in the limit of N large the probability $\mathscr{P}_{N+1}[w, q]$ can be written in explicit form as function of $\mathscr{P}_N[w, q]$. Symbolically we get

$$\mathscr{P}_{N+1} = \mathscr{R}[\mathscr{P}_{\mathscr{N}}] \tag{53}$$

The probability $\mathscr{P}_\infty$, which is at the heart of the replica approach, can be obtained by solving the fixed point equation

$$\mathscr{P}_\infty = \mathscr{R}[\mathscr{P}_\infty] \tag{54}$$

The probability distribution (embedded with an ultrametric structure) which was found by using replica theory turns out to be a solution of this fixed point equation. Alas, it is not known if it is the only solution.

Chaoticity is a very important property of spin glasses. It amounts to say that if we consider a finite system and we add to the total Hamiltonian a perturbation $\delta\mathcal{H}$ such that

$$1 \ll \delta\mathcal{H} \ll N \tag{55}$$

the unperturbed and the perturbed system are as different as possible. As usual chaoticity may be formulated in terms of equilibrium expectation values of observables. In the typical chaotic case

$$q(\delta H) \equiv \frac{1}{N} \sum_{i=1,N} \langle \sigma_i \rangle_H \langle \sigma_i \rangle_{H+\delta H} \tag{56}$$

is equal to the minimum allowed overlap q_m as soon as δH satisfies the previous bound (55). Chaoticity can also be formulated by saying that the states of the perturbed systems have minimal overlap (i.e., q_m) with the states of the system in absence of the perturbation.

Here is a list of some examples:

- Chaoticity with respect to a random energy perturbation.

This is a trivial effect. The weights w are of order 1. Because of this fact a random perturbation in the energy function, which acts differently on different states, completely changes the weights w as soon as it is much larger than 1 (or much larger than $\frac{1}{N}$ if we look at the energy density).

- Chaoticity in magnetic field.

This has been the first example of chaos in spin glasses that has been discovered.[3] If we have two systems with the same couplings J but different magnetic fields h_1 and h_2, their equilibrium overlap becomes the minimum one allowed (that we call q_m) as soon as $(h_1 - h_2)^2 N \gg 1$. The difference in magnetic field acts more or less as a random energy perturbation.

- Chaoticity in temperature.

This effect[45–48] is maybe present in some models and absent in others (surely p spin infinite range spherical models).[49] It is related to the fact that states with the same total free energy may have different energy and entropy, and therefore a different dependence of the free energy on the temperature.

- Chaoticity when changing the number of spin.

Chaoticity when changing the number of spin[4, 7, 8, 50] is at the heart of the cavity approach and it is responsible of the differences among the predictions for the free energy of the replica exact and the replica broken theory.[4] When we go from N to $N+1$ spin the weights w change of a factor of order 1. Because of that we must write evolution equations for the whole population of states and not for a single state. This crucial and well known effect has been also discussed for the short range model by refs. 7 and 8: in this context it takes the name of "chaotic volume dependence" (see also ref. 50 for related work).

This form of chaoticity tell us that we cannot speak of the properties of a given state in the infinite volume limit, but the decomposition into states must be done for each value in N. Moreover one must pay a particular attention in taking the infinite volume limit. Local quantities like the expectation value of a the spin at a given point do not have a limit, at least in a naive sense, when N goes to infinity.

A simple case of chaotic dependence on the volume is the one of an Ising ferromagnet in presence of a random symmetric distribution of magnetic field at low temperature. The total magnetization is well approximated by sign $\sum_{i=1,N} h_i$ (where the h_i are the random fields) and this quantity changes in a random way when N goes to infinity.

5. THE ORDER PARAMETER IN THE RSB ANSATZ

At this point of our discussion the reader could be worried about the thermodynamical stability of RSB construction. We are dealing here with a new and peculiar phenomenon: even in the infinite volume limit the leading free energy differences are of order 1, as opposed to a difference of order N in the usual thermodynamical systems. It is important to reach a better understanding of such an unusual behavior, in order to eliminate possible doubts about the relevance of RSB. Indeed one may be worried by the fact that by choosing a suitable perturbation one can select only one of the ground states and arrive to a situation in which the function $P(q)$ is trivial. This is correct, but in order to reach this goal the perturbation must be very carefully tuned (but see ref. 12 for a different point of view). If the perturbation is random the effect will be different, as discussed in the Section 6. This section will be devoted to discussing various methods which can be used to derive an expression for the function $q(x)$ (or equivalently for $P(q)$) only considering the expectation values of intensive quantities, which can be computed in the infinite volume limit.

We will start by introducing a construction that puts the overlap order parameter in a more familiar perspective (5.1) (like the magnetic field for ordinary statistical systems). We will give a specific example of physical relevance of such order parameter (5.2), and show a computation that is very clarifying from a theoretical point of view (5.3) (since it allows to base the RSB results on the analysis of intensive quantities in the infinite volume limit). At last we will show that, under some hypothesis, the probability distribution of the order parameter can be reconstructed by means of a dynamical approach (5.4).

5.1. Two Coupled Replicas

Following reference[51] we will show here that we can discuss the two replica overlap as the order parameter of the theory in a very natural way. We consider two copies of the system with the same realization of the couplings J, and we add to the Hamiltonian an external field which couples the two real replicas σ and τ:

$$\mathscr{H} \equiv -\sum_{i,j} J_{ij}\sigma_i\sigma_j - \sum_{i,j} J_{ij}\tau_i\tau_j - h\sum_i (\sigma_i + \tau_i) - \varepsilon \sum_i \tau_i\sigma_i \tag{57}$$

Considering the two cases of positive and negative ε leads to a discontinuity in the expectation value of the overlap in the limit where $\varepsilon \to 0$ (in complete analogy with the usual symmetry breaking one has in a ferromagnet when $h \to 0^+$ and $h \to 0^-$). In this way we give a definition of the two bounds of the overlap support, q_m and q_M, that we had already introduced earlier, by using a purely thermodynamical approach.

In the RSB Ansatz of ref. 2 one finds that[51] in the mean field theory the expectation value of the overlap q between the replicas τ and σ, that we denote as $q(\varepsilon)$, is a discontinuous function of ε as $\varepsilon \to 0$. One has that

$$\lim_{\varepsilon \to 0^+} q(\varepsilon) = q_M \tag{58}$$

(where q_M coincides with q_{EA}), but

$$\lim_{\varepsilon \to 0^-} q(\varepsilon) = q_m \tag{59}$$

This discontinuity at $\varepsilon = 0$ is a striking consequence of replica symmetry breaking: the mean field predictions prediction for $\varepsilon > 0$ is $q(\varepsilon) = q_{\mathrm{EA}} + A\varepsilon^b$, where A is a constant and $b = \frac{1}{2}$. It is possible that even under the same Replica Symmetry Breaking Ansatz of the mean field theory, the value of b is changed in finite dimensions (a very naive guess could be $b = \frac{1}{2}$ for $D \geqslant 6$, $b = \frac{D-2}{D+2}$ for $D < 6$).

In a theory without replica symmetry breaking one finds a very different result:

$$\lim_{\varepsilon \to 0^+} q(\varepsilon) = \lim_{\varepsilon \to 0^-} q(\varepsilon) = q_{\mathrm{EA}} \tag{60}$$

Continuing our discussion of Section 2.4 about more general definitions of overlaps and distances in configuration space (we have discussed for example the energy overlap and the link overlap) we can base our modified action on the energy overlap, i.e.,

$$\mathcal{H} \equiv -\sum_{i,j} J_{ij}\sigma_i\sigma_j - \sum_{i,j} J_{ij}\tau_i\tau_j - \varepsilon \sum_{i,j} \tau_i\tau_j\sigma_i\sigma_j \tag{61}$$

Again the expectation value of the energy overlap $q_E(\varepsilon)$ in a theory with replica symmetry breaking is a discontinuous function at $\varepsilon = 0$, while $q_E(\varepsilon)$ is continuous at $\varepsilon = 0$ in systems without replica symmetry breaking.

5.2. Physical Relevance of the Order Parameter

In the previous section we have made clear the physical relevance of q_M, i.e., of the q_{EA} defined in (45) (the overlap of two replica's in the same state). We have to be more careful when considering quantities like, for example

$$q_J \equiv \int dq\, P_J(q)\, q \tag{62}$$

(where we have chosen the simplest interesting quantity, and, as usual, we assume we are in non-zero magnetic field), and taking their disorder average by

$$q_a \equiv \overline{q_J} \tag{63}$$

q_J is not a self-averaging quantity: even for arbitrary large volume it takes different values for different realizations of the couplings. Its value is determined by differences in the free energies which are of order 1.

We will show here that in a specific (but very interesting) case q_a [52, 53] has a direct physical meaning. We consider[53] the model defined by the Hamiltonian

$$\mathcal{H} \equiv -\sum_{ij} \sigma_i J_{ij} \sigma_j - \sum_i \sigma_i r_i \tag{64}$$

where the r_i are quenched random Gaussian magnetic fields with zero mean and variance r_0^2, and the couplings J_{ij} are the usual spin glass quenched random couplings. We define the infinite volume staggered magnetization

$$m_s \equiv \lim_{N\to\infty} \frac{1}{N} \sum_i \overbrace{r_i \langle \sigma_i \rangle} \tag{65}$$

where $\widetilde{(\cdots)}$ denotes the double average over the couplings J_{ij} and over the random magnetic field (r_i). A simple integration by parts tells us that

$$m_s = r_0^2 \beta (1 - q_a) \tag{66}$$

i.e., establishes a relation among the staggered magnetization and the average quenched overlap q_a. Such a simple identity (in the style of the relations of refs. 5, 6, and 54) reveals that the order parameter can be directly related to a well defined thermodynamical parameter (note that m_s is a self-averaging quantity).

5.3. Random Field and Coupled Replicas

Now, following ref. 51, we art able to establish a relation among the results of the two former sections, and to establish some further interesting analytic evidence. We consider a spin glass in a random magnetic field, with the Hamiltonian (64). we call $\mathscr{Z}^N[r]$ the partition function of a system with N spins, and with a random field r distributed according to $d\mu(r)$. We define a generalized free energy density as

$$F(s, r_0^2) \equiv \lim_{N \to \infty} -\frac{1}{\beta s N} \log \left[\int d\mu(r) \left(\frac{\mathscr{Z}^N[r]}{\mathscr{Z}^N[0]} \right)^s \right] \tag{67}$$

$F(s, r_0^2)$ is a well defined thermodynamic quantity. For integer values of s the integrals can be solved and we find a system of s coupled replicas:

$$\mathscr{H} = \sum_{a=1}^{s} \mathscr{H}_0[\sigma^a] - \frac{r_0^2}{2} \sum_{i=1}^{N} \sum_{a,b=1}^{s} \sigma_i^a \sigma_i^b \tag{68}$$

where $\mathscr{H}_0$ is the zero field Hamiltonian, and r_0^2 is the ε of the Hamiltonian (57). We are interested in the behavior of the free energy F for small positive values of r_0^2. We define

$$\aleph(s) = \left. \frac{\partial F(s, r_0^2)}{\partial r_0^2} \right|_{r_0^2 = 0^+} \tag{69}$$

Analogously to what happens in Section 5.1 we get that[51]

$$\aleph(s) = 1 + (s-1)\, q_{\mathrm{EA}} \tag{70}$$

Let us see why. The term $\aleph(s)$ is proportional to the expectation value of the interaction term in Eq. (68). In this term there are s diagonal entries that contribute with one $(a = b)$, and $s(s-1)$ non-diagonal entries that contribute with q_{EA}.

Next we discuss what happens for non-integer values of s, $0<s<1$. In this case using the mean field RSB Ansatz one can explicitly compute that

$$\aleph(s)=1-\int_s^1 du\, q(u) \tag{71}$$

It would be interesting to check if this formula is valid in general or if it is only valid in the mean field ultrametric approach.

The probabilistic meaning of this construction has been discussed in detail in ref. 51. For example in the simple case where the function $q(x)$ has a discontinuity at $x=m$ one finds that for $s<m$ the integral over r is dominated by the generic configurations of the random magnetic field r, while for $s>m$ the integral is dominated by those rare configurations of the magnetic field which point in the same direction of one of the possible magnetizations of the system.

The non-linearity of the function $\aleph(s)$ for sufficiently small values of s is a signal of replica symmetry breaking. One can show in general that

$$\aleph(0)=\int_0^1 dq\, P(q)(1-q) \tag{72}$$

and $(d\aleph(s)/ds)|_{s=1}=q_{EA}$.

This result is interesting from a theoretical point of view, since it leads to the construction of a not trivial order parameter which signals the presence of replica symmetry breaking in a purely thermodynamic way, i.e., by only computing intensive quantities. Unfortunately the quantity $\aleph(s)$ is extremely difficult to compute numerically but for very small systems.

5.4. The Dynamical Approach

In this section we will give a definition of the function $P(q)$ based on the behavior of the systems when it is slightly off-equilibrium. This will imply that it is possible to define $P(q)$ as a function of "well-defined" physical observable quantities, like the magnetization of the system.

In principle we can considered two different off-equilibrium situations

- The system is driven off-equilibrium by an external force, or by a time dependent Hamiltonian. For example we can assume that the couplings J are not time independent, but that they change at random on a time scale τ, which is assumed to be very large but finite. In this case we reach a stationary, off-equilibrium situation, in which the correlation functions depend only on the time difference of the observables.

• The system is drifting toward equilibrium because it was not at equilibrium at time $t_0 = 0$. In this case, also if equilibrium is eventually reached, the system is slightly out equilibrium at finite time. The correlation functions will be no more translationally invariant.

In this note we will consider only the second situation, but similar considerations apply to the first case.

We consider the quantity $A(t)$ that depends on the local variables of the unperturbed Hamiltonian $\mathscr{H}$. We define the associated autocorrelation function

$$C(t, t') \equiv \langle A(t)\, A(t') \rangle \tag{73}$$

where the brackets $\langle \cdots \rangle$ imply a double average, over the dynamical process and over the disorder (as it wild be in all this section). We also define the response function

$$R(t, t') \equiv \left. \frac{\delta \langle A(t) \rangle}{\delta \varepsilon(t')} \right|_{\varepsilon = 0} \tag{74}$$

where we have perturbed the original Hamiltonian by a small contribution

$$\mathscr{H}' = \mathscr{H} + \varepsilon(t)\, A(t) \tag{75}$$

In the following we will specifically select $A(t) = (1/N) \sum_i \sigma_i(t)$. When looking at the dynamics of the problem and assuming time translational invariance it is possible to derive the *fluctuation-dissipation* theorem (thereafter FDT, see for example ref. 24), that reads as

$$R(t, t') = \beta \theta(t - t')\, \frac{\partial C(t, t')}{\partial t'} \tag{76}$$

The fluctuation-dissipation theorem holds in the equilibrium regime, i.e., when

$$|t - t'| \ll t \tag{77}$$

We expect a breakdown of its validity in the region where Eq. (77) does not hold. Under general assumptions one finds that[55] the FDT theorem gets modified as

$$R(t, t') = \beta X(t, t')\, \theta(t - t')\, \frac{\partial C(t, t')}{\partial t'} \tag{78}$$

It has also been suggested[55, 56] that the function $X(t, t')$ turns out to be a function of the autocorrelation function:

$$X(t, t') = X(C(t, t')) \tag{79}$$

Under this hypothesis one can generalize FDT. The off-equilibrium fluctuation-dissipation relation, which should hold in the aging regime of the dynamics, reads

$$R(t, t') = \beta X(C(t, t'))\, \theta(t - t')\, \frac{\partial C(t, t')}{\partial t'} \tag{80}$$

The previous equation can be related to observable quantities like the magnetization. The magnetization in the dynamics is a function of the time, and a functional of the magnetic field (that is itself a function of the time: $h = h(t)$). We denote it by $m[h](t)$. Using a functional Taylor expansion and the definition of the response function we can write

$$m[h](t) = \int_0^t dt'\, R(t, t')\, h(t') + \mathrm{O}(h^2) \tag{81}$$

that is nothing but the linear-response theorem where the terms proportional to h^2 have been neglected. By applying (80) we derive the dependence of the magnetization over time in a generic time-dependent magnetic field (with a small strength),[12] $h(t)$

$$m[h](t) \simeq \beta \int_{-\infty}^t dt'\, X[C(t, t')]\, \frac{\partial C(t, t')}{\partial t'}\, h(t') \tag{82}$$

Now we can perform the following experiment. We let the system to evolve in absence of magnetic field from $t = 0$ to $t = t_w$, and then we turn on a constant magnetic field, h_0. The time dependent magnetic field is[13] $h(t) = h_0 \theta(t - t_w)$, and

$$m[h](t) \simeq h_0 \beta \int_{t_w}^t dt'\, X[C(t, t')]\, \frac{\partial C(t, t')}{\partial t'} = h_0 \beta \int_{C(t, t_w)}^1 du\, X[u] \tag{83}$$

where we have performed the change of variables $u = C(t, t')$ and we have used the fact that $C(t, t) \equiv 1$. In the equilibrium regime (where FDT holds, and $X = 1$) we must find that

$$m[h](t) \simeq h_0 \beta (1 - C(t, t_w)) \tag{84}$$

[12] Here the symbol $\simeq$ means that the equation is valid in the region of small fields. One must be careful because the strength of the non-linear effects often increases as a power of t.[57]

[13] In our notation we ignore the fact that $m[h](t)$ depends on t_w.

i.e., $(m[h](t)\, T)/h_0$ is a linear function of $C(t, t_w)$ with slope -1. A precise relation connecting the function X to the equilibrium behavior of the system has been conjectured.[55, 56] In the limit where t and t_w go to ∞ and $C(t, t_w) = q$ one expects that $X(C)$ converges to the $x(q)$ of Eq. (13). Obviously $x(q)$ is equal to 1 for all $q > q_{EA}$, and in this region we recover FDT. It follows that, if the previous conjecture is true, it is possible to define $P(q)$ in terms of the magnetization of the system, i.e.,

$$P(q) = -\frac{1}{h_0 \beta} \frac{d^2 m[h](t)}{dC^2}\bigg|_{C=q} \tag{85}$$

In the last section we shall see how this approach gives results for the function $P(q)$ which are very similar to those one can obtain by its direct definition.

6. STOCHASTIC STABILITY

Stochastic stability is a property which is valid in the mean field approximation: it is reasonable to conjecture that is valid in general also for short range models. It has been introduced quite recently[5, 6, 54, 58, 67] and strong progresses have been done on the study of its consequences.

In order to decide if a system with Hamiltonian H is stochastically stable, we have to consider the free energy of an auxiliary system with the following Hamiltonian:

$$H + \varepsilon H_R \tag{86}$$

If the average (with respect to H_R) free energy is a differentiable function of ε (and the limit where the volume goes to infinity commutes with the derivative with respect to ε), for a generic-choice of the random perturbation H_R inside a given class and ε close to zero, the system is said to be *stochastically stable*. In the nutshell stochastic stability tells us that the Hamiltonian H does not has any special features and that its properties are analogous to those of similar random systems (H can contain quenched random disorder).

It is simpler to compute the properties of the stochastically perturbed system than those of the original system, since any possible accidental symmetry is washed out by the random perturbation. For example spin glasses at exactly zero field are not stochastically stable because of the symmetry $\sigma \to -\sigma$ which is destroyed by a random perturbation. Stochastic stability may hold only for spin glasses in presence of a non-zero magnetic field.

The definition of stochastic stability may depend on the class of random perturbations we consider. Quite often it is convenient to chose as a random perturbation an infinite range Hamiltonian, e.g.,

$$H_R^3 = \sum_{i,k,l} J_{i,k,l} \sigma_i \sigma_k \sigma_l \tag{87}$$

where the sum runs over all the N sites of the system and the J's are random uncorrelated variables with variance $\frac{1}{N}$. In the same way we can define a random perturbation H_R^p where the interaction involves p spins.

A simple integration by part tells us that in finite volume

$$R^p(\varepsilon) = \frac{\langle H_R \rangle_\varepsilon}{\varepsilon} = \int dq\, P_\varepsilon(q)(1 - q^p) \tag{88}$$

where $P_\varepsilon(q)$ is the average over the random perturbation of the overlap distribution probability. Adding terms with different values of p we can reconstruct the whole function $P(q)$.

The quantity $R^p(\varepsilon)$ is a well defined thermodynamic quantity like the internal energy, whose expectation value may be ambiguous only at exceptional points of first order phase transitions. It can also be obtained as the derivative of the ε dependent free energy.

Stochastic stability is a very strong property. Many properties can be derived from stochastic stability, in particular the overlap sum rules (14) and their generalizations. Let us discuss a few examples which should help to understand some implications of stochastic stability.

- Let us consider two different systems with two different non-trivial functions $P_1(q_1)$ and $P_2(q_2)$, and let us suppose that each of the systems is stochastically stable. The union of the two systems, if they are non interacting, will not be stochastically stable anymore, as can be easily seen: the relation (14) is no more valid for the union system. Stochastic stability describes a situation in which the whole system remains strongly correlated, as opposed to the one in which the function $P(q)$ is non trivial because of the formation of interfaces among two possible phases.

- When the overlap may only take two values, or equivalently the function $P(q)$ is simply given by

$$P(q) = A\delta(q - q_m) + (1 - A)\,\delta(q - q_M) \tag{89}$$

stochastic stability implies that the usual Mean Field Ansatz gives the correct result.

• The identity among the dynamic $X(q)$ function and the static $x(q)$ function can be proved to be a consequence of stochastic stability.[58, 59]

We have seen that stochastic stability strongly constrains the properties of the system, and that many of the qualitative results of the replica approach can be derived as mere consequences of stochastic stability. Stochastic stability apparently does not imply ultrametricity, which seems to be an independent property.[54] This independence problem is still open as far as the only probabilities distribution of the free energies of the states that have been constructed in an explicit form are ultrametric.

7. THE INFINITE VOLUME PURE STATES

The free energy is a very basic quantity to analyze when studying the infinite volume limit of a physical system. In many cases it is easy to prove (at least for the lattice model) the existence of the free energy in the infinite volume limit. At first sight that could seem to be enough for deriving the thermodynamics and for computing intensive quantities, by derivating the free energy with respect to the external field.

However when we consider the free energy as a function of some parameter we can find out that there are points where it is not differentiable, more precisely where the left and the right derivatives do differ. The typical example is the case of the spontaneous magnetization where

$$F(h) = F(h=0) + m\,|h| + O(h^2) \tag{90}$$

In this case we can obtain different values of the magnetization by considering the two limits $h \to 0^{\pm}$. The same Hamiltonian (with zero magnetic field) could give different result for the magnetization in the limit $N \to \infty$ and $h \to 0$. In this way we say that we end up in one of two different allowed states of the infinite volume system. A crucial reason for the direct introduction of pure states for an infinite volume system is to make life simpler, giving an intrinsic definition of pure states, avoiding the necessity of considering the response of the system all possible forms of the external fields.

7.1. Generalities

We will try to clarify here the language we need in order to proceed further, and we will give a few needed mathematical definitions.

The word state is often used in mathematics, with different underlying meanings. A possible definition is the following. Let $\mathscr{A}$ be the B^* algebra of observables, which in classical statistical mechanics form an Abelian algebra with identity. We say that a linear functional ρ is a state if

$$A \geqslant 0 \Rightarrow \rho(A) \geqslant 0 \qquad \|\rho\| = 1 \tag{91}$$

where this second condition (the norm of ρ is one) implies that $\rho(A=1)=1$.

In a finite volume a state is a normalized probability distribution: we can associate to it an expectation value. The notion of a state can be extended to an infinite system. If a compact set of states is convex, we can consider the extremal points of this set and call them pure states. Any state of the set can be written in an unique way as a linear combination of these pure states.

The introduction of the notion of pure states in statistical physics has the main goal, as we said before, to allow a clear definition of symmetry breaking. A crucial notion is the one of *clustering*: a state is called clustering if connected correlation functions computed in such state go to zero at large distance. There exist systems for which the finite volume equilibrium state goes to an infinite volume one with the unwanted property that its correlation functions do not satisfy the clustering properties (consider for example a ferromagnetic system at zero external magnetic field in the low temperature region, where there is a spontaneous magnetization: in a typical situation volume N will have a magnetization plus with probability 0.5 or minus with probability 0.5, volume $N+1$ again a magnetization plus or minus and so on. The infinite volume limit of these pure states will be a statistical mixture of the plus and the minus states). Physical consistency requires that if a system is in a given phase intensive quantities do not fluctuate, that is possible only if correlation functions are clustering.

For a class of models (i.e., models without quenched disorder with translational invariant Hamiltonians) it has been established that, if translational invariance is not spontaneously broken, the equilibrium state obtained as the infinite volume limit of finite volume states can be decomposed in an unique way as the convex combination of translational invariant states, in which the clustering property is satisfied. This is a remarkable result. This procedure has been generalized by introducing local equilibrium states (DLR states[43]) for an infinite system with short range Hamiltonian. A DLR state satisfies all the identities on conditional probabilities that would be valid for a Boltzmann–Gibbs state and involve only a finite number of variable. The DLR states form a convex set and their extremal points are clustering pure states. To find the structure of all extremal clustering infinite volume states for a given system is a non trivial task, which has been solved only in a few cases (typically for a ferromagnetic model).

This formalism in principle would allow to write formulae of the kind

$$\langle \cdot \rangle_{\mathbf{B\text{–}G}} = \sum_{\alpha} w_{\alpha} \langle \cdot \rangle_{\alpha} \tag{92}$$

where $\langle \cdot \rangle_{\mathbf{B\text{–}G}}$ is the infinite volume limit of the Boltzmann–Gibbs probability distribution defined for finite volume, and α labels the extremal DLR states. The sum must be replaced by an integral if the DLR states are not a numerable set.[14] Of course we are assuming the far from evident existence of $\langle \cdot \rangle_{\mathbf{B\text{–}G}}$.

The proofs which are needed are very simple[15] if one uses the appropriate mathematical setting.[(41)] Hard problems start when one has to show that this construction is not empty, i.e., when one has to prove that local equilibrium states do exist directly for the the actual infinite system without obtaining it as a limit of finite volume measures.[16]

The simplest way to define something in the infinite volume limit is to consider a finite volume system and to show that the infinite volume limit of the Boltzmann–Gibbs probability exists. In this construction there is the freedom to chose the boundary conditions of the system, that could lead to different local equilibrium states. If the boundary conditions are chosen in an appropriate way (e.g., all spins up in a ferromagnet) one obtains a pure state. Unfortunately such a procedure can be carried out only in a very few cases: in general when the volume goes to infinity the Boltzmann–Gibbs probability does not have a limit, at the opposite of what we could naively think (we give a simple example of such a system in Section 7.2).

The proof of the existence of the free energy density in the infinite volume limit for short range lattice systems is quite Simple in the case of non random systems and not too complex for disordered systems. The crucial point in the proof is that we can modify the total Hamiltonian without changing the free energy density by adding a contribution which diverges with the volume, but diverges with a slower rate than the volume itself. It is intuitive that in the infinite volume limit the free energy density cannot depend by any boundary effect (the surface to volume ratio goes to zero).

[14] This happens when a continuous symmetry group is broken. The most familiar example is the Heisenberg ferromagnet, where the DLR states are labeled by an unit vector, giving the direction where the spontaneous magnetization points.

[15] The only delicate point is to prove the clustering property for pure states.

[16] We do not want to arise the point that an actual infinite random system quite likely does not make sense from Brower's constructivistic point of view.

On the contrary when we try to control the expectation values over the probability distribution we find that a change in total Hamiltonian of a quantity of order 1 may completely change the result.

It always true that using compactness argument we can prove that if we consider a sequence of systems inside a box of side L we can find a sequence $L(k)$ (with $\lim_{k \to \infty} L(k) = \infty$), such that the local expectation values go to a finite limit when k goes to infinity.[9] However there can be infinitely many of such sequences, so that in this way we may obtain many different infinite volume expectation values. Given the non constructive nature of compactness arguments it is also difficult to discuss the clustering properties of the resulting states.

The nature and the number of the states of the infinite system is a crucial issue. A priori there RSB Ansatz does not give an answer, that can turn out to be different for different systems: detailed computations and the analysis of theoretical ideas are needed to understand what exactly happens. One has to consider 3 main possibilities: first the number of states can be finite, second it can be infinite with states forming a countable set, and as a third possibility the states can form an uncountable set. The RSB Ansatz applied to the theory of spin glasses turns out to imply that the number of finite volume states of a system becomes infinite in the infinite volume limit. That implies that the second or the third case hold. A detailed computation (see Section 7.5) shows that the third possibility is the correct one.

We will also briefly mention the metastate, which is a powerful mathematical tool. The metastate has been constructed by two different approaches, first in ref. 60 based on averaging over couplings and later in ref. 7 based on a Cesàro average over the volumes, where the two approaches were shown to yield the same metastate. In the latter approach we consider a (reasonable enough) function $f_J^{(N)} \equiv f(\rho_J^{(N)})$ defined on a lattice of volume N and define its Cesàro average as

$$f_J^C \equiv \lim_{M \to \infty} \frac{1}{M} \sum_{N=1}^{M} f_J^{(N)} \tag{93}$$

7.2. The Naive Infinite Volume Limit Does Not Exist

We will give now an example of a situation where the B–G distribution does not have a limit when the volume diverges.[7, 8] We consider a ferromagnetic Ising model with a small random magnetic field and a small temperature in three dimensions.

The heuristic analysis goes as follows. In a finite box there are two relevant finite volume states, the one with positive magnetization and the one with negative magnetization. In a first approximation, valid at small field and temperature, the difference in free energy of the two states is proportional to $2\sum_i h_i$, which is a number of order $N^{3/2}$. Therefore (but for rare choices of the random field) fores a given value of L one state will dominate. However when increasing L one will switch an infinite number of times from the situation where the magnetization is positive to a state with negative magnetization. The magnetization itself does not have a limit when the volume goes to infinity.

A definite limit may be obtained by taking the limit by subsequences (i.e., choosing only those value of L for which the magnetization is positive or negative). The other possibility is in taking the average over L and using the fact that the Cesàro limit (93) of m exists.

Once the infinite volume limit has been taken we can decompose the state in extremal DLR states. Here the typical relevant states for the infinite volume limit are those with positive or negative magnetization. If we choose the first approach (limit by appropriate subsequences) we will find a pure state that is a clustering state. In the case of the Cesàro limit we will obtain a 50% mixture of the two extremal states.

Similar and more complex phenomena are frequent both in random and in non random system (e.g., those having quasi periodic ground states). Care is needed in order to obtain the infinite volume limit. Statements about chaoticity are basically about the fact that the naive infinite volume limit does not converge (see refs. 4 and 7, 8, and 50).

7.3. Non Self-Averageness and the Infinite Volume Limit

At this stage it is clear that we need a lot of ingenuity in order to be able to define the B–G distribution for an infinite system.

The replica approach only deals with very large but finite systems, and it does not ask what happens in an actual infinite systems. It should also be clear that the two approaches, the replica analysis of the finite volume correlations functions (and the results which can be stated in a simple and intuitive way by using the idea of decomposition into states of the Boltzmann–Gibbs measure) and the construction of pure states for an infinite system, give different information, which can be hardly compared one with the other.

In the replica method one obtains information only on those states whose weight w does not vanish in the infinite volume limit.[17] All local

[17] As it stands this sentence may be misleading because it could seem to describe the properties of a given state when we change the volume. A more precise (but heavier) formulation is the following: for each system with large fixed volume N the replica method gives information on the states (defined for that particular model) whose weight w is not too small.

equilibrium states have the same free energy density: however the differences in the total free energy may grow as $L^{(D-1)}$. From an infinite volume point of view all these states are equivalent, while from a finite volume point of view only the state with lower free energy and the states whose total free energy differ from the ground states by an amount of order one are relevant.

For example in the ferromagnetic case (in more than two dimensions at sufficient low temperature) there are equilibrium states which have positive magnetization in half of the infinite volume and negative magnetization in the other half.[7] These states are invisible in the replica method because their weight (when restricted to a finite volume system) goes to zero as $\exp(-AL^{D-1})$, A being an appropriate constant (as we have already discussed special techniques, i.e., coupling replicas, may be used to recover, at least partially, this information). In the replica method the states are weighted with the corresponding Boltzmann–Gibbs weight and this weight can be hardly reconstructed from an analysis done directly at infinite volume (but see ref. 8 for a different point of view).

Therefore one cannot expect a priori that formulae like the relation (35) are valid in the infinite volume limit (although that could happen): on the contrary, according to the facts we have discussed in the last paragraphs, one would better expect that the mathematical properties of an infinite system could be quite different from the ones of a finite large system. The usual formalism of the replica theory does not concern the properties of the states of an actual infinite system.

7.4. A Comparison of the RSB Theory with Some Rigorous Results

In a recent paper[9] the authors have obtained new exact results about the behavior of finite dimensional spin glasses. Here we discuss this interesting issue in some detail, and we observe that these results are in perfect agreement with the predictions of the RSB Ansatz that we have been discussing in the former sections. We will stress how important it is to be careful to the real meaning of the objects that are defined.

- We consider a spin glass at low temperature. The system is in a box of side L, volume $V=L^D$, with fixed boundary condition. The Hamiltonian depends on a set of quenched variables J. We consider the overlap q and its probability distribution $P_J(q)$. In the spin glass phase the function $P(q)$ (9) is not a simple delta function, but it has a more complex structure.

- If the function $P(q_1)$ is not a delta function, one finds that the function $P_J(q_1)$ does depend on J and it is not a self-averaging quantity. In other words the quantity $P(q_1, q_2) \equiv \overline{P_J(q_1)\, P_J(q_2)}$ is not given by the product $P(q_1)\,P(q_2)$ (rigorous arguments in this direction have been recently given in refs. 5 and 6).

• In the same realization of the quenched random couplings we consider two systems which have a mutual overlap $\bar{q}$ in the $L \to \infty$ limit. In this case the probability of finding a region of size R where the overlap is $p \neq \bar{q}$ goes to zero as $\exp(-R^{\alpha} f(p, \bar{q}))$. The authors of ref. 61 have estimated the exponent α to be equal to $(D - \frac{5}{2})$.

• In the infinite volume limit the two spin configurations σ and τ defined with quenched disordered couplings J which differ in a finite (arbitrarily small) portion of the lattice links turn out to have an overlap which is always equal to the minimum allowed overlap q_m.[62]

The work of ref. 9 describes an apparent contradiction with the results of the RSB Ansatz. In ref. 9 the authors give two new definitions of a probability distribution of the overlaps q (which we indicate, with abuse of language, again by $P_J(q)$). Such $P_J(q)$ do not depend on J in the large volume limit. The point we want to stress is that the objects that the authors define are different from the ones we usually encounter in the literature. Such J-independence turns out to be in perfect agreement with the RSB Ansatz.

Let us list the predictions of the RSB approach for the quantities that are defined in ref. 9. The authors present different constructions: we will analyze them trying to translate them in a lay language.

We consider a system of size L, and we focus our attention on what happens in an internal box of size R. We call q_R the overlap of two replicas in this box. We call I the couplings inside the box and E those outside the box. The couplings J are determined by E and I ($J = I \oplus E$).

Following the first construction of ref. 9 we define

$$P_I^{(1)}(q) \equiv \int d\mu(E)\, P_J^R(q) \tag{94}$$

where $P_J^R(q)$ is the probability distribution of the overlap q_R, i.e., of the overlap restricted to the region R.

Let us first send $L \to \infty$, or if we prefer, let us consider the case $L \gg R$. When R goes to infinity, still being much smaller than L, replica theory implies that q and q_R are equal: the equality of these two quantities has been discussed in detail in Section 2.2 and it is a consequence of the clustering properties of the correlations function in the ensemble at fixed q. As a consequence $P_I^{(1)}(q)$ coincides with $\int d\mu(E)\, P_J(q)$. This last integral does not depend on I, so for large R replica theory predicts that

$$P_I^{(1)} = P(q) \tag{95}$$

and it is independent from I, in perfect agreement with the general results proven in ref. 9.

Let us discuss a second definition, $P^{(2)}(q)$, which is inspired by the second construction of ref. 9. Here things become more interesting because we have a construction for the B–G measure in the infinite volume limit as the convergent limit of measures of finite volume. If we skip technical details the main idea is the following. As in the previous case we consider a system of size L and we concentrate our attention on what happens in a box of size R. We call I the couplings inside the box and E those outside the box. If $\mathscr{C}$ is a configuration of the spins inside the smaller box and $\mathscr{D}$ that of the spin outside the box we can define a probability

$$P_I(\mathscr{C}) \equiv \overline{P_{I \oplus E}(\mathscr{C} \oplus \mathscr{D})} \tag{96}$$

where the upper bar stands for an average over the external couplings E and the external spins $\mathscr{D}$. In other words we consider a system of size R and we average its properties over the external world. (Compactness argument may be used to prove that the probability distribution $P_I(\mathscr{C})$ has a limit (as usual at least by subsequences) when L goes to infinity first and R goes to infinity later. Let us call the corresponding state $\rho_J^{\text{B–G}}$.

Armed with this infinite volume probability for an infinite system one can compute the probability distribution of the overlap and one can prove that it does not depend on the internal couplings I. This would be hardly a surprise because we have obtained this B–G distribution by an average process over an infinitely large system, which naturally destroys non-self-averageness. If we compute it in the framework of the RSB approach we find that the overlap is always zero.

The argument runs as follows: we consider two systems, one with couplings $J_1 = I \oplus E_1$ and the other with couplings $J_2 = I \oplus E_2$ (i.e., the couplings are equal in the internal box and different in the external box). We consider the distribution probability of the overlaps q_R and q among a configuration of the first system and a configuration of the second system, the first overlap (q_R) being restricted to the region of size R (where the couplings are I for both systems). we introduce the corresponding probability distributions which obviously depend on the couplings I, E_1 and E_2. We define

$$\begin{aligned} P_I^{(R2)}(q_R) &\equiv \int d\mu(E_1)\, d\mu(E_2)\, P^R_{I,\,E_1,\,E_2}(q_R) \\ P_I^{(2)}(q) &\equiv \int d\mu(E_1)\, d\mu(E_2)\, P_{I,\,E_1,\,E_2}(q) \end{aligned} \tag{97}$$

Also in this case $P_I^{(R2)}(q_R)$ and $P_I^{(2)}(q)$ coincide in the large R limit. $P_I^{(2)}(q)=\delta(q)$, due to the chaotic nature of spin glasses. $P_I^{(2)}$ is independent from I, as proven in ref. 9, and it is different from $P_I^{(1)}$.

It is clear that there are alternative definition of the function $P(q)$, which are less interesting as far as they display a less rich behavior. The reader should notice that it is only a bad notation to call these functions with the same name, as far as they describe very different properties of the system.[18] In studying the properties of all these functions the RSB approach gives the correct answer, i.e., it declares self-averaging objects which are self-averaging and non-self-averaging quantities that are likely to be non-self-averaging.

7.5. On Infinite Volume States

We will discuss here about some rigorous results,[60, 7] that have been used to allow a construction of the infinite volume limit of the quenched state. There are two main possibly starting points for such a task: the first is the construction described in the previous section, where we average over the couplings in an external region. This approach generates the states that we have called $\rho_J^{\text{B–G}}$. In the second approach (which can be used for the construction of the metastate, see below) we consider periodic boxes of size L, and we denote by $\rho_J^{(L)}$ the expectation value with respect to the usual B–G distribution. Using Eq. (93) we define the quenched state as the Cesàro average ρ^C. Both procedures construct the infinite volume quenched state. One can prove[8] that the two constructions lead to the same infinite volume equilibrium state. If one changes the boundary conditions, e.g., if one uses antiperiodic boundary conditions, the result will not change.[12] In this way we have a natural definition of an infinite B–G state, which however involves in one way or another some kind of average.

It is crucial to note that the limits mentioned before should be read in a weak sense. In other words for any given quantity A which is a function of only a *finite* number of spins we have that

$$\rho_J^C(A)=\lim_{M\to\infty}\frac{1}{M}\sum_{L=1}^{M}\rho_J^{(L)}(A) \tag{98}$$

This equality does not have to hold for observable quantities which contain an explicit L-dependence.

[18] It would be not wise to conclude that they must have the same properties because they have been called with the same name.

This equilibrium state can be decomposed into extremal DLR states (which we label by the index λ). We have

$$\rho_J^{\text{B–G}} = \int d\mu(\lambda)\, \rho_J^{\lambda} \tag{99}$$

In this way we find a natural measure $d\mu(\lambda)$ over the extremal states. This measure is not yet the metastate. In order to obtain the metastate we have to consider not only the expectation values themselves, but the products of expectation values. At this end we can define

$$\rho_J^2(A, B) = \lim_{M \to \infty} \frac{1}{M} \sum_{L=1}^{M} \rho_J^{(L)}(A)\, \rho_J^{(L)}(B) \tag{100}$$

One finds that[60, 7]

$$\rho_J^2(A, B) = \int dv(s)\, \rho_J^s(A)\, \rho_J^s(B) \tag{101}$$

where s denotes a generic state (pure or a mixture) and $v(s)$ is a measure on the states. This measure is called the *metastate* and it is the generalization of the measure $\mu(\lambda)$ defined in Eq. 99. This construction may be generalized took the products of more expectations values.

The results of the RSB Ansatz imply that the set of states on which this measure $\mu(\lambda)$ is concentrated cannot be countable. Indeed if that was the case the previous formula (Eq. 99) could be written as

$$\rho_J^{\text{B–G}} = \sum_{\lambda=1}^{\infty} w(\lambda)\, \rho_J^{\lambda} \tag{102}$$

and the probability of finding two configurations in the same pure state would be given by

$$\sum_{\lambda=1}^{\infty} w(\lambda)^2 > 0 \tag{103}$$

But we have shown in the previous discussion that the RSB theory predicts that the overlap distribution in the state $\rho_J^{\text{B–G}}$ (the quenched state) is a delta function at zero overlap, so that the probability of finding two configurations in the same pure state must be zero, in contradiction with the previous formula.

We are ready now to illustrate the main flaw of a series of papers (see refs. 12, 9 and references therein), where the metastate approach was used to claim the presence of an internal inconsistency in the predictions of the RSB theory. The starting point of these papers was the heuristic assumption that the finite volume state can be approximately decomposed as the sum of infinite volume states:

$$\rho_J^L \approx \sum_{\lambda=1}^{\infty} w^L(\lambda)\, \rho_J^\lambda \tag{104}$$

This formula looks innocent and similar to the one that it is used as a starting point of the RSB approach, (35), but it is indeed rather different: in the RSB theory the sum in the r.h.s. runs over the *finite volume states*, while in (104) the sum runs over the *infinite volume states.*

Before further discussing if the heuristic results of refs. 12, 9 are correct we should investigate if their starting hypothesis (104) makes sense. We will show here that (104) can be sometimes (not always) correct for ferromagnets, but it is unnatural when dealing with spin glasses (see also ref. 7 for earlier work on the invisibility of the interface states). In the case of spin glasses equilibrium configurations of a system of size L with periodic boundary condition when embedded in a larger system will have a much higher energy than the equilibrium configurations. Naively one would expect an energy increase on the surface of the order of L^{D-1}, but the actual increase may be smaller due to possible adjustments of the interface. The spins at $i=1$ and $i=L$ would be chosen in such a way to minimize the free energy with periodic boundary conditions, but would be out of place when merging the spin configuration in a larger system.

The previous formula also fails in some ferromagnetic cases. Let us consider the case which we have discussed before in Section 2.3 of a ferromagnet with antiperiodic boundary conditions. We consider the three dimensional case, with temperature not too far from the critical one (or equivalently the two dimensional case). In these conditions the interface is rough and it has a width increasing like $L^{1/2}$ in three dimensions (in two dimensions the width is always proportional to $\log(L)$).

The divergence of the width of the interface has absolutely no consequences on the analysis of states in finite volume (we classify the configurations in states by the average position of the interface; the correlation functions are clustering but for a region close to the interface, which can be neglected since it is a fraction of the volume which asymptotically goes to zero), but it implies that in the infinite volume limit there are only two pure equilibrium states: the ones with uniform positive and uniform negative magnetization. The state with positive magnetization in half space and negative magnetization in the other half space exists only when the interface is not rough. That shows that the relation (104) is not satisfied even in this very simple case.[19] The opposite conclusion would be valid in three dimensions (but not in two dimensions) at positive temperatures smaller than the roughening temperature, because in this case the interface would have a finite width also in the infinite volume limit.

Of course it is true that the probability distribution $P_J^{R,L}$ of the variables in a region of fixed size R inside a box of size L with periodic boundary conditions can be written as

$$\rho_J^{R,L} \approx \int d\mu_J^{R,L} \rho_J^{\lambda} \tag{105}$$

where $L \gg R$, $\rho_J^{R,L}$ is the state associated to $P_J^{R,L}$, and the difference among the r.h.s. and the l.h.s. goes to zero when L goes to infinite.[20] As we have discussed it is crucial that (105) fails in many cases for $R = L$. In the replica approach $\rho_J^{L,L}$ plays a central theoretical role, and the other probability distributions (e.g., $\rho_J^{R,L}$ for $R < L$) are derived quantities.

The existence of rigorous arguments which prove that the relation (104) cannot hold even in some simple cases, and of heuristic arguments which imply that it is not valid for spin glasses, strongly suggests that it would be unwise to use it as the starting point of any argument. It is not a surprise that this formula (which is one of the starting points of the non-standard SK picture) leads to contradictory conclusions. The true RSB Ansatz (the so-called SK picture or mean field picture) that we have discussed in the previous sections (and that, following the wording of refs. 9 and 12, is different both from what refs. 9, 12 call the standard SK picture and from what they call the non-standard SK picture), does not lead to obvious contradictions: as far as we know there are no generic arguments which question its validity.

The metastate approach, is telling us something about the behavior of the properties of a fixed region of space in the infinite volume limit (essentially that there is a natural way to define such a limit if we average over the appropriate regions). This allows us to introduce a natural measure over pure DLR states. However this infinite volume states are states in presence of a quenched random environment: they are different from the

[19] A similar analysis of the $3D$ ferromagnet implies that (104) is never valid if we take antiperiodic boundary conditions in two directions, e.g., x and y.

[20] To claim that the r.h.s. goes to the l.h.s. when L goes to infinity would be incorrect, because both sides of (105) do not have a limit when $L \to \infty$: only their difference (which goes to zero) has a limit.

finite volume states of the replica theory and they are not directly related to the global behavior of systems in a finite volume.

As stressed in ref. 63 and in ref. 54 the crucial problem in order to compare the rigorous approach to the RSB Ansatz predictions consists in studying the behavior of the probability distribution of two (or more) identical replicas, $P(\sigma, \tau)$ and to verify the existence of correlations among the replicas. In particular if we study a system with the n-replicated Hamiltonian (3), with positive integer n, we can construct the infinite volume probability distribution for this n-replicated system. The predictions of the replica approach can be translated in predictions about the values of the overlaps among these replicas. Replica symmetry breaking corresponds to the existence of correlations among replicas which can be exposed by introducing additional replicas.

More precisely we can Consider a system done of n real replicas of size L. We concentrate our attention on what happens in a box of size $R<L$. We consider the $n \times n$ matrix $q_R^{a,b}$ of the overlaps in the box of size R. Using the same notation as before we define:

$$P_I(\mathbf{q}) \equiv \int d\mu(E)\, P_J^R(\mathbf{q}) \tag{106}$$

where $P_J^R(\mathbf{q})$ is the probability distribution of the overlap matrix $q_R^{a,b}$.

The probability distribution should go to a finite limit when $L \to \infty$ first and $R \to \infty$ later. We can also consider the probability distribution of only some elements of this matrix. In particular we have already remarked that $P(q_{1,2})$ coincides with the probability distribution $P(q)$. Moreover (and this is a crucial issue) the fact that $P_J^L(q)$ depends on J translate in this language as a lack of factorization of this probability:

$$P(q_{1,2}, q_{3,4}) \neq P(q_{1,2})\, P(q_{3,4}) \tag{107}$$

Spontaneous replica symmetry breaking corresponds to a non-independence of the replicas and to the presence of correlations among them. It is possible to translate the predictions of the RSB Ansatz into this formalism, which can be also used to prove udder general assumptions the validity of relations like (14).[5, 6]

One can obtain similar results also using the metastate, defining

$$P^R(\mathbf{q}) \equiv \lim_{M \to \infty} \frac{1}{M-R} \sum_{L=R}^{M} P^{R,L}(\mathbf{q}) \tag{108}$$

and sending $R \to \infty$ at the end.

This approach is promising. The framework can also be used for studying systems without quenched disorder.[(64)] Using this formalism it is possible to investigate the issue of replica symmetry breaking also for systems without disorder like structural glasses. For reasons of space we will not discuss here this important point in more details.

8. NUMERICAL RESULTS

In this last part of the paper we will review briefly the large mass of numerical results that support the fact that replica symmetry is spontaneously broken in finite dimensional spin glasses. In particular we will discuss numerical results for the three and four dimensional Ising spin glass with Gaussian couplings and with binary couplings (that can take the two values ± 1).

We will extract from published papers only those evidences which are relevant to show that the real finite dimensional systems behave as implied from the predictions of the RSB Ansatz, and we will refer to the original references for more details. We will also discuss some new numerical results (about a precise determination of the finite size effects that affect the infinite volume sum rules of the theory and about simulations with coupled replicas) that we will describe here in detail.

We notice that the biggest systems which are fully thermalized in numerical simulations contain at most 10^4 spins. This number is not very different from what can be realized experimentally: there are some indications that in a typical experiment it is possible to thermalize only regions containing 10^5 spins at most.[(57)] If replica predictions would fail for systems of size bigger than 10^6, this fact would be unobservable both in computer simulations done with the present computer technology and (more important) in real experiments.

8.1. The Phase Transition

In this section we have chosen four figures in order to make clear some basic facts, i.e.:

1. The $3D$ EA spin glass undergoes a true phase transition (Fig. 1).
2. The Edward–Anderson order parameter does not vanish in the thermodynamical limit (Figs. 2 and 3).
3. The low temperature phase is mean-field-like (Figs. 2 and 4).

In the next paragraphs we will discuss these three issues in better detail. For a complete discussion we address the reader to refs. 18, 34, and 35.

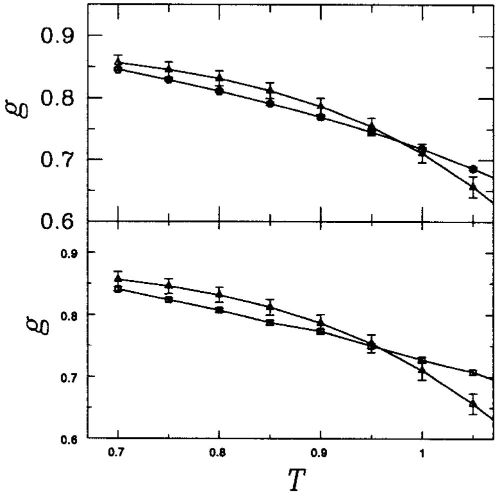

Fig. 1. The Binder cumulant versus T for the $3D$ Ising spin glass with Gaussian couplings. In the upper figure we show the crossing of the $L=8$ and $L=16$ curves. In the lower figure are the crossing of the curves for $L=4$ and $L=16$.

In Fig. 1 we show the best available evidence for the existence of a phase transition. We plot the Binder cumulant g defined as

$$g \equiv \frac{1}{2}\left(3 - \frac{\overline{\langle q^4 \rangle}}{\overline{\langle q^2 \rangle}^2}\right) \tag{109}$$

The crossing of the curves of the Binder cumulant for different lattice sizes is considered as the standard signature of the existence of a phase transition. This evidence has been first given by Kawashima and Young,[32] and is also supported by calculations of Berg and Janke.[33]

As discussed in detail in the literature (see for example ref. 18) the $3D$ case is atypical, in which we sit very close to the lower critical dimension D_c^L. The signature for a transition we have shown in 1 is indeed atypical, since more than a crossing of the different Binder parameter curves we observe a merging. Again, this is a signature of the fact that D_c^L is very close to 3. For example in the $4D$ spin glass[65, 66] the crossing is a very typical, clear cut crossing of the type one finds for the usual Ising model.

After establishing the existence of a phase transition we want to characterize the low T phase. A replica symmetry broken phase has to be characterized by establishing in a clear way its peculiar properties in the infinite volume limit.

For the (as we already said atypical) case of the $3D$ spin glass, we start by discarding the possibility, suggested by the little separation between different Binder cumulant curves for $T < T_c$, of the presence of a Kosterlitz–Thouless phase transition without a non-zero order parameter. In this case the order parameter would become zero, in the infinite volume limit, even in the low T region. We have computed the probability distribution of the overlap, that we show in Fig. 2. Using these probability distributions we have computed the behavior of the positions of the maximum as a function of the lattice size for a temperature well below T_c, as shown in Fig. 3. From Fig. 3 it is clear that the possibility that $\lim_{L \to \infty} q_M = 0$ is unnatural (the power -1.5 that we use in the horizontal scale comes from a best fit to the data). Our best fit to the form $q_\infty + a/L^b$ (that we have also plotted in Fig. 3) gives us an infinite volume order parameter, $q_{\rm EA} = 0.70 \pm 0.04$ very close to the estimate one finds using dynamical methods (given by the q value where the equilibrium regime ends, see Fig. 21 and later in the text). In spite of this accurate estimate, and of the strong qualitative evidence suggested by Fig. 3, a fit with $q_\infty = 0$ and a convergence with a very small power exponent (i.e., 0.2) would have a greater χ^2 but cannot be excluded from our data.

Once we have characterized the transition point and we have ruled out the scenario of a transition with no order parameter we show our evidence of a broken replica symmetry in $3D$ spin glasses.

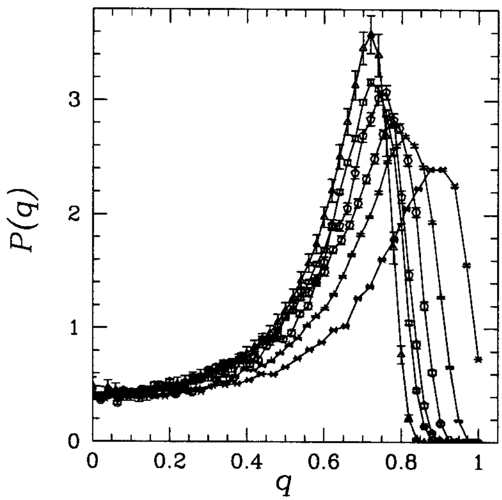

Fig. 2. The probability distribution of the overlap for the $3D$ ising spin glass with Gaussian couplings below the critical temperature ($T = 0.7 T_c$). The data are for $L = 4$, 6, 8, 10, 12 and 16 and increasing the size the peak becomes sharper and higher.

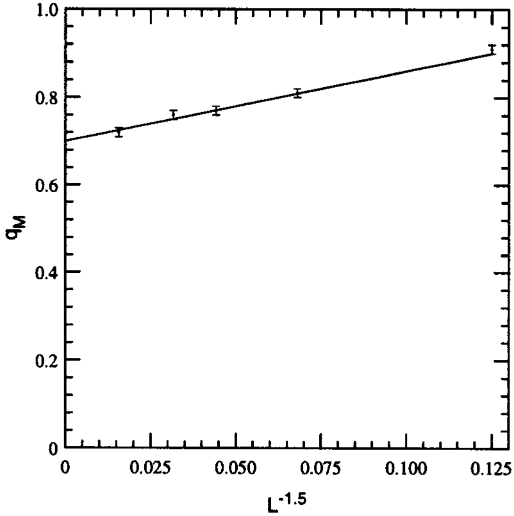

Fig. 3. The value q_M where $P(q)$ is maximum versus $L^{-1.5}$ in the $3D$ ising spin glass with Gaussian couplings below the critical temperature ($T = 0.7T_c$).

We plot in Fig. 4 the value of the Binder cumulant at $T = 0.7T_c$ as a function of the lattice size. In an usual ferromagnetic phase this points extrapolate to 1 in all the broken phase, for $T < T_c$. It is clear from the figure that in our data we do not see any evidence of such a limit value. In a broken replica symmetry phase one predicts, on the contrary, a non trivial shape of $P(q)$ in the whole broken phase, and a non one limit of the Binder parameter, that is, according to Fig. 4, far more plausible.

For sake of completeness we report here our best estimates of the critical exponents and for the critical temperature:

$$T_c = 0.95 \pm 0.04, \qquad \nu = 2.00 \pm 0.15, \qquad \frac{\gamma}{\nu} = 2.36 \pm 0.06 \tag{110}$$

These estimates of ν and γ agree very well with those of refs. 32, 33 for the $3D$ model with binary couplings.

8.2. Sum Rules

We describe here some original work dealing with numerical verification (in the finite dimensional case) of some typical sum rules first derived for mean field spin glasses.[26, 5, 6, 54]

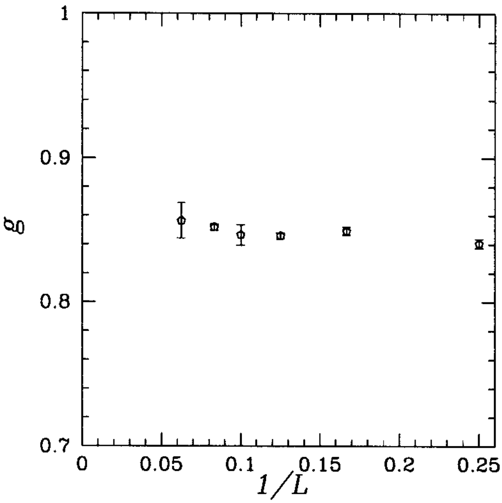

Fig. 4. The Binder cumulant as a function of L for the $3D$ Ising spin glass with Gaussian couplings below the critical temperature ($T = 0.7T_c$).

These equalities are related to the stochastic stability of the system, and give relations among the joint overlap averages of *real replicas* (i.e., a finite number of copies of the system in the same realization of the quenched disorder). One can show[5] that under very general assumptions of continuity (that turn out to be well verified[67]) they are also valid in finite dimensional models. In the following we will show numerically, through Monte Carlo simulations, that they are very accurately verified in the $3D$ Ising spin glass with binary couplings.

We define by

$$E(\cdots) \equiv \overline{\langle \cdots \rangle} \tag{111}$$

the global average, taken both over the thermal noise and over the quenched disorder. In the infinite volume limit the following equalities, among others, hold:

$$E(q_1^2, q_{3,4}^2) = \tfrac{2}{3} E(q_{1,2}^2)^2 + \tfrac{1}{3} E(q_{1,2}^4) \tag{112}$$

$$E(q_{1,2}^2 q_{2,3}^2) = \tfrac{1}{2} E(q_{1,2}^2)^2 + \tfrac{1}{2} E(q_{1,2}^4) \tag{113}$$

In order to study this problem we have run simulations of the $3D$ Ising spin glass with binary couplings (that allows 32 or 64 systems to be updated at the same time, with a large amount of computer time saving).

Table I

L	Thermalization	Equilibrium	Samples	N_β	δT	$T_{\min}$	$T_{\max}$
6	50000	50000	2048	19	0.1	0.5	2.3
8	50000	50000	2048	19	0.1	0.5	2.3
10	70000	70000	2048	37	0.05	0.5	2.3
12	70000	70000	2048	37	0.05	0.5	2.3

We have used the *parallel tempering* technique[68–70] that allows to thermalize large systems deep in the broken phase. Thanks to Cray T3e runs of a multi-spin-coded program we have been able to obtain a very high statistics. For each value of the lattice size $L = 6, 8, 10, 12$, we have considered 2048 different realization of the quenched disorder to define the sample averages. For each sample we have simulated 4 replicas with separate and independent evolutions. At every sweep we have measured the energy and the mutual overlaps of the four replicas. Monte Carlo simulation parameters such as the number of sweeps used for thermalization, the number of sweeps during which observables were measured, the number of samples, the number of β values allowed in the parallel tempering procedure,[69, 70] the minimum and maximum T value and the temperature increment are summarized in in Table I.

The temperature swapping process (the parallel tempering needs this condition to be satisfied in order to have an acceptable efficiency). The allowed temperature range (assuming $T_c \simeq 1.1$ as in refs. 32 and 71) is approximately $0.5T_c < T < 2T_c$.

Let us now discuss the results. In Fig. 5 we plot the quantity

$$1.0 - \frac{2/3E(q_{12}^2)^2 + 1/3E(q_{12}^4)}{E(q_{12}^2 q_{34}^2)} \tag{114}$$

(i.e., 1 minus the ratio of the left hand side and the right hand side of the equality (112)) versus T for each value of L. As it should be at high temperature the limiting value is $-2/3$, since in the high T region $P(q)$ is a Gaussian centered around $q = 0$. Conversely at low T the content of Eq. (112) is highly non-trivial. there the function $P(q)$ is not a simple δ-function: it is non-trivial, and for example $E(q^4) = O(1)$ and it differs from $E(q^2)^2$ of a quantity of order 1 (typically in the low T phase their difference is of order 30%). It is very appealing that in this regime (112) is verified up two significant digits, as can be deduced from Figs. 6 and 7.

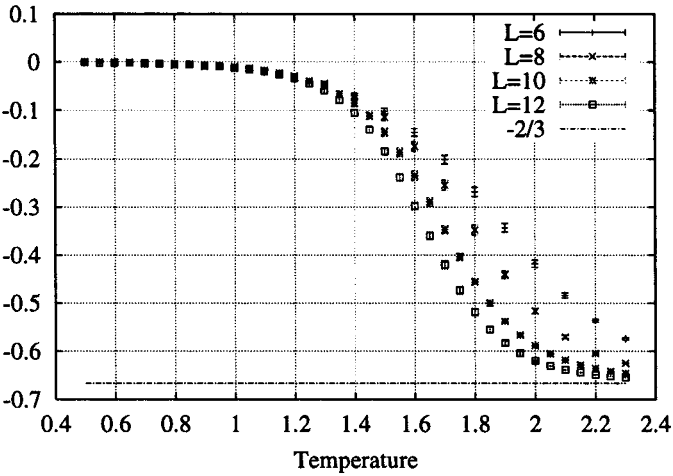

Fig. 5. The quantity (114) versus T for different values of L.

Figure 6 shows that in the broken phase the relation (112) is satisfied in a non-trivial way (i.e., not through $0 = 0$). For high T values (112) just tells us that zero equal zero, but in the broken phase the left hand side and the right one are non-zero (we have already shown that by finding that the value of q_M such that $P(q_M)$ is maximum does not go to zero when $L \to \infty$, and Fig. 6 confirms it.

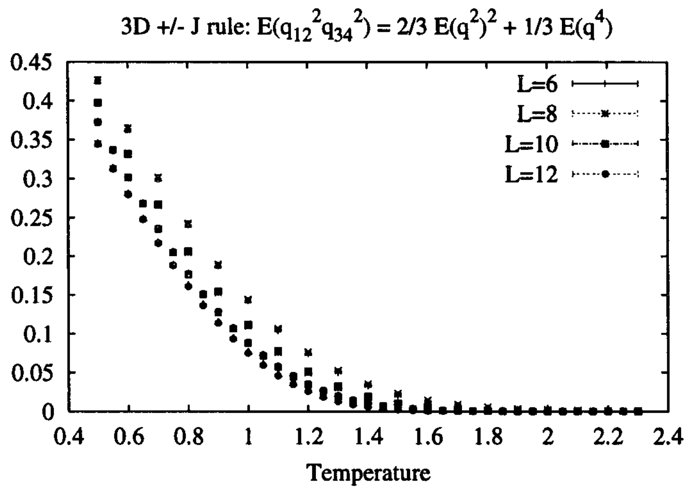

Fig. 6. The (indistinguishable on this scale) left hand side and right hand side of the relation (112) for different values of L. For all values of L on this scale the curves are perfectly superimposed within the error bars.

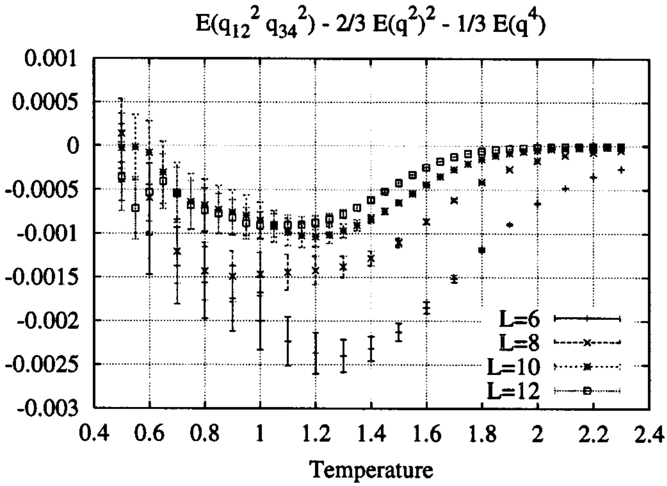

Fig. 7. Difference between the left hand side and the right hand side of the relation (112) versus T for different values of L.

Figure 7 shows us how relation (112) is violated on a finite lattice. Clearly (112) is exact in the infinite volume limit, and one get finite size corrections on finite lattices. It is remarkable that these corrections are already small on small lattices: they are maximum close to the critical point, decrease when going far from T_c, and go smoothly to zero with increasing lattice size.

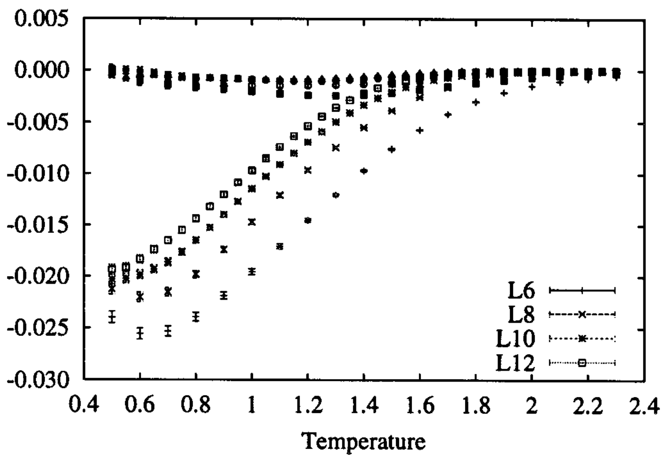

Fig. 8. As in Fig. 7, but we also plot the quantities (115) for different values of L.

The cultivated reader can notice that relation (112), for example, is also satisfied in' a droplet like situation, where all the relevant expectation values are constant. In order to stress the difference among this situation and the one observed in numerical simulations we replot in Fig. 8 the same curves of Fig. 7, adding the quantities

$$E(q_{1,2}^2 q_{3,4}^2) - \tfrac{1}{3} E(q_{1,2}^2)^2 - \tfrac{2}{3} E(q_{1,2}^4) \qquad (115)$$

where we have interchanged the factors $\frac{1}{3}$ and $\frac{2}{3}$, by putting them in the wrong places. In a droplet picture this relation would work as well as relation (112): Fig. 8 shows clearly that this is not the case, as is implied by a RSB picture. Only in the warm phase both realizations are satisfied (trivially, since all the relevant expectation values are zero in the infinite volume limit).

The results related to the equality (113) are even more appealing. Here at least 3 real independent replicas are needed to implement (113) ((112) can also be implemented with only two real replicas, since $E(q_{1,2}^2 q_{3,4}^2) = \overline{\langle q^2 \rangle^2}$). These three replicas are Constrained by the ultrametricity constraints: the fact that the relation (113) is verified in $3D$ with an accuracy of two significant digits is a strong hint toward the existence of a non-trivial (ultrametric) structure of *pure states* in realistic short-range models.

As before the high T region of Fig. 9 tells us that in the high T phase $P(q)$ is Gaussian, while the low T is not.

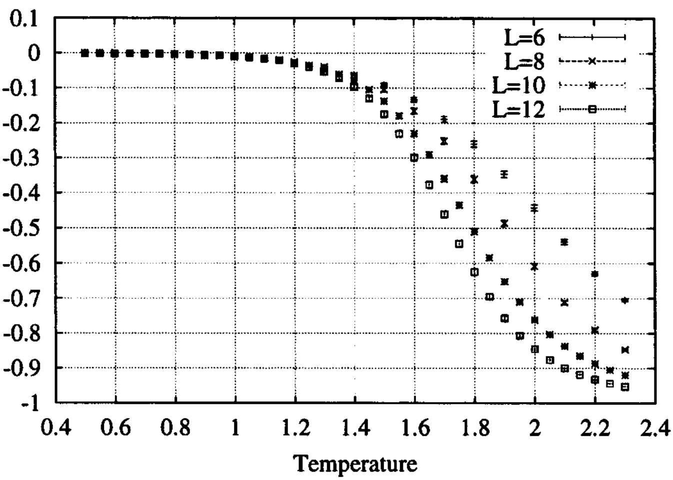

Fig. 9. As in Fig. 5 but for the relation (113).

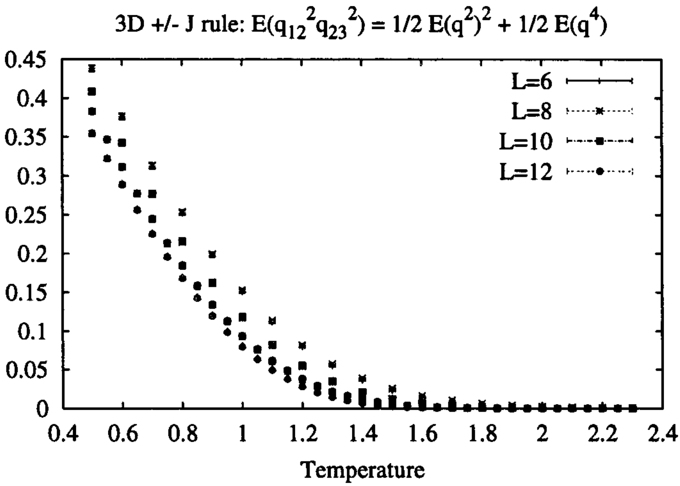

Fig. 10. As if Fig. 6 bur for the relation (113).

Figure 10 shows (like Fig. 6 does for (112)) the values of the two sides of the relation (113). The numerical values are again perfectly superimposed within the limit of our statistical errors.

Finite size effect related to (113) are shown in Fig. 11. Also here the same discussion done for Fig. 7 is valid.

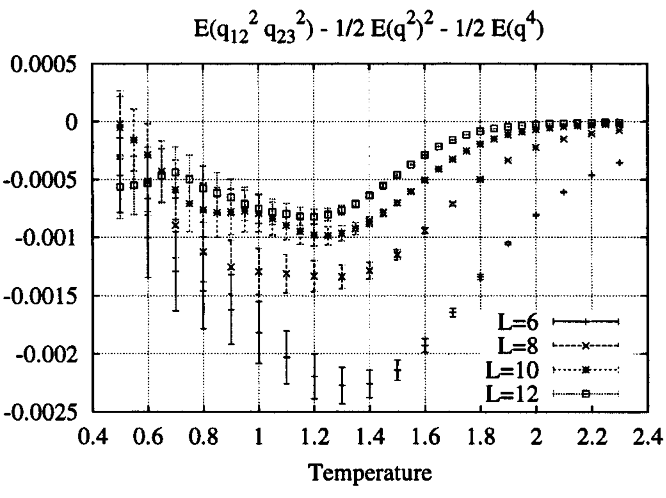

Fig. 11. As in Fig. 7 but for the relation (113).

We have always estimated the statistical errors that we have used in our plots by using a direct jack-knife analysis (see for example ref. 72). The amount of the violation of the sum rule that one can see in Figs. 7 and 11 close to T_c decreases in a statistically significant way with L: scaling fits are possible, and a power law explains it all, but there are not enough points (and the statistical error over such a very small number is not small enough) to make the fit reliable.

8.3. Correlation Functions

In this subsection we study the equilibrium and the quasi-equilibrium overlap-overlap correlation functions. These results have been published in refs. 73 and 34. We have discussed the issue of correlation function in the RSB formalism in Section 2.2: we will discuss here a few numerical results supporting our theoretical framework.

Let us discuss first the definitions of quasi-equilibrium correlation functions. We have run quasi equilibrium simulations following two different procedures. The first method is based on a sudden quench of the system from a $T=\infty$ configuration to $T=T_f<T_c$. In the second approach (an annealing procedure) one starts the simulation at a large value of T and slowly cools the system down to T_f, systematically decreasing the temperature of a small dT. We have always used $T_f=0.7T_c$. In both cases we run a simulation for a very large system of a size L which can be considered infinite in a first approximation. At a given time t we measure the correlations function of the local overlap among two replicas of the systems $(C_L(x, t))$.

We can define the quasi-equilibrium correlation function as

$$C(x)=\lim_{t\to\infty}\left(\lim_{L\to\infty} C_L(x, t)\right) \tag{116}$$

The order of the two limits matters. The overlap density among the two replicas remains zero. It can be argued that $C(x)$ is equal to the equilibrium correlation function of a system where two replicas are constrained to have zero overlap.

We show in Fig. 12 four different curves that represent the $q-q$ correlation function for a $3D$ spin glass with Gaussian couplings, computed using different approaches.

1. The lower curve is the infinite time extrapolation of the correlation function $(C(x, t))$ computed by using the first quasi-equilibrium method described in the previous paragraph.

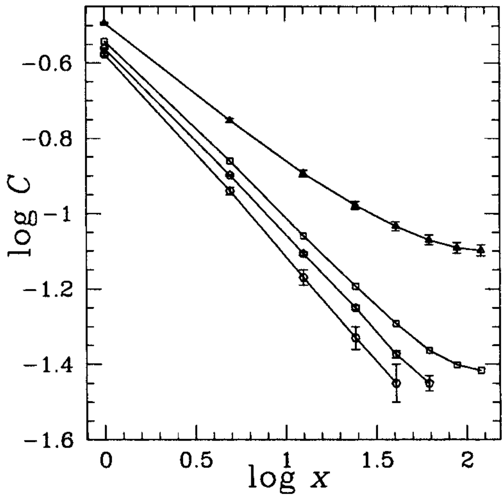

Fig. 12. Correlation functions at equilibrium and quasi-equilibrium for the $3D$ Ising spin glass with Gaussian couplings in a double logarithmic scale. The two lower curves correspond to an quasi-equilibrium simulation with an infinite time extrapolation. The third curve (from the bottom) corresponds to an equilibrium computation selecting couples of configurations with $q \simeq 0$. The upper curve is for the equilibrium correlation function. $T = 0.7T_c$.

2. The next curve (bottom to top in the figure) has been obtained with the second quasi-equilibrium method after an extrapolation to infinite time.

3. The third curve is the equilibrium $q-q$ correlation function at equilibrium computed only on configurations that have a mutual overlap $q < 0.01$.

4. Finally the uppermost curve is the total $q-q$ correlation function at equilibrium without any constraint.

The lowest two curves (quasi-equilibrium curves) have been obtained simulating a very large system ($L = 64$, which does not approaches equilibrium on the time scale of our numerical simulations), while the two upper curves have been obtained at equilibrium (using parallel tempering[68–70]) on a $L = 16$ lattice (so that they can undergo sizable finite size effects, and they surely do when the distance becomes close to $\frac{L}{2}$).

The quasi-equilibrium correlation function does not depend much on the method one uses to estimate it. During the quasi-equilibrium runs, since the lattice size is very large and the initial conditions are random ($T = \infty$, i.e., $q = 0$), the overlap stays zero (in our statistical accuracy) uring the whole simulation. As we have remarked it looks safe to assume that in these conditions the infinite time extrapolation gives us the true equilibrium value restricted to the $q=0$ subspace.

In the infinite time limit $C(x) \propto x^{-\alpha}$ with $\alpha \sim 0.5$. If replica symmetry is broken it is useful to write the correlation function in the form

$$C(x) = \int dq\, P(q)\, C_q(x) \tag{117}$$

where $C_q(x)$ is the correlation function restricted to the set of equilibrium configurations with fixed mutual overlap q.

In the RSB approach $C_q(x)$ depends on q, which can assume any value between 0 and q_{EA}. The two curves obtained via the infinite time extrapolation of the quasi-equilibrium data give an estimate of $C_0(x)$. In the droplet approach the system at equilibrium is supposed: to be always at q_{EA}. If the picture of a droplet phase was valid the $q=0$ three lower curves of Fig. 12 would coincide with the full equilibrium upper curve. On the contrary Fig. 12 shows the clear difference between $C(x)$ and $C_0(x)$.

The $q=0$ correlation functions shown in Fig. 12 are *non connected* (i.e., $\lim_{x \to \infty} C_q(x) = q^2$): the asymptotic value of C_0 is zero in the RSB approach and q_{EA}^2 in the simple Migdal–Kadanoff picture. Computations by de Dominicis *et al.* (see for example ref. 27 and references therein) show that in the RSB approach one expects a pure power law decrease for the $q=0$ ergodic component of the correlation function. The pure power law decrease observed in Fig. 12 is very clear, calling for an asymptotic approach to zero, as in the RSB theory.

The infinite time extrapolation of the quasi-equilibrium correlation functions ($C(x,t)$) coincides indeed with the true equilibrium result. This is clear from Fig. 12 where the three lower curves follow a power law behavior with the same exponent.

An expected discrepancy from a pure power law appears in the large x region for the $L=16$ equilibrium runs. This is the point where the correlation function starts to feel the effect of the periodic boundary conditions (on the large, $L=64$ lattice where we have computed the quasi-equilibrium curves, we expect to observe the effect of the periodic boundary conditions for $\log(x) \simeq 3.5$).

We have also analyzed the probability distribution of $C(x)$ at thermal equilibrium. We have shown in the upper curve of Fig. 12 the expectation value of $C(x)$, but there is more information in the full distribution probability (for fixed x). We show in Fig. 13 the histogram of the $x=2$ component of the equilibrium correlation function. We have also marked in this figure the extrapolated value of the quasi-equilibrium correlation function (the one of the lowest curve in Fig. 12). One can distinguish a clear peak

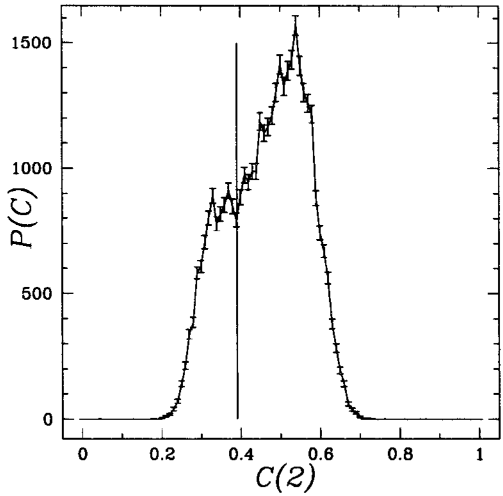

Fig. 13. Probability distribution of the $q-q$ equilibrium correlation function $C(x)$ at distance $x=2$.

(in the region of large $C(2)$ values) and an incipient maxima (or flex point located close to the quasi-equilibrium value.

From Fig. 13 we can extract another interesting conclusion. If we assume, naively, a dependence of the form $C(x) = a(x) + b(x)\, q^2$ and a mean-field-like shape for the $P(q)$ we expect the probability distribution of $C(x)$, to have the form of a double peak shape, with the two peaks located at non-zero value of q. This is what we see in Fig. 13: the equilibrium histogram and the quasi-equilibrium values of the $q-q$ correlation function agree well with all predictions of the broken replica symmetry theory.

8.4. Quasi-Equilibrium Window Overlap

The so called *window overlap* has an important role in qualifying the behavior of the system independently from the boundary conditions. We have already introduced and discussed the window overlaps in Sections 2.2 and 2.3. We will show here some numerical results that help in clarifying the picture.

Let us repeat that the window overlap is computed using only the spins belonging to part of the $3D$ lattice:

$$q_B = \frac{1}{B^3} \sum_{x=0}^{B-1} \sum_{y=0}^{B-1} \sum_{z=0}^{B-1} \sigma(x, y, z)\, \tau(x, y, z) \tag{118}$$

where σ and τ are defined under the same realization of the quenched disorder. We will denote the probability distribution of q_B by $P_B(q)$.

Here we consider the behavior of the window overlap during a quasi-equilibrium simulation (see ref. 73). As usual we start from two random configurations, which we quench suddenly well below the critical temperature. We monitor the value of the window overlap (for different sizes of the small region, B, where we have computed the overlap). By computing its probability distribution, $P_B(q, t)$, we derive the Binder cumulant of $P_B(q, t)$: $g(B, t)$.

We find that the values of $g(B, t)$ collapse on a single curve when using for the dynamical exponent the value found at this temperature by analyzing the correlation functions (see the former section and references therein). In Fig. 14 we show this scaling plot. It is clear that the data collapse very well for all different values of the size of the small region where the overlap was computed. Moreover it is possible to obtain a safe extrapolation for the infinite volume value of this Binder cumulant. We estimate a value of 0.64, that is clearly different from the droplet model prediction, $g = 1$, and is not too far from the value of full volume Binder cumulant g at the critical point.

Recent experimental data[74] find that real spin glasses are well fitted by the same scaling law we have shown in Fig. 14.

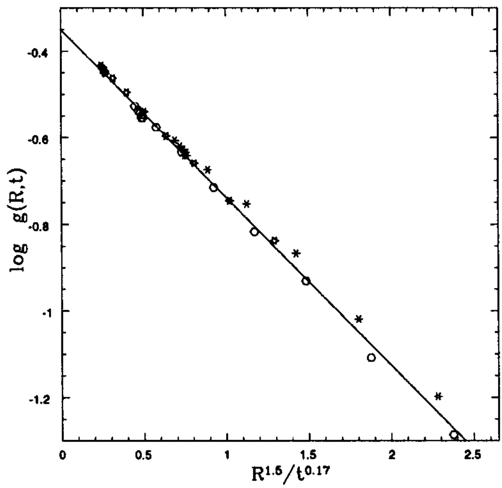

Fig. 14. Logarithm of the Binder cumulant $g(R, t)$ of the window overlap q_R (measured in a cubic box of linear size R) versus the rescaled ratio of the window size R and the Monte Carlo time t. Stars are for $R = 2$, hexagons are for $R = 3$ and asterisks for $R = 4$.

8.5. Equilibrium Window Overlap

Window overlaps have also been analyzed at equilibrium 75. The main goal of such a measurement is to check the theoretical ideas discussed in Sections 2.2 and 2.3: it turns out to give crucial hints about the behavior of the system.

In Fig. 15 we show the probability distribution of the window overlap (measured in a box of volume 4^3) for two different lattices: $L=8$ and $L=12$. If interfaces were playing a crucial role (see the discussion in Section 2.3) one would expect this distribution to tend toward a pair of δ function as $L \to \infty$ for fixed window size B. From Fig. 15 it is clear that this is not the case. The shape of the two probability functions is basically the same independently of the lattice size.

In Fig. 16 we show the probability distribution of the window overlaps as a function of the window size for a fixed lattice size, $L=12$. The shape of the probability distribution does not change much with B (the largest change is when B reaches L, and we recover the usual overlap that is more sensitive to the presence of a finite lattice than smaller observables). Moreover the behavior of the value of the probability distribution near the origin (in the region of small overlaps) is opposite to the one we would get if the model was building a simple droplet structure (i.e., this value does not go to zero for small B values, and it is on the contrary slightly enhanced due to the finiteness of the window size).

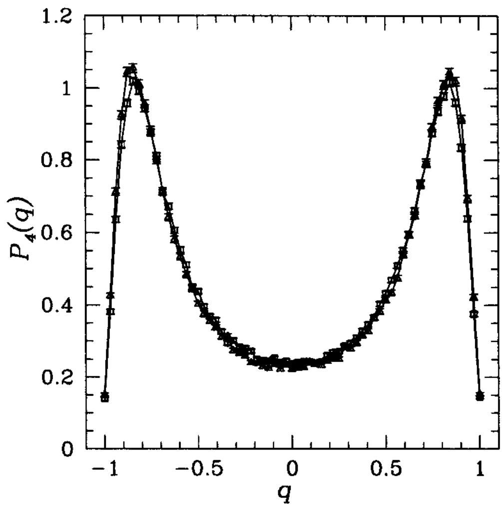

Fig. 15. $P_4(q)$ for the $3D$ Ising spin glass with Gaussian couplings below the critical temperature ($T=0.7T_c$): triangles for $L=8$, squares for $L=12$.

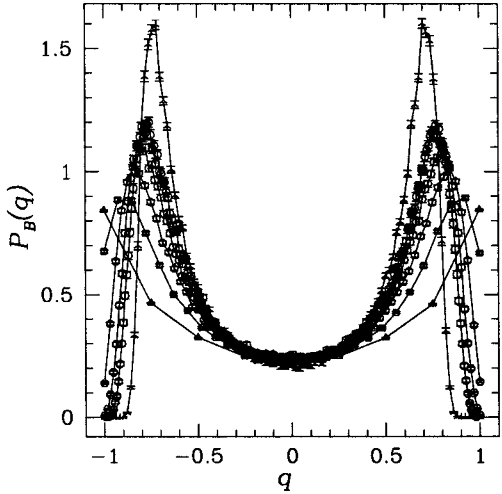

Fig. 16. $P_B(q)$ for the $3D$ Ising spin glass with Gaussian couplings below the critical temperature ($T = 0.7T_c$) and $L = 12$: $B = 2$ (triangles), $B = 3$ (squares), $B = 4$ (pentagons), $B = 5$ (hexagons), $B = 6$ (heptagons) and $B = 12$ (three line stars). B is increasing with the height of the two maxima.

It is clear that the distinctive features characterizing the broken phase do not depend on the exact definition of the overleap: the full and the window overlaps describe the same picture of the low temperature phase.

8.6. Zero Temperature

An interesting and open problem is what happens in the zero temperature limit. In this limit it is clear the minimum energy configuration σ^* dominates the partition function. It is less clear if the limit $T \to 0$ and the limit $N \to \infty$ can be freely interchanged (always *cum grand salis*).

A naive picture is the following: let us call σ^r the local minima of the Hamiltonian and let us order them according to increasing value of the energy. Let us restrict the discussion to the case of models where the coupling constant change continuously in such a way that with probability one no degeneracy of the states is allowed. At small finite temperature we would like to write

$$Z(\beta) \approx \sum_r e^{-\beta E^r} \tag{119}$$

This formula looks very similar to the relation

$$Z(\beta) = \sum_{\alpha} e^{-\beta F^{\alpha}} \tag{120}$$

where the sum runs now over the finite volume states, and F^{α} is the corresponding free energy. One is therefore tempted at low temperature to identify the finite temperature finite volume states with the local minima of the Hamiltonian, and to use the properties of the firsts to deduce the properties of the latters.[21]

However there may be some problems in this proposals: indeed in a little more refined approach one would write

$$Z(\beta) \approx \sum_{r} e^{-\beta E^{r} + S^{r}} \tag{121}$$

where the entropy S^r could be approximatively computed taking care of one spin excitations, i.e.,

$$S^{r} = \sum_{i} s(m_i^r) \tag{122}$$

where

$$s(m) = \frac{1+m}{2} \log\left(\frac{1+m}{2}\right) + \frac{1+m}{2} \log\left(\frac{1+m}{2}\right) \tag{123}$$

and the local magnetization can be computed at low temperature using mean field like equations

$$m_i^r = \tanh\left(\beta \sum_{k} J_{i,k} m_k^r\right) \tag{124}$$

The point is not if this particular choice of the entropy is adequate, but that some entropy corrections are present. It may happen (this effect should be carefully investigated) that these entropy corrections, that are proportional to N, have a variation from state to state proportional to $N^{1/2}$, and these terms completely upset the mapping among finite temperature states and the zero temperature minima. As far as we expect that

[21] We neglect the fact that some of the minima correspond to two spins excitation of the ground states, and at finite temperature they are mapped into the same finite volume states where the ground state is mapped. A more detailed analysis is needed to cope with this problem, and we will not discuss it here.

$S \propto NT$ in short range models, we could expect a crossover region at $T \propto N^{1/2}$.

This could not happen at least for two different reasons:

- For some reasons, the fluctuations in the entropy are smaller than $N^{1/2}$. If they are finite, they give only an irrelevant reweighting of the states.
- Although it is not possible to have a one to one correspondence of the finite temperature states with the local minima, the statistical properties of the two sets are similar.

If any of the last two scenario is valid, one has that the function $P(q, T)$ and the corresponding function $x(q, T)$ are smooth functions of the temperature close to zero temperature also for large N, and no crossover region exists.

No evidence does exist in either directions, but, just for the sake of the discussion, let us assume that this zero temperature smoothness conjecture is correct, as it is often done in the literature. Let us define $E(q)$ as the energy gap between the ground state and all the states with overlap in modulus less than q with the ground state. If we call $P_q(E)$ its distribution, the previous approach can be used to derive that at small temperature

$$\int dE\, P_q(E)\, e^{-\beta E} = x(q, T) \tag{125}$$

In this way we find that[22]

$$P_q(0) = \lim_{T \to 0} \frac{x(q, T)}{T} \equiv y(q) \tag{126}$$

If $y(q)$ is different from zero we have that $P_q(E)$ is different from zero at finite E when the volume goes to infinity, and local minima with different q have a finite energy gap and difference in energy: if we close our eyes on energy differences which are of order 1 the ground state turns out to be non degenerate. Obviously the opposite conclusion holds if $y(q) = 0$.

What do we know about the function $y(q)$? In the SK model one finds that $y(q) \neq 0$, and it is qualitatively of the form $y(q) \simeq q(1-q)^{-1/2}$. We do not have analytic informations on other models (like diluted ones) and numerical simulations in the low temperature region are not frequent.[(76)] Quite recently new optimization techniques have been used which allow the computation of the ground states on relative large lattices (i.e., up to

[22] In the usual mean field approximation, the probability distribution $P_q(E)$ can be computed analytically: one finds that $\langle E(q) \rangle \approx y(q)^{-1}$.

10^3 or 10^3).[77–81] For example the results by Palassini and Young[80, 81] seem to favor the hypothesis that in the infinite volume limit the first excited state is similar to the ground state (even if fitting ambiguities are in this case relevant, and the $3d$ result is largely compatible with the survival of a non-degenerate scenario). If replica symmetry breaking is present at non zero temperature, such a result could be interpreted by saying that $y(q)=0$: however a more carefully analysis is needed, especially on the extrapolation to the infinite volume limit. Moreover the possible existence of a crossover region in T should be investigated before reaching definite conclusions.

8.7. Coupled Replicas

A very useful approach is based on coupling two lattice spin glass systems (of the same size and with the same realization of the quenched random couplings) by their mutual overlap. We define an Hamiltonian:

$$\mathcal{H}_{J,\varepsilon}[\sigma,\tau] \equiv \mathcal{H}_J[\sigma] + \mathcal{H}_J[\tau] - \frac{\varepsilon}{V}\sum_i \sigma_i\tau_i \tag{127}$$

where $\mathcal{H}_J$ is the usual disordered Hamiltonian defined in Eq. (2). We present here original results for the $4D$ Ising spin glass with Gaussian couplings: we will define in detail the procedure we have followed. Older results of the same kind (with smaller lattices and a smaller statistical sample) can be found in refs. 82 and 83.

We have studied (on a parallel computer of the APE series[84]) $4D$ systems of very large size: we have set $L=24$ ($V=L^4$), and averaged over 6 different coupled systems. We have worked at zero magnetic field and set $T=1.35 \simeq 0.75T_c$. We have investigate a set of ε values going from 0.1 down to 0.006. We have used 10^5 Monte Carlo sweeps of the system for $\varepsilon=0.1$, $5 \cdot 10^5$ for $\varepsilon=0.03$, 10^6 for $\varepsilon=0.01$ and $1.5 \cdot 10^7$ for $\varepsilon=0.006$. For each run we have checked that the measured overlap had reached a stable plateau (see Fig. 17).

The presence of the interaction term $(\varepsilon/V)\sum_i \sigma_i au_i$ with a positive value of ε forces the two copies of the system to stay closer than for $\varepsilon=0$: $q_\varepsilon(t) \equiv (\sum_i \sigma_i(t)\,\tau_i(t))/V$ will tend as $t \to \infty$ to a value greater than the equilibrium value with $\varepsilon=0$.

For ε not too small taking the infinite time limit of $q_\varepsilon(t)$ is easy. The forcing makes the correlation length (and time) small: the overlap tends to its asymptotic value in a reasonable time and we can obtain $q_\varepsilon(t=\infty)$ directly from the value of the plateau, without any risky extrapolation

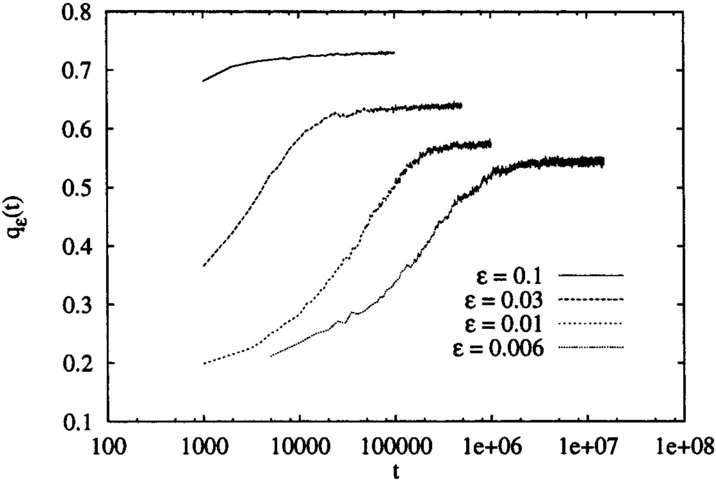

Fig. 17. Time evolution of the overlap between two coupled replicas for the 4*D* Ising spin glass with Gaussian couplings. The coupling strength, ε, is smaller for the lower curve.

procedure. We plot in Fig. 18 the value $q_\varepsilon(t=\infty) \equiv q_\varepsilon$ extrapolated to infinite time.

Next we have to estimate the limit for $\varepsilon \to 0$ of $q(\varepsilon)$. In the simplified picture of a rugged free energy landscape, made of many valleys, the coupling between two copies forces them into the same valley, and so we expect

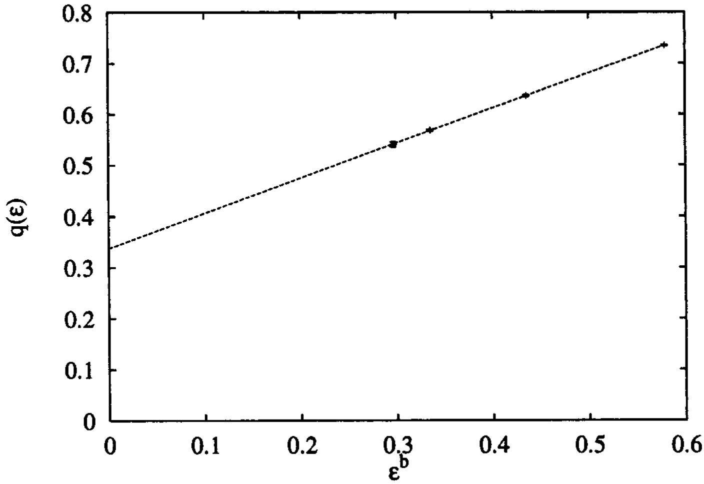

Fig. 18. The value $q_\varepsilon(t=\infty)$ extrapolated to infinite time as a function of ε^b. We used the exponent found in our best fit: $b = 0.24 \pm 0.03$.

to obtain in that limit an information about the mean size of a valley. Such information, in the theory of spin glasses, is encoded in the Edward–Anderson order parameter (q_{EA}) defined as the average overlap between two replicas within the same pure state.

We can reach the same conclusion following a different way of reasoning: the presence of the $\varepsilon > 0$ term is equivalent to a potential favoring bigger overlaps, so that at equilibrium ($t \to \infty$) $q(\varepsilon)$ will be the maximum overlap allowed for $\varepsilon = 0$ plus a term due to the interaction,

$$q(\varepsilon) = q_{\max} + a\varepsilon^b \tag{128}$$

For $\varepsilon = 0$ the probability distribution function of the absolute value of the overlap has support $[0, q_{EA}]$: the order parameter of the theory, $q_{EA} = q_{\max}$ can be obtained via the limit $\varepsilon \to 0$.

We have fitted the behavior of (128) for the data shown in Fig. 18. On the best fit:

$$q_{EA} = 0.34 \pm 0.03 \tag{129}$$

$$a = 0.69 \pm 0.02 \tag{130}$$

$$b = 0.24 \pm 0.03 \tag{131}$$

In the mean-field theory $b = \frac{1}{2}$, while in previous work[82] in 4*D* the authors found $b \simeq \frac{1}{3}$. The value found for the order parameter q_{EA} is in good agreement with the one found in ref. 65, where off-equilibrium measurement were suggesting $q_{EA}(T = 1.35) = 0.30 \pm 0.05$.

8.8. Energy Overlap

We will show here results that implement the ideas discussed in Sections 2.4 and 5.1. We will show numerical computations based on the Hamiltonian (61). The data we show here are from the work of some of us in ref. 85. They have been used in the debate about the hints that one can hope to get from the Migdal–Kadanoff approximation when studying spin glass systems.[85, 86]

We have analyzed the 3*d* EA model by numerical simulations (using a tempering algorithm and an annealing scheme, checking convergence and averaging over 64 or more samples), with binary couplings and the Hamiltonian (61). We compare these data to the results obtained in the Migdal–Kadanoff approximation of the same model.

It turns out that one can see a clear difference, already at $T = 0.7$ on medium-size lattices, among the MKA and the EA model.

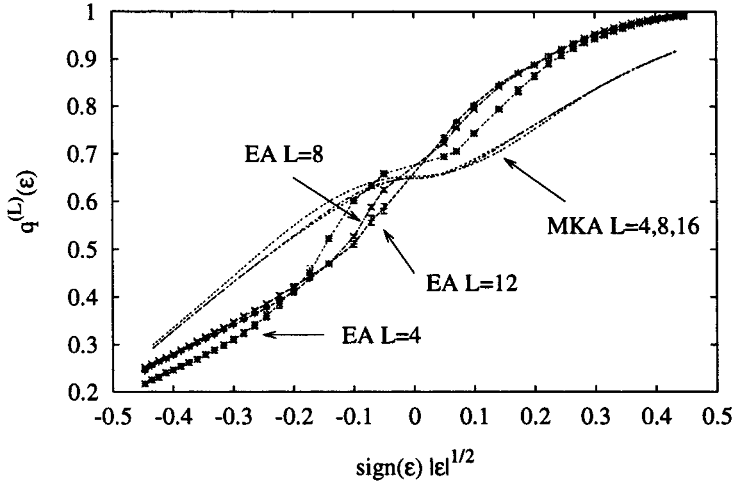

Fig. 19. $q^{(L)}$ from numerical simulations in the $3d$ EA spin glass (lines with points) and in the Migdal–Kadanoff approximation.

In Fig. 19 we show our results for $q^{(L)}(\varepsilon)$ versus $e^{1/2}$. The MKA gives a smooth behavior: for small ε, $q^{(L)}(\varepsilon)$ behaves like e^{λ}, with $\lambda \simeq 1$. Finite size effects look very small for these sizes (from 4 to 16). The EA model behaves in a completely different way. Here finite size effects are large, and the behavior for small ε becomes more singular for larger sizes. The $L=4$ lattice is reminiscent of the MKA behavior, but already at $L=8$ the difference is clear. From our data we are not able to definitely establish the existence of a discontinuity, but the numerical evidence is strongly suggestive of that. The data are suggestive of the building up of a discontinuity as $L \to \infty$, i.e., $q = q_+ + A_+ \varepsilon^{\lambda}$ for $\varepsilon > 0$ and $q = q_- + A_- |\varepsilon|^{\lambda}$ for $\varepsilon < 0$, with $q_+ \neq q_-$ and an exponent λ close to $\frac{1}{2}$: a continuous behavior (i.e., $q_+ = q_-$) cannot be excluded from these data, but in this case we find an upper limit $\lambda < 0.25$, totally different from the behavior of MKA, $\lambda \simeq 1$.

8.9. Ultrametricity

The ultrametric organization of the equilibrium states is one of most distinctive and striking features of the RSB solution of the spin glass mean field theory. Checking if an organization of the same kind still rules the state distribution in finite dimensional models is a task of large interest.[87]

The issue of the ultrametricity in a finite number of dimensions has been checked numerically in ref. 87. The most convincing numerical tests have been done in four dimensions, since there the phase transition is more

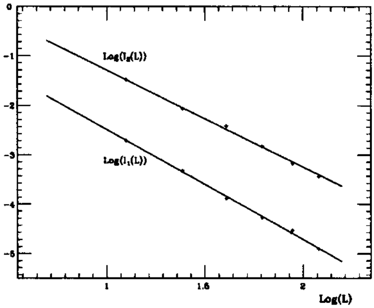

Fig. 20. The probability of a forbidden overlap I^L as a function of L. For the lower points we have fixed $q_{1,2} = q_{2,3}$, for the upper points $q_{1,2} \neq q_{2,3}$.

clear. In Fig. 20 we plot the probability (I^L) of the appearance of an overlap which is forbidden by ultrametricity as a function of the lattice size. This probability goes to zero as $L \to \infty$ with a power law in L, and the power law (i.e., an exponent of 2.21) is consistent with expectations coming from mean field analytic computations (for more details see ref. 87). The support to the existence of a low temperature phase with an ultrametric structure of states is very strong.

Other numerical simulations done with a different technique in three dimensions on systems with side from 4 to 12 are compatible with ultrametricity, but the approach to zero seems to be much slower that in four dimension and at the present moment it is difficult to reach a definite conclusion.[89, 90] This problem should be better investigated in the future.

We recall that is also possible to show,[88] by using the set of sum rules we have discussed before that if the states are organized ultrametrically in a finite dimensional spin glass the detailed structure of the ultrametric organization has to be exactly the same of the mean field solution. This fact does not prove ultrametricity, but once ultrametricity has been detected (for example numerically) it allows to establish many other important results about the structure of the system.

8.10. Dynamics

The analysis of the dynamical behavior of spin glasses can give a large amount of information (see Section 5.4 earlier in the text for a first discussion and references). Here we summarize some nice numerical results concerning the dynamical determination of the overlap probability distribution, from ref. 91.

As we have already discussed, the basic ingredients of the dynamical approach are the autocorrelation function $C(t, t')$ and the integrated response function. We use a magnetic field that jumps at time t_w:

$$h(t) = h_0 \theta(t - t_w) \tag{132}$$

In this way by computing the function $X[u]$ one can test numerically the validity of the relation (84), that relates the magnetization and the correlation function. In other words we try to check that the function X depends only on the value of the correlation function $C(t, t')$ (and not on the times t and t') even for large but finite times. A second interesting goal is to check that X is given by the integrated probability distribution of the overlap.

We have simulated four couples of spin samples, with Gaussian couplings, on a $L = 64$ lattice in three dimensions. We have used two different values of the magnetic fields in order to control the validity of the linear response approximation.

We show in Fig. 21 the results for the function X. We have also plotted the equilibrium behavior, where the FDT theorem holds (i.e., the straight line $1 - C$). This method also gives us a way to estimate the order parameter of the system as the point where the function X departs from the FDT regime. From Fig. 21 we can estimate the value of the order parameter as $q_{\mathrm{EA}} \simeq 0.68$, in very good agreement with the equilibrium value quoted before ($q_{\mathrm{EA}} = 0.70 \pm 0.02$) (see Fig. 3). We remind the reader that

$$x(q) = \int_0^q \mathrm{d}q' \, P(q') \tag{133}$$

where $P(q)$ is the equilibrium probability distribution of the overlap.

From 21 it is clear that for not too large waiting time the function X depends only on the value of the correlation function. Moreover the equilibrium $x(q)$ matches extraordinarily well the X function.

It is clear that $x(q)$ does not have the form suggested by a droplet like picture. The droplet picture predicts a linear region with slope -1 (the equilibrium regime, $q \in [q_{\mathrm{EA}}, 1]$) and another regime where we have a horizontal line ($q \in [0, q_{\mathrm{EA}}]$). Figure 21 rules out this possibility.

9. CONCLUSIONS

In this note we hope we have succeeded in clarifying better the precise nature of the predictions of the Replica Symmetry Breaking approach, and the numerical and analytical evidences available to support its validity in finite dimensional, realistic spin glasses. It is clear that there are many

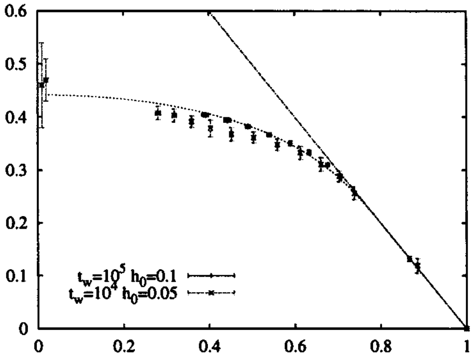

Fig. 21. The function $X(c) \equiv Tm/h_0$ versus C (see text) for a $3D$ Ising spin glass with Gaussian couplings. $L = 64$ and $T \simeq 0.7T_c$. The curve is the function $x(C)$ obtained integrating the equilibrium probability distribution of the overlap. The straight line is the FDT prediction (i.e., the straight line $1 - C$). Data are from two different numerical simulations, one with $t_w = 10^5$ and $h_0 = 0.1$ and the other one with $t_w = 10^4$ and $h_0 = 0.05$.

issues that need clarification: for example working out a field theory describing finite dimensional systems would be crucial. Also numerical simulations need to be improved, and pushed to lower T values (where the effect of the critical point at T_c is not obscuring too much the real low T structure of the system).

Let us stress again the points of bigger relevance. Correlation functions have been studied in detail in finite dimensional systems, and they confirm a RSB picture. The proposal that a nontrivial function $P(q)$ is an artifact due to the presence of interfaces among two equilibrium states has been analyzed and falsified: the study of window overlaps confirms that the non-trivial shape of $P(q)$ is not due to the presence of interfaces. Coupling replicas helps again in observing clear signatures of replica symmetry breaking. We have discussed in detail about states, by stressing the importance of finite volume states. We believe this is a crucial notion for understanding a disordered system. We have analyzed the implications of RSB on the finite volume states and discussed the hierarchical organization of states. We have discussed in detail the difficulties connected to the study of infinite volume states, and why we believe that the recent rigorous results by Newman and Stein[7, 12] strongly support RSB. We have discussed numerical results that confirm this point of view.

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