General properties of overlap probability distributions in disordered spin systems. Toward Parisi ultrametricity.

Stefano Ghirlanda* Francesco Guerra**

* Zoologiska Institutionen, Stockholms Universtitet, S-106 91 Stockholm, Sweden
** Dipartimento di Fisica, Università di Roma "La Sapienza", I-00185 Roma, Italy & INFN, Sezione di Roma 1.

Abstract

For a very general class of probability distributions in disordered Ising spin systems, in the thermodynamical limit, we prove the following property for overlaps among real replicas. Consider the overlaps among s replicas. Add one replica $s+1$. Then, the overlap $q_{a,s+1}$ between one of the first s replicas, let us say a, and the added $s+1$ is either independent of the former ones, or it is identical to one of the overlaps q_{ab}, with b running among the first s replicas, excluding a. Each of these cases has equal probability $1/s$.

1 Introduction

In this paper we focus on general properties of overlap distributions in statistical-mechanical models made up of Ising spins (see below for definitions). Historically, these properties have been considered for the first time in spin-glass models [7], so that for convenience we take them as a starting point in our discussion, and generalise our results later on.

The problem of finding the phase structure of short-ranged models for spin glasses has proved extremely difficult, and yet remains unsolved. An important result, though, has been achieved with Parisi's solution of the Sherrrington-Kirkpatrick (SK) model (a mean-field approximation to more realistic ones), whose hamiltonian we recall:

$$\mathcal{H}_J\{\sigma\} = -\frac{1}{\sqrt{N}} \sum_{(ik)} J_{ik}\sigma_i\sigma_k \, . \tag{1}$$

The σ_i's ($i = 1, \ldots, N$) are Ising spins and the J_{ik}'s (collectively noted J) are random variables drawn from independent unit normal distributions, with the constraints $J_{ik} = J_{ki}$ and $J_{ii} = 0$. The sum runs over all couples (ik), with $1 \leq i < k \leq N$. Parisi solution for this model implies a countable infinity of pure states (below the critical temperature), that turn out to be organised in a very remarkable geometric structure, of the type called ultrametric [7].

This structure is clearly seen by introducing a replicated system, made up of non-interacting, identical copies (replicas) of an SK system. These are usually called "real" replicas to distinguish them from the replicas used in the replica method, which requires a limit to zero replicas. In this way the Boltzmann state of the replicated system is simply the following product state:

$$\Omega_J(\cdot) = (\omega_J^{(1)} \otimes \cdots \otimes \omega_J^{(s)})(\cdot)\,, \tag{2}$$

where $\omega_J^{(i)}$ is the state of replica i for a given realisation of the J's. We call σ_i^a the variables associated to replica a, on which $\omega_J^{(a)}$ acts. Notice that all replicas have the *same* noise J. We will write $\mathbb{E}(\cdot)$ the average over the coupling distribution.

The overlap between the spin configurations of different replicas a and b is defined as:

$$Q_{ab} = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^a \sigma_i^b\,. \tag{3}$$

Notice that Q_{aa} would be trivially equal to one. We introduce now the random variables q_{ab} (referred to also as overlaps) by requiring that for any smooth function $F_s(Q)$ of the configuration overlaps among s replicas (summarised by Q in the notation) the following equality holds:

$$\mathbb{E}(\Omega_J(F_s(Q))) = \langle F_s(q) \rangle\,, \tag{4}$$

where $\langle\cdot\rangle$ is by definition the average with respect to the distribution of the q's. According to (4), this implies both Boltzmann and J averages. Although the replicas are independent so long as the thermal average is considered, they are coupled by the J average, for they all share the same realisation of the couplings. In fact the Parisi solution gives the following joint distribution for the overlaps q_{12} and q_{13} among three replicas, labelled 1, 2, and 3:

$$\rho_{12,13}(q_{12}, q_{13}) = \frac{1}{2}\rho(q_{12})\rho(q_{13}) + \frac{1}{2}\rho(q_{12})\delta(q_{12} - q_{13})\,, \tag{5}$$

where $\rho(\cdot)$ is the probability distribution of the overlap between any two replicas. Formula (5) says that the two overlaps are independent with probability one half, and identical with the same probability. Even when we consider two overlaps between two distinct couples of replicas, the correlation remains strong:

$$\rho_{12,34}(q_{12}, q_{34}) = \frac{2}{3}\rho(q_{12})\rho(q_{34}) + \frac{1}{3}\rho(q_{12})\delta(q_{12} - q_{34})\,. \tag{6}$$

The difference with formula (5) is just that the probability of the two overlaps being identical has reduced to one third, and accordingly the probability of their being independent is two thirdies.

In general, the underling ultrametric structure allows all joint probability distributions of the overlaps among replicas to be expressed as functions of the distribution $\rho(\cdot)$ of a single overlap. We refer to the literature [7] for a thorough exposition of this geometrical structure, but here we want to stress the well known fact that this situation requires $\rho_J(\cdot)$, i.e. the overlap distribution at fixed J, to be non-self-averaging with respect to J, that is to depend on the realisation of the couplings even after the thermodynamical limit has been taken. In fact, since $\rho(q) = \mathbb{E}(\rho_J(Q))$:

$$\begin{aligned} &\rho_{12,34}(q_{12}, q_{34}) = \mathbb{E}(\rho_{J\,12,34}(Q_{12}, Q_{34})) \\ &= \mathbb{E}(\rho_J(Q_{12})\rho_J(Q_{34})) \neq \mathbb{E}(\rho_J(Q_{12}))\mathbb{E}(\rho_J(Q_{34}))\,, \end{aligned} \tag{7}$$

i.e. $\rho_J(\cdot)$ fluctuates with J.

While a complete mathematical proof of the Parisi solution is still lacking, the latter is widely believed to be correct due to extensive computer simulations [6, 5] and mathematical arguments, see [4, 11, 13, 2] and references therein. On the other hand, doubts about the relevance of the ultrametric structure to realistic models have been raised in the last years, and in particular the existence of non-self-averaging quantities in the thermodynamical limit has been questioned [8], see however [9]. In our opinion, since Parisi's method seems very difficult to generalise beyond the mean-field approximation, a deeper understanding of the ultrametric geometry in the simpler SK model is a necessary first step in order to consider its relevance to short-ranged models. In this paper, following the ideas outlined in [4, 3], we are able to prove that some features of the ultrametric geometry arise naturally in the SK model as a consequence of the self-averaging of thermodynamical quantities, e.g. the internal energy.

Moreover, by a careful limiting procedure we establish the same results for short-ranged models. We do not address the very difficult question of the number of phases in the glassy regime of spin-glass models, but show that, whichever this number be, the overlap distributions (as previously defined) have some ultrametric features.

In section two we recall some known results, and find their consequences for the overlap distributions in the SK model. In section three we generalise these arguments in order to construct a well-defined set of such distributions, independently from Parisi's work and in agreement with it. Section four is devoted to the extension of these results to short-ranged models. A short concluding section summarises our arguments.

2 Consequences of self-averaging

For the sake of convenience let us define:

$$A_J\{\sigma\} \stackrel{\text{def}}{=} -\frac{1}{N}\mathcal{H}_J\{\sigma\}\,. \tag{8}$$

We start our arguments by recalling a known theorem, stating the self-averaging of $A_J\{\sigma\}$ with respect to the $\langle\cdot\rangle$ average in the thermodynamical limit [4, 3]:

$$\lim_{N\to\infty}\left(\langle A_J\{\sigma\}^2\rangle - \langle A_J\{\sigma\}\rangle^2\right) = 0\,. \tag{9}$$

By following [4, 3], let us sketch the proof of (9). Let us write the $\langle\cdot\rangle$ mean square deviation in (9) as a sum of two terms in the form

$$\begin{aligned}\langle A_J\{\sigma\}^2\rangle - \langle A_J\{\sigma\}\rangle^2 = \mathbb{E}\omega_J(A_J\{\sigma\}^2) - (\mathbb{E}\omega_J(A_J\{\sigma\}))^2 = \\ \mathbb{E}(\omega_J(A_J\{\sigma\}^2) - \omega_J^2(A_J\{\sigma\})) + (\mathbb{E}\omega_J^2(A_J\{\sigma\}) - (\mathbb{E}\omega_J(A_J\{\sigma\}))^2).\end{aligned} \tag{10}$$

The second term is the $\mathbb{E}$ mean square deviation of the internal energy. Since Pastur and Scherbina [11] have proven the self-averaging of the free energy, standard thermodynamical reasoning based on convexity gives also self-averaging for the internal energy [4, 12]. This may fail in principle only for a zero measure set of values for β. Due to the lack of complete control on the thermodynamical limit, it is also necessary to exploit subsequences, as explained in [4]. Therefore, the second term in (10) goes to zero as $N\to\infty$. The first term is equal to $N^{-1}\partial_\beta\mathbb{E}\omega_J(A_J\{\sigma\})$. Since $\mathbb{E}\omega_J(A_J\{\sigma\})$ is finite, the N^{-1} term forces also the first term in (10) to go to zero as $N\to\infty$, with the possible exclusion of a set of zero measure of values for β. Therefore we have established (9). This, in turn, implies that:

$$\lim_{N\to\infty}\left(\langle A_J\{\sigma^a\}F_s(q)\rangle - \langle A_J\{\sigma\}\rangle\langle F_s(q)\rangle\right) = 0\,, \tag{11}$$

where by $A_J\{\sigma^a\}$ we intend that $A_J\{\sigma\}$ is calculated on replica a, that we take to be one of the replicas in $F_s(q)$. This result is achieved from (9) via a simple Schwarz inequality:

$$\begin{aligned}
\lim_{N\to\infty} \left(\langle A_J\{\sigma^a\}F_s(q)\rangle - \langle A_J\{\sigma\}\rangle\langle F_s(q)\rangle\right)^2 &= \\
\lim_{N\to\infty} \langle \left(A_J\{\sigma^a\} - \langle A_J\{\sigma\}\rangle\right) F_s(q)\rangle^2 &\leq \\
\lim_{N\to\infty} \langle \left(A_J\{\sigma^a\} - \langle A_J\{\sigma\}\rangle\right)\rangle^2 \langle F_s(q)\rangle^2 &= 0\,,
\end{aligned} \tag{12}$$

by virtue of (9). We express now (11) in terms of overlaps, using the fact that integration by parts gives $\langle J_{ik} f(J)\rangle = \langle \partial_{J_{ik}} f(J)\rangle$, for a generic function $f(\cdot)$, since the J's are normally distributed. From this formula we get:

$$\mathbb{E}\left(\partial_{J_{ik}}\Omega_J(F_s(Q))\right) = \frac{1}{\sqrt{N}}\sum_{a=1}^{s}\mathbb{E}\left(\Omega_J(F_s(Q)\sigma_i^a\sigma_k^a) - \Omega_J(F_s(Q))\Omega_J(\sigma_i^a\sigma_k^a)\right) \tag{13}$$

by explicit calculation. Applying these formulae, the first term in (11) is written as:

$$\begin{aligned}
\langle A_J\{\sigma^a\}F_s(Q)\rangle &= \frac{\beta}{N^2}\sum_{(ik)}\mathbb{E}\left(\Omega_J\left(\sigma_i^a\sigma_k^a F_s(Q)\sum_{b=1}^{s}\sigma_i^b\sigma_k^b\right) - \right. \\
&\qquad \left. \Omega_J\left(\sigma_i^a\sigma_k^a F_s(Q)\right)\Omega_J\left(\sum_{b=1}^{s}\sigma_i^b\sigma_k^b\right)\right) \\
&= \frac{\beta}{2}\left\langle\left(\sum_{b=1}^{s} q_{ab}^2 - s q_{a,s+1}^2\right)F_s(q)\right\rangle\,,
\end{aligned} \tag{14}$$

while the second one is simply:

$$\langle A_J\{\sigma\}\rangle\langle F_s(q)\rangle = \frac{\beta}{2}\left(1 - \langle q^2\rangle\right)\langle F_s(q)\rangle\,. \tag{15}$$

Using (14) and (15) in (11) we get:

$$\lim_{N\to\infty}\left\langle F_s(q)\left(\sum_{b=1}^{s} q_{ab}^2 - s q_{a,s+1}^2 - \left(1 - \langle q^2\rangle\right)\right)\right\rangle = 0\,. \tag{16}$$

Since $F_s(\cdot)$ is a generic function, we can introduce conditional expectations $\mathbb{E}(\cdot|\mathcal{A}_s)$ with respect to the algebra $\mathcal{A}_s$ generated by the overlaps among s replicas, and write:

$$\mathbb{E}\left(q_{a,s+1}^2|\mathcal{A}_s\right) = \frac{1}{s}\langle q^2\rangle + \frac{1}{s}\sum_{b\neq a} q_{ab}^2\,, \tag{17}$$

where the unity in (16) has canceled with the term $a = b$ in the sum. We shall leave understood that (17), as others formulae obtained in the following, holds exactly only in the thermodynamical limit.

Using (17) we can write equalities relating averages of squared overlaps, the simplest of which is:

$$\langle q_{12}^2 q_{13}^2 \rangle = \frac{1}{2}\langle q^4 \rangle + \frac{1}{2}\langle q^2 \rangle^2 \,, \tag{18}$$

in full agreement with the Parisi probability distribution (5).

Moreover, from (17) we can easily derive an expression for the conditioned expectation $\mathbb{E}\left(q_{s+1,s+2}^2 | \mathcal{A}_s\right)$ as well, starting by writing (17) in the case of $s+2$ replicas and $a = s+1$:

$$\mathbb{E}\left(q_{s+1,s+2}^2 | \mathcal{A}_{s+1}\right) = \frac{1}{s+1}\langle q^2 \rangle + \frac{1}{s+1}\sum_{b=1}^{s} q_{b,s+1}^2 \,. \tag{19}$$

Keeping in mind that $\mathbb{E}\left(\mathbb{E}\left(\cdot | \mathcal{A}_{s+1}\right) | \mathcal{A}_s\right) = \mathbb{E}\left(\cdot | \mathcal{A}_s\right)$, we have:

$$\begin{aligned} \mathbb{E}\left(q_{s+1,s+2}^2 | \mathcal{A}_s\right) &= \frac{1}{s+1}\langle q^2 \rangle + \frac{1}{s+1}\sum_{b=1}^{s} \mathbb{E}\left(q_{b,s+1}^2 | \mathcal{A}_s\right) \\ &= \frac{1}{s+1}\langle q^2 \rangle + \frac{1}{s+1}\left(\langle q^2 \rangle + \frac{1}{s}\sum_{b=1}^{s}\sum_{c\neq b}^{1,s} q_{bc}^2\right) \,, \end{aligned} \tag{20}$$

that is:

$$\mathbb{E}\left(q_{s+1,s+2}^2 | \mathcal{A}_s\right) = \frac{2}{s+1}\langle q^2 \rangle + \frac{2}{s(s+1)}\sum_{a<b\leq s} q_{ab}^2 \,. \tag{21}$$

¿From (21) we can derive other known ultrametric equalities, for example:

$$\langle q_{12}^2 q_{34}^2 \rangle = \frac{1}{3}\langle q_{12}^4 \rangle + \frac{2}{3}\langle q_{12}^2 \rangle^2 \,, \tag{22}$$

again in agreement with (6) obtained from Parisi's solution. In the following section we generalise formulae (17) and (21) to arbitrary (integer) powers of overlaps.

3 Auxiliary interactions and overlap probability distributions

Let us consider the SK model in the presence of an external field:

$$A_{J,J'}\{\sigma\} \stackrel{\mathrm{def}}{=} A_J\{\sigma\} + \frac{\lambda}{N}\sum_{i=1}^{N} J_i' \sigma_i$$

$$\stackrel{\text{def}}{=} \quad A_J\{\sigma\} + \lambda I_{J'}\{\sigma\}\,, \tag{23}$$

where the random variables J'_i are independt from the J_{ik}'s and with the same distribution. We assume that λ is "small", since in the end we will take it to zero to recover the free SK model.

Theorem (11) can be generalised to the present case, since it only relies on self-averaging of the internal energy:

$$\lim_{N\to\infty} \left(\langle A_{J,J'}\{\sigma^a\} F_s(q)\rangle - \langle A_{J,J'}\{\sigma\}\rangle\langle F_s(q)\rangle\right) = 0\,, \tag{24}$$

where now $\langle\cdot\rangle$ implies averaging over the J' variables as well. Using the same procedure as in the preceding section, but now integrating and deriving with respect to the J' variables, we get the completely analogous formula:

$$\mathbb{E}\left(q_{a,s+1}|\mathcal{A}_s\right) = \frac{1}{s}\langle q\rangle + \frac{1}{s}\sum_{b\neq a} q_{ab}\,, \tag{25}$$

which continues to hold when λ is taken to zero (after having taken the thermodynamical limit). The only difference between this formula and (17) is that here overlaps appear at the first power.

It is now clear that we can consider auxiliary interactions of the general form:

$$\lambda_r I_r\{\sigma\} \stackrel{\text{def}}{=} \frac{\lambda_r}{N^{(r+1)/2}} \sum_{(i_1\ldots i_r)} J'_{i_1,\ldots,i_r}\sigma_{i_1}\cdots\sigma_{i_r}\,, \tag{26}$$

the former case being $r=1$. So we end up with the formula:

$$\mathbb{E}\left(q^r_{a,s+1}|\mathcal{A}_s\right) = \frac{1}{s}\langle q^r\rangle + \frac{1}{s}\sum_{b\neq a} q^r_{ab}\,, \tag{27}$$

valid for the free SK model when $\lambda_r \to 0$. A similar formula is valid for $\mathbb{E}\left(q^r_{s+1,s+2}|\mathcal{A}_s\right)$ as a generalisation of (21). We have thus obtained the main result of this paper:

THEOREM. *Given the overlaps among s real replicas, the overlap between one of these and an additional replica is either independent of the former overlaps or it is identical to one of them, each of these cases having probability $1/s$:*

$$\rho_{a,s+1}(q_{a,s+1}|\mathcal{A}_s) = \frac{1}{s}\rho(q_{a,s+1}) + \frac{1}{s}\sum_{b\neq a}\delta(q_{a,s+1} - q_{ab})\,, \tag{28}$$

where $\rho_{a,s+1}(\cdot|\mathcal{A}_s)$ is the conditioned distribution of $q_{a,s+1}$ given the overlaps in $\mathcal{A}_s$.

PROOF. The theorem is proved by (27) and the fact that the overlaps are bounded.

COROLLARY: *The distribution of $q_{s+1,s+2}$ conditioned to the overlaps in $\mathcal{A}_s$ is given by:*

$$\rho_{s+1,s+2}(q_{s+1,s+2}|\mathcal{A}_s) = \frac{2}{s+1}\rho(q_{s+1,s+2}) + \frac{2}{s(s+1)} \sum_{a<b\leq s} \delta(q_{s+1,s+2} - q_{ab}) \,. \tag{29}$$

PROOF: The proof is the same as that leading from (17) to (21).

We shall comment on theorems (28) and (29) in the concluding section. Notice that the general relations found in the previous theorem imply also the constraints on overlap distributions found in [1].

4 Extension to short-ranged models

While we have been dealing with the SK model so far, it is easy to establish the same results for short-ranged models by carefully taking the thermodynamical limit. Suppose that a given model has M pure states at a given temperature, that we label $\omega_i(\cdot)$, $i = 1, \ldots, M$. The value of M is immaterial for our argument (but see the concluding section). Each of these states can be reached in the thermodynamical limit by means of a suitable field h_i, that for disordered systems such as spin-glasses is presently unknown.

Let us now note $\mathcal{H}\{\sigma\}$ the hamiltonian of the considered short-ranged model, and let us add to it both the field h_i and a perturbation of the SK type (26) (now written as $\mathcal{H}_{SK}\{\sigma\}$), in such a way that the hamiltonian becomes:

$$\mathcal{H}\{\sigma\} + h_i + \lambda\mathcal{H}_{SK}\{\sigma\} \,, \tag{30}$$

where λ is a "small" parameter.

If, after the thermodynamical limit, λ is taken to zero, the system is left in the state $\omega_i(\cdot)$ selected by the field h_i, if the SK interaction has been kept "small enough" throughout the whole process, and provided that the considered model is not unstable with respect to the perturbation $\mathcal{H}_{SK}\{\sigma\}$.

While λ is different from zero, the SK interaction enables us to perform the same calculations as shown in the preceding sections, and to establish the same relations (28) and (29) relatively to the considered states of the system.

In general, we can state that the basic property of the overlaps, given by theorem (28), holds for all states that can be reached by adding a small spin glass interaction of the type (26) to the original interaction, by taking the infinite volume limit, and then by removing the added spin-glass fields.

5 Concluding remarks and outlook

In the preceding sections we have seen how an analysis of fluctuations has contributed a deeper understanding of the structure of the SK model, and how the same arguments can be extended to general models in statistical mechanics. Theorem (28) is a strong constraint that all overlap probability distributions have to satisfy, but it is not the same as ultrametricity. It appears instead to be the same as the hypothesis of "replica equivalence" in the framework of the replica method. As Parisi has shown [10], this hypothesis enables one to express all joint overlap distributions in terms of only those that refer to a *complete set* of overlaps among each given number s of replicas (the simplest case beyond $\rho(\cdot)$ being $\rho_{12,13,23}(\cdot,\cdot,\cdot)$ for $s=3$). Moreover, it can be shown that, under the hypothesis of replica equivalence, the only ultrametric solution is the usual Parisi solution [10], and the same conclusion remains true if one starts from (28) instead that from replica equivalence.

The fact that theorems (28) and (29) hold for basically all statistical mechanical models, compels us to remind that their consequences can be trivial, when a particular model is considered. This happens, for example, in the high temperature regime, when all overlaps take a constant value.

As stated in the introduction, the question of what case applies to short-ranged spin glass models still stays open.

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