On the probabilistic formulation of the replica approach to spin glasses

Giorgio Parisi
Dipartimento di Fisica, Università La Sapienza
INFN Sezione di Roma I
Piazzale Aldo Moro 2, Roma 00185, Italy

October 28, 2018

Abstract

In this paper we review the predictions of the replica approach on the probability distribution of the overlaps among replicas and on the sample to sample fluctuations of this probability. We stress the role of replica equivalence in obtaining relations which do not depend on the form of replica symmetry breaking. A comparison is done with the results obtained with a different rigorous approach. The role of the ultrametricity and of other algebraic properties is discussed. It is shown that the ultrametric solution can be obtained from a variational principle.

1 Introduction

The mean field theory for spin glasses has been originally derived by finding the solution of the Sherrington Kirkpatrick model \[1,2\]. The replica method was used in the first derivation. Probabilistic tools (based the cavity method) can be used instead of the replica approach, the formalism being more explicite at the price of being more heavy \[1,2,3\].

The probabilistic method and the replica approach are conceptually equivalent. In both cases the ultrametric structure of the states was assumed from the beginning. In order to present a definitive proof of the proposed solution, one should prove that the ultrametric Ansatz is the unique stable solution of the mean field equations, or, if there are more stable solutions, one should show that the ultrametric one has been chosen. This proof is lacking because of the difficulties in considering a generic non ultrametric Ansatz.

The aim of this note is to perform a small step in this direction by combining probabilistic methods and the replica techniques and by showing that the usual ultrametric solution can be selected by using a variational principle. In section II and III we briefly review the replica technique and the meaning of spontaneously broken replica symmetry. In section IV we spell out some of the consequences of replica equivalence and its connections with rigorous results. In section V we study ultrametricity and in section VI we show how the ultrametric solution may be singled out using an appropriate variational principle. In section VII we mention the existence of two extra symmetry, translational invariance in replica space and separability, which strongly constrain the probability distribution.
2 The real replica approach

In this paper many of the considerations will not depend on the detailed form of the interaction. We will study a system whose dynamical variables are Ising spins \( \sigma_i = \pm 1 \), \( i = 1, N \). The total number of degrees of freedom is \( N \) which is assumed to be quite large but finite. The system is at thermal equilibrium at a temperature \( T = \beta^{-1} \).

The Hamiltonian will depend on some control variables \( J \). A standard procedure consists in considering an ensemble of systems, which differ by the value of the control parameters \( J \) and to compute the average over \( J \) \([1]\). In many cases, i.e. spin glasses, the number of parameters \( J \) is proportional to \( N \); another possibility consists in considering a fixed value of \( J \) and averaging over \( N \) inside a given interval (e.g. \( N_0 - \Delta < N < N_0 + \Delta \) with \( \Delta \) large \([2]\)). In the following the average over the \( J \) variables (or over \( N \)) will be denoted by a bar.

Let us firstly study what happens at a given value of \( J \) (or \( N \)). It is useful to consider \( m \) replicas of the same system (\( m \) being arbitrary, may be infinite) and to define the overlaps

\[
q_{s,t} = \frac{\sum_{i=1}^{N} \sigma_i^s \sigma_i^t}{N},
\]

where \( s \) and \( t \) denote the replica.

Here the number of replicas \( m \) is a positive integer, which remain fixed and will not go to zero at the end of the computation; this number should not be confused with \( n \), the number of replicas that are used to compute the statistical expectation values, which eventually is taken to be equal to zero. These replicas are just \( m \) copies of the same system; their properties are in principle experimentally observables (they can be studied with numerical simulations) and some times they are called real replicas \([3]\).

We want to explore the possibility that the quantity \( q \) still fluctuates also for very large (obviously finite) systems. For each choice of the parameters \( J \) we can study the probability distributions of the overlaps. We can define various functions, the simplest one \( P_J(q) \) defined

\[
\int dq P_J(q) f(q) \equiv \langle f(q_{1,2}) \rangle = \langle f(q_{s,t}) \rangle_J.
\]

where \( s \) and \( t \) are arbitrary different replicas (all replicas are intrinsically equal!). In other words \( P_J(q) \) is the probability that two different equilibrium configurations have overlap \( q \).

In we consider more overlaps together, we have to introduce other probability distributions: e.g. \( P_J^{12,23,31}(q_{1,2}, q_{2,3}, q_{3,1}) \) defined as:

\[
\int dq_{1,2} dq_{2,3} dq_{3,1} P_J^{12,23,31}(q_{1,2}, q_{2,3}, q_{3,1}) f(q_{1,2}, q_{2,3}, q_{3,1}) = \langle f(q_{1,2}, q_{2,3}, q_{3,1}) \rangle_J.
\]

There are other probability distributions which can be trivially obtained as functions of others. An example is given by \( P_J^{12,34}(q_{1,2}, q_{3,4}) \) defined as

\[
\int dq_{1,2} dq_{3,4} P_J^{12,34}(q_{1,2}, q_{3,4}) f(q_{1,2}, q_{3,4}) = \langle f(q_{1,2}, q_{3,4}) \rangle_J.
\]

It is obvious that all the configurations \( \sigma_i^s \) have the same probability independently from the value of \( s \), so that the probability distribution of the overlaps will be symmetric under the exchange of the replica indices. We thus have

\[
P_J(q_{1,2}) = P_J(q_{3,4}), \quad P_J^{12,34}(q_{1,2}, q_{3,4}) = P_J(q_{1,2}) P_J(q_{3,4}).
\]

By increasing the number of replicas we find that more and more probability functions are needed. Each system (for given \( J \) and \( N \)) may have the functions \( P \) which differs from

\[
\int dq P_J(q) \quad (q = \pm 1).
\]
those of an other system. Indeed at low temperature, where these functions are not given by a single $\delta$ function, they change of a quantity of order 1 when the total Hamiltonian changes of a quantity of order 1 (e.g. when we change the form of the Hamiltonian in one point).

The actual form of the functions $P$ for a given systems has the disappointing property of not being thermodynamical stable, i.e. it changes completely under any perturbation. As we shall see later, this is the price to pay in order to have that the probability distribution of the functions $P$, i.e. $\mathcal{P}[P]$, is stable with respect to a wide class of perturbations [7, 8].

In order to get a feeling of the meaning of the fluctuations of the overlap, let us suppose that the Boltzmann average for finite but large $N$ can be decomposed into different pure states or valleys:

$$<\cdot> = \sum_{\alpha} w_{\alpha} <\cdot>_{\alpha} \quad (6)$$

and the expectation value in each of the pure state $\alpha$ satisfy the cluster property for the correlations functions, i.e. intensive quantities do not fluctuate.

The name pure state is abusive from a strict point of view: intensive quantities do always have fluctuations of order $N^{-1}$ and for $N$ fixed (albeit large but finite) we do not have any criterion (apart common sense) to distinguish fluctuations which are of order 1 from those that are of order $N^{-1}$.

In the usual ordered case one can easily define the states for the actual infinite system. In disordered systems the limit $N \to \infty$ may be rather tricky and it is quite possible that the expectation values of local observables do not have a limit (i.e. they oscillate) when $N \to \infty$. Here we do not want to enter into rather sophisticated mathematical arguments and we limit ourselves to study finite and large systems and to perform the limit $N \to \infty$ only after the average over $J$ (or $N$).

If we assume that equation (6) can be approximately written for also for finite system, we can approximately write (using the asymptotic vanishing of the connected correlations within a pure state):

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

$$P_J^{12,23,31}(q_{1,2}, q_{2,3}, q_{3,1}) = \sum_{\alpha,\gamma,\beta} w_{\alpha} w_{\gamma} w_{\beta} \delta(q_{\alpha,\gamma} - q_{1,2}) \delta(q_{\alpha,\beta} - q_{2,3}) \delta(q_{\beta,\gamma} - q_{3,1}). \quad (7)$$

In general these probabilities are $J$-dependent. It is interesting to consider their average over the $J$’s, which for simplicity we will indicate removing the suffix $J$:

$$P(q_{1,2}) = \overline{P_J(q_{1,2})}, \quad P^{12,23,31}(q_{1,2}, q_{2,3}, q_{3,1}) = \overline{P_J^{12,23,31}(q_{1,2}, q_{2,3}, q_{3,1})},$$

$$P^{12,34}(q_{1,2}, q_{3,4}) = \overline{P_J^{12,34}(q_{1,2}, q_{3,4})}. \quad (8)$$

The number of independent probability distributions is infinite. The replica method of next section consists in coding all this infinite set of functions into a $n \times n$ matrix $Q$. The value of $n$ is originally an integer. At a later stage non integer values of $n$ are allowed and eventually the limit $n \to 0$ is performed.

### 3 Breaking the replica symmetry

The replica method uses a $n \times n$ matrix $Q$. The free energy can be written as function of $Q$ in the limit $n \to 0$ and is invariant under the action of the permutation group of $n$ elements acting on indices of $Q$. In this section we will study the relations among the properties of the matrix $Q$ and the probability distributions introduced in the previous section.
When replica symmetry is exact all the off diagonal elements of the matrix $Q$ are equal (the diagonal elements of $Q$ are equal to zero). When replica symmetry is spontaneously broken, we must consider a matrix $Q$ which is not invariant under the permutations of replicas. If $\Pi$ is a permutation and $\Pi(a)$ is the value of the index $a$ after a permutation, the value of

$$Q_{\Pi(a),\Pi(b)} \equiv Q^{\Pi}_{a,b},$$

for fixed $a$ and $b$, depends on the permutation $\Pi$. We can thus introduce the function $P^R(q_{1,2})$ which is the probability distribution of the quantity $Q^{\Pi}_{1,2}$ averaged over all $n!$ permutations $\Pi$ with equal weight. In other terms we define the function $P^R(q_{1,2})$ as follows:

$$\sum_{\Pi} f(Q^{\Pi}_{1,2}) \equiv \int dq_{1,2} P_R(q_{1,2}) f(q_{1,2}),$$

$f$ being an arbitrary test function. In the same way we can define other functions, e.g.

$$\sum_{\Pi} f(Q^{\Pi}_{1,2}, Q^{\Pi}_{3,4}) \equiv \int dq_{1,2} dq_{3,4} P^{12,34}_R(q_{1,2}, q_{3,4}) f(q_{1,2}, q_{3,4}).$$

For each matrix $Q$ for a given $n$ we define a set of probability functions $P_R$, which are in one to one correspondence with the previous introduced functions $^1$.

The main assumption of the replica method is that there exists a matrix $Q$ such that for a given value of $n$ (in particular for $n = 0$) the $P_R$ functions defined in this way do coincide with the homologous probabilities $P$ previously defined with the real replicas. The case $n = 0$ seems rather strange; it is defined by considering the previous formulae for integer $n$ and perform the analytic continuation to $n = 0$. At the present moment it is not clear how much restrictive this hypothesis is. The space of all possible matrix $Q$ analytically continued at $n = 0$ is infinite dimensional and it is not easy to prove that a given set of $P$ functions cannot be obtained in this way.

In other words we have traded an infinite matrix $q_{a,b}$ (if $m = \infty$), which fluctuates also for very large systems, with a matrix $n \times n$ matrix $Q$ (which does not fluctuate) in the limit $n \to 0$. We have coded the infinite number of functions, which characterize the probability distribution of $q$, in the structure of the matrix $Q$.

As we said in the introduction the only well studied example of matrix $Q$ is such that the probability distribution of the overlaps is ultrametric, i.e. if $q_{1,2} > q_{1,3}$ and $P(q_{1,2}, q_{2,3}, q_{3,1}) > 0$ then $q_{2,3} = q_{1,3}$. In this ultrametric scheme the relevant quantity is $P(q_{1,2})$ and (as we shall see later) all other high order functions can be obtained from it by algebraic manipulations $^1, ^2, ^3$.

### 4 Replica Equivalence

#### 4.1 Introducing Replica Equivalence

Let us now consider a more general case in which ultrametricity is not assumed. There are general arguments which imply that the form of the matrix $Q$ is not completely arbitrary $^1$. It has been argued that also when replica symmetry is broken the matrix $Q$ must be

---

1 If we are not interested to consider the overlap of a configuration with itself, that for Ising spin is 1, we can consider only the off diagonal terms of the matrix $Q$, which it is conventionally taken to be zero on the diagonal.
such that no replica has different characteristics from the others. Observables which involve only one replica must be replica symmetric. In particular we must have that

$$\sum_b f(Q_{a,b})$$

(12)
does not depend on $a^2$. This property is called replica equivalence. It is likely connected to the fact that the expectation values of intensive ($J$-independent) quantities do not change from one state to the other.

This hypothesis implies automatically in the replica formalism that the free energy is finite. Indeed in the replica approach the free energy can be written as function of the matrix $Q$ (see eq. (37)). If replica equivalence is correct, the term $1/n$ in the free energy cancels automatically with the sum over $n$. Moreover adding the appropriate terms in the Hamiltonian we can generate an extra term proportional to

$$\frac{\sum_{a,b} f(Q_{a,b})}{n}$$

(13)

This term is automatically finite if condition (12) is satisfied.

It is interesting to note that this argument is quite similar to those which have been used by Guerra [7] in his rigorous derivation of some of the following equations. The replica equivalence conditions is also deeply related to the stability conditions of Aizenman and Contucci [8].

### 4.2 Two overlaps

Condition (12) has interesting consequences. In the simplest case we can consider the following equations:

$$\sum_{c,d} Q_{a,c}^{k_1} Q_{b,d}^{k_2} = (\sum_{c,d} Q_{a,c}^{k_1})^2 = \int dq_1 P(q_1) q_1^{k_1} \int dq_2 P(q_2) q_2^{k_2}. \quad (14)$$

The previous equation holds both for $a = b$ and for $a \neq b$. Let us spell its consequences in the first case. Its l.h.s can be written as

$$\left( \sum_{c,d; c \neq d} + \sum_{c,d} \delta_{c,d} \right) \left( Q_{a,c}^{k_1} Q_{a,d}^{k_2} \right). \quad (15)$$

In the first sum there are $(n-2)(n-1)$ non zero terms ($Q_{a,a} = 0$) and in the second sum there are $(n-1)$ non zero terms. Each term of the first and second sum give a contribution equal respectively to

$$\int dq_{1,2} dq_{1,3} P^{12,13}(q_{1,2}, q_{1,3}) q_{1,2}^{k_1} q_{1,3}^{k_2} \quad \int dq_{1,2} P(q_{1,2}) q_{1,2}^{k_1+k_2}. \quad (16)$$

Putting everything together we obtain the relations

$$P^{12,13}(q_{1,2}, q_{1,3}) = \frac{1}{2} P(q_{1,2}) P(q_{1,3}) + \frac{1}{2} P(q_{1,2}) \delta(q_{1,2} - q_{1,3}). \quad (17)$$

A similar equation can be obtained if we consider the case $a \neq b$. Indeed after a similar algebra and using the previous results we get

\[ ^2 \text{This is essentially equivalent to assume that each line is a permutation of other lines, which would be true for example in the case of Knuth's combinatorial matrices [1].} \]
Many relations of this kind may be derived and it is quite likely that all can be derived from replica equivalence can also proved using the method of [7, 8].

Some of these relations have been derived in [8] using a different technique.

For example we could spell the consequences of the condition

$$P_{12,31}^{12,34}(q_{12}, q_{34}) = \frac{2}{3}P(q_{12})P(q_{34}) + \frac{1}{3}P(q_{12})\delta(q_{12} - q_{34}).$$

(18)

These relations have a peculiar standing because they have been proved by Guerra [7] under quite general conditions. We can thus safely assume that they are correct, without any further reference to the replica method.

### 4.3 Three overlaps

Using the same method as before we obtain that replica equivalence implies the following relations:

$$6P_{12}^{12,13,14}(q_1, q_2, q_3) = P(q_1)P(q_2)P(q_3) + \delta(q_1 - q_2)P(q_1)P(q_3) + \delta(q_1 - q_3)P(q_1)P(q_2) + \delta(q_2 - q_3)P(q_1)P(q_2) + 2\delta(q_1 - q_2)\delta(q_2 - q_3)P(q_1).$$

(19)

$$6P_{12}^{12,13,34}(q_1, q_2, q_3) = 2P_{12}^{12,23,31}(q_1, q_2, q_3) + P(q_1)P(q_2)P(q_3) + \delta(q_1 - q_2)P(q_1)P(q_3) + \delta(q_2 - q_3)P(q_1)P(q_2) + \delta(q_1 - q_2)\delta(q_2 - q_3)P(q_1).$$

(20)

$$12P_{12}^{12,34,15}(q_1, q_2, q_3) = 2P_{12}^{12,23,31}(q_1, q_2, q_3) + 3P(q_1)P(q_2)P(q_3) + \delta(q_1 - q_2)P(q_1)P(q_3) + 3\delta(q_1 - q_3)P(q_1)P(q_2) + \delta(q_2 - q_3)P(q_1)P(q_2) + 2\delta(q_1 - q_2)\delta(q_2 - q_3)P(q_1).$$

(21)

$$15P_{12}^{12,34,56}(q_1, q_2, q_3) = 2P_{12}^{12,23,31}(q_1, q_2, q_3) + 5P(q_1)P(q_2)P(q_3) + 2\delta(q_1 - q_2)P(q_1)P(q_3) + 2\delta(q_1 - q_3)P(q_1)P(q_2) + 2\delta(q_2 - q_3)P(q_1)P(q_2) + 2\delta(q_1 - q_2)\delta(q_2 - q_3)P(q_1).$$

(22)

Some of these relations have been derived in [7] using a different technique.

It is remarkable that all the probability functions involving three overlaps can be computed from that with one overlap plus $P_{12}^{12,23,31}$. This last function if quite important because it contains the main information on the validity of ultrametricity.

### 4.4 Further consequences

If we look in more details to replica equivalence there are further relations that must be satisfied. For example we could impose that

$$T_a = \sum_{b,c}q_{b_1}^{k_1}q_{b_2}^{k_2}q_{b_3}^{k_3}$$

(23)

does not depend on $a$.

For example we could spell the consequences of the condition

$$\frac{\sum_a T_a^2}{n} = (\frac{\sum_a T_a}{n})^2$$

(24)

If we proceed as before we find that

$$6P_{12}^{12,23,31,14,45,51}(q_1, q_2, q_3, q_4, q_5, q_6) + P_{12}^{12,23,31}(q_1, q_2, q_3)\delta(q_4 - q_1)\delta(q_5 - q_2)\delta(q_6 - q_3) = P_{12}^{12,23,31}(q_1, q_2, q_3)P_{14,45,51}^{12,23,31}(q_4, q_5, q_6) + (25)

+ 3(P_{12}^{12,23,31,24,41}(q_1, q_2, q_3, q_5, q_6)\delta(q_4 - q_2) + P_{12}^{12,23,31,14,43}(q_1, q_2, q_3, q_4, q_5)\delta(q_3 - q_6).$$

Many relations of this kind may be derived and it is quite likely that all the equation that can be derived from replica equivalence can also proved using the method of [7, 8].
5 Ultrametricity

The ultrametricity condition states that the function $P_{12,23,31}$ can be written as

$$P_{12,23,31}(q_{12}, q_{23}, q_{13}) = \theta(q_{12} - q_{13})\delta(q_{23} - q_{13})A(q_{12}, q_{13}) + 2 \text{ cyclic permutations} + B(q_{12})\delta(q_{12} - q_{13})\delta(q_{23} - q_{13})$$

(26)

It is already been shown [15] that this condition and the previous relations, in particular eq. (17), implies that

$$A(q_{12}, q_{1,3}) = P(q_{12})P(q_{1,3})$$

$$B(q_{12}) = x(q_{12})P(q_{12})$$

(27)

where

$$x(q) = \int_0^q dq' P(q')$$

(28)

and we have assumed for simplicity that the support of the function $P(q)$ is within the interval [0-1].

This relation has been proved [15] by noticing that

$$\int_0^1 dq_{23} P_{12,23,31}(q_{12}, q_{23}, q_{13}) = P_{12,13}(q_{12}, q_{13}).$$

(29)

The r.h.s is given by eq. (17) while the l.h.s. is given by

$$A(q_{12}, q_{13}) + \int q_{12} dq' (A(q_{12}, q')\delta(q_{12} - q_{13}) + B(q_{12})\delta(q_{12} - q_{13})).$$

(30)

We finally find that the usual result (27) is correct.

In the same way it can be proved that in the ultrametric case also the other probability distribution involving more overlaps e.g. $P_{12,23,34,41}(q_{12}, q_{23}, q_{34}, q_{41})$ are uniquely determined in terms of the only independent function $P(q)$.

The argument is quite similar to the previous one. Ultrametricity implies that

$$P_{12,23,34,41}(q_{12}, q_{23}, q_{34}, q_{41}) = \theta(q_{12} - q_{13})\theta(q_{23} - q_{34})\delta(q_{34} - q_{14})A(q_{12}, q_{23}, q_{34}) + \text{ permutations + delta functions}.$$  

(31)

On the other hand

$$\int dq_{41} P_{12,23,34,41}(q_{12}, q_{23}, q_{34}, q_{41}) = P_{12,23,34}(q_{12}, q_{23}, q_{34})$$

(33)

and the r.h.s is known from replica equivalence.

Generally speaking ultrametricity implies that the probability distribution of the overlaps of $m$ replicas, which is a priori a function of $m(m - 1)/2$ variables, depends only on $m - 1$ variables and therefore, using the relations coming from the replica equivalence, is determined by the probability distribution with a smaller number of replicas.

Given the function $P(q)$ there is one and only one ultrametric set of probabilities satisfying the principle of replica equivalence. We shall see in the next section how the ultrametric distribution may be characterized using a variational principle.
6 A variational approach

6.1 The variational equations

We now apply this formalism to the study of the infinite range Sherrington Kirkpatrick model near \( T_c \).

The model is defined as follows:

\[
H = \frac{1}{2} \sum_{i,k=1,N} J_{i,k} \sigma_i \sigma_k, \tag{34}
\]

where the \( J \)'s are random Gaussian variables with zero average and variance \( N^{-1/2} \).

In the replica approach the free energy density can be obtaining by finding the minimum with respect to the matrix \( Q \) the function \( F(Q) \) defined as:

\[
F(Q) = \frac{\beta^2}{2n} \text{Tr} Q^2 - \frac{1}{n} \ln(\sum_{a,b} \exp(\sum_{a,b} Q_{a,b} \sigma_a \sigma_b)). \tag{35}
\]

The definition of minimum is rather tricky: we say that \( F(Q) \) has a minimum if its Hessian

\[
\mathcal{H}_{ab,cd} = \frac{\partial^2 F}{\partial Q_{ab} \partial Q_{cd}} \tag{36}
\]

has non negative eigenvalues. This condition may result as a minimum or as a maximum condition as function of the parameters on which the matrix \( Q \) depends.

Near the critical temperature, where \( Q \) is small, \( F(Q) \) can be approximated (neglecting terms which do not play a crucial role) as:

\[
F(Q) = \frac{1}{n} (-\frac{\tau}{2} \text{Tr}(Q^2) + \frac{1}{3} \text{Tr}(Q^3) - \frac{y}{4} \sum_{ab} Q_{ab}^4). \tag{37}
\]

Let us concentrate our attention on the function \( F(Q) \). Its value is given by

\[
W[\mathcal{P}] = \int dq_{12} P(q_{12})(\frac{\tau}{2} q_{12}^2 + \frac{y}{4} q_{12}^4) - \frac{1}{3} \int dq_{12} dq_{13} dq_{23} P^{12,23,31}(q_{12}, q_{13}, q_{23}) q_{12} q_{13} q_{23}, \tag{38}
\]

where we indicate with \( \mathcal{P} \) the whole set of \( P \) functions, which can be computed in terms of the matrix \( Q \). Near \( T_c \), where we can approximate the \( F(Q) \) with a polynomial, only a finite number of \( P \) functions are relevant.

Now there is a apparently strange phenomenon. We have remarked that the matrix \( Q \) is a compact form for coding the probability functional \( \mathcal{P} \) and it does not contains extra information. We would thus expect that the equations we get from the condition

\[
\frac{\partial W}{\partial Q_{a,b}} = 0 \tag{39}
\]

are the same that those obtained from the condition

\[
\frac{\delta W}{\delta \mathcal{P}} = 0. \tag{40}
\]

This is not the case. Equation (39) implies that

\[
\tau Q_{a,b} + y Q_{a,b}^3 = \sum_c Q_{a,c} Q_{c,b}. \tag{41}
\]
This equation correspond to an infinite set of equations for the probability distribution. For example if we multiply it by $Q^k_{a,b}$ for arbitrary $k$ we arrive to the equation

$$P(q)(\tau q + yq^3) = \int dsdtP^{12,23,31}(q, s, t)st$$  \tag{42}

If we square it and we multiply again by $Q^k_{a,b}$ for arbitrary $k$ we arrive to the equation

$$P(q)(\tau q + yq^3)^2 = \int dsdtP^{12,23,31}(q, s, t)s^2t^2$$
$$+ \int dsdtdudvP^{12,23,31,24,41}(q, s, t, u, v)stuv.$$  \tag{43}

On the other hand the equation (40) depends only on the probabilities with one or three overlaps. Different forms of the matrix $Q$ which gives the same probability distributions with one and three overlaps, will give the same value of the free energy.

In the usual approach we do not see any difference among equations (40) and (39). The key point is separability (discussed in the next section) which is satisfied in the usual approach. Separability implies that the equation (43) is a consequence of equation (42). In the usual approach the construction of the matrix $Q$ has been done using symmetry principles. The matrix $Q$ depends on a sets of parameters $q$ and the equation (39) is equivalent to

$$\frac{\partial F}{\partial q} = 0.$$  \tag{44}

If we work from a general point of view, the two equations looks rather different. It is clear that (39) contains more information than (40) if we stay in case in which the separability conditions does not hold, however the last one should be enough to compute the free energy in any case.

Let us try to spell out the consequences of eq. (40). It is clear that we cannot change all the $P$ in an independent way.

- The probability with more than one overlaps are obviously related to that with less overlap.
- We have the constraint that the probabilities are not negative.
- On top of all these requirements Guerra’s relations should be satisfied.

We propose the following variational principle which should equivalent the the usual one: the free energy and the correct probability distributions are obtained by finding the maximum of the functional $W[P]$ with respect to the function $P(q)$ and finding the minimum with respect to the other function $P^{12,23,31}$. This principle is applied in the region where all the previous constraints are satisfied. In other words we suppose the probability are non negative and that

$$\int dq_{1,2}P^{12,23,31}(q_{1,2}, q_{1,3}, q_{2,3}) = P^{12,23}(q_{1,2}, q_{2,3}) = \frac{1}{2}P(q_{1,2})P(q_{1,3}) + \frac{1}{2}P(q_{1,2})\delta(q_{1,2} - q_{1,3})$$  \tag{45}

The equation (45) is extremely important because it tell us we cannot change the function $P^{12,23,31}(q_{1,2}, q_{1,3}, q_{2,3})$ in an arbitrary way.

It may looks strange to maximize with respect to one parameter and to minimize with respect to an other, but this is quite a common situation in the replica approach [1].
We will argue now that this variational principle gives the usual ultrametric solution. It is clear that if ultrametricity is assumed, we recover the older approach, where the free energy is maximized with respect to $P(q)$. The only thing we have to prove is that the minimization with respect to $P_{12,23,31}$ at fixed $P(q)$ implies ultrametricity. In order to see how it could be done let us consider two simple case.

6.2 An example: the overlap has two possible values

In the first case the overlap can take two values $q_0$ with probability $p_0$ and $q_1$ with probability $p_1$ (we suppose $q_0 < q_1$). For the three overlaps we have four possibilities (all three are equal to $q_1$, two to $q_1$ and one to $q_0$ . . . ) and the corresponding probabilities are denoted $p_{111}, p_{110}, p_{100}, p_{000}$ with obvious notation. The free energy is thus

$$F = P_0 \left(\frac{\tau}{2} q_0 + \frac{y}{4} q_0^3\right) + P_1 \left(\frac{\tau}{2} q_1 + \frac{y}{4} q_1^3\right) - \frac{1}{3} \left(p_{111} q_1^3 + 3p_{110} q_1^2 q_0 + 3p_{100} q_1 q_0^2 + p_{000} q_0^3\right)$$

We have that:

$$p_{111} + p_{110} = p_{11} = \frac{1}{2}(p_1^2 + p_1),$$
$$p_{110} + p_{100} = p_{10} = \frac{1}{2}p_1 p_0,$$
$$p_{100} + p_{000} = p_{10} = \frac{1}{2}(p_0^2 + p_0).$$

The second equalities of each line follow from Guerra’s relations. The previous relations can be written as

$$p_{111} = \frac{1}{2}(p_1^2 + p_1) - u,$$
$$p_{110} = u,$$
$$p_{100} = \frac{1}{2} p_1 p_0 - u,$$
$$p_{000} = p_0^2 - u.$$

Let us concentrate our attention on the dependence of the free energy on $u$. We find that

$$F(u) = F(0) + u(q_1 - q_0)^3.$$  

The coefficient of $u$ is positive and the minimum of the free energy with respect to $u$ is located at the minimum value of $u$, i.e. $u = 0$. It is crucial to note that $u = 0$ is just the condition which follows from the ultrametricity condition. Using the result $u = 0$ the remaining parameters and be computed as usual.

6.3 An other example: the overlap has three possible values

The same phenomenon happens if we consider a more complicated situation: three of more values of the overlap. Let us study what happens for three possible values of the overlap. After some algebra one finds

$$p_{222} = \frac{1}{2} (p_2 + p_2^2) - a - b, \quad p_{221} = a, \quad p_{220} = b,$$
One finds finally the free energy depends on $a$, $b$, $c$ and $d$ as follows

$$F(a, b, c, d) = F(0, 0, 0, 0) + a(q_2 - q_1)^3 + b(q_2 - q_0)^3 + d(q_1 - q_0)^3 + c(q_1 - q_0)^2(3q_2 - q_1 - 2q_0).$$

All the coefficients are positive definite in the region where $q_0 < q_1 < q_2$. The minimum of the free energy is reached at $a = b = c = d = 0$, and the ultrametricity conditions are satisfied.

In general the distribution probability of three replicas can be written as a form which satisfies the ultrametricity relations plus a reminder. The dependence of the free energy on the reminder is linear and therefore its minimum is located just at the boundary of the allowed region. The sign structure is crucial to obtain that the boundary which corresponds to a minimum is located at the point at which the ultrametricity violations have the minimum possible value (i.e. zero). Once that the ultrametricity structure is recovered, the expression for the free energy is the usual one.

We are thus in the strange situation: in order to obtain the ultrametric solution we must maximize the free energy with respect to the function $P(q)$, but minimize it with respect to the other parameters which describe the violations of the ultrametricity.

On the other hand, the other possibility, the one which correspond to maximize everything, produces a maximal violation of the ultrametricity which would give rather nonsensical results. Indeed in the first case we would get $p_{100} = 0$ and $p_{110} > 0$, which would clash with the interpretation in terms of states. If $q_{1,2} = q_1$ 1 and 2 belongs to the same state and if $q_{1,3} = q_1$ 1 and 3 belongs to the same; by transitivity 1 and 3 must belong to the same state and consequently $q_{13} = q_1$.

It is also not clear if the non ultrametric solution does have a replica interpretation, i.e. there is an associated matrix $Q$.

It is likely worthwhile to look again to the equations coming from the cavity approach using as far as possible a general approach in which the ultrametricity is not assumed in order to see if there exists a non-ultrametric solution. Equation (40) or equivalently its consequences eqs. (41, 42) should be derivable in the framework of the cavity approach. It may be possible that subleading terms must be considered in order to obtain interesting results.

## 7 Other algebraic structures

We have seen in the previous section that ultrametricity is an extremely powerful constraint and that there is only one ultrametric probability distribution at fixed $(P(q))$. In this section we explore other algebraic properties that are present in the usual solution. The aim is to characterize as far as possible the probability distribution in order to find how much space there is for non ultrametric solutions, which should still have good properties.

The properties which we are going to consider are translational invariance in replica space and separability.
7.1 Translational invariance

Replica equivalence implies that all replicas are equivalent. The simplest way to implement it is to assume that there is a group \( G \) (a subgroup of the group of permutation of \( n \) elements) which leaves the matrix \( Q \) invariant and acts transitively on the space of indices (i.e. for any pairs \( a, b \) there is element \( g \) of the group such that \( g \cdot a = b \)).

The simplest group we can think of, as suggested by Kondor, is the translational group, i.e. the group generated by the operation \( a \to a + 1 \) (all sums and differences are done modulo \( n \), in this section). It was later realized by Sourlas that by reshuffling the indices the usual form of matrix \( Q \) in presence of replica symmetry breaking can be put in such a way to be translational invariant. In this new base we have

\[
Q_{a,b} = q(a - b). \tag{52}
\]

Translational invariance is quite useful at the technical level: the matrix product becomes now a convolution which can be easily done by Fourier transform. Using this fact, if we call \( s \) the variable of the Fourier transform, one finds that there exists a function \( F(q, s) \) such that

\[
\int d\mu(s) F(q_1, s) F(q_2, s) = P(q_1) \delta(q_1 - q_2),
\]

\[
\int d\mu(s) F(q_1, s) F(q_2, s) F(q_3, s) = P_{12,23,31}(q_1, q_2, q_3). \tag{53}
\]

Similar relations can be found for probabilities involving a high number of \( q \) (i.e for \( P_{12,23,34,41}, P_{12,23,34,45,51} \) and so on). These relations are not on the same standing of the ones derived in the previous sections because they do not allow us to write algebraic equations involving a finite set of probability distributions; they however strongly constrain the set of allowed probability distributions.

At this stage it is not clear how to exploit the consequences of translational invariance on the probability distribution. It seems reasonable to assume that not all the probability distributions which satisfy replica equivalence can be generated by a matrix \( Q_{a,b} \) which is translational invariant, but it is no so easy to find a counterexample. It is not clear if the alternative scheme introduced in can be extended in such a way to have a probability interpretation.

An answer to these questions would be interesting, because it would help us to elucidate the origine of the rather mysterious translation invariance in replica space.

7.2 Separability

Separability (or non degeneracy) correspond to the following algebraic statement. Let us consider all the matrices which can be generated from the matrix \( Q \) in a permutational covariant fashion. Some example are

\[
Q_{ab}^k, \sum_c Q_{ac} Q_{cb}, \sum_{c,d} Q_{ac} Q_{ad} Q_{cd} Q_{cb} Q_{db}. \tag{54}
\]

Separability states that if we take two pair of indices \((ab \text{ and } cd)\), we have that

\[
Q_{ab} = Q_{cd} \longrightarrow M_{ab} = M_{cd} \tag{55}
\]

where \( M \) is a generic matrix of the set generated by the rules (54). In other words pairs of indices which have different properties have a different values of \( Q \).
In the usual approach when replica symmetry is broken there is subgroup of the group of permutations that commutes with the matrix $Q$. Let us consider the orbits in the space of pairs of indices. It evident that the values of the elements of the matrix $Q$ and of any matrix derived using the rules are constant of the orbits. If we assume that different orbits have different value of the matrix $Q$ we obtain the condition (57).

The separability condition is extremely powerful in determining the expectation values of higher order moments of the probability distribution.

Let us study a simple example and let us consider a matrix $M$ constructed with the rules (54). It is evident that if

$$
\sum_b Q_{a,b}^k M_{a,b} = \int dq P(q) M(q) q^k, \quad \sum_b Q_{a,b}^k R_{a,b} = \int dq P(q) R(q) q^k
$$

we have that

$$
\sum_b Q_{a,b}^k M_{a,b} R_{a,b} = \int dq P(q) M(q) R(q) q^k.
$$

If we apply the previous formula to the case where $M$ and $R$ have the form

$$
M_{ab} = \sum_c Q_{ac}^{k_1} Q_{cb}^{k_2}, \quad R_{ab} = \sum_c Q_{ac}^{k_3} Q_{cb}^{k_4}
$$

we find the rather surprising formula

$$
3 P_{12,13,32,14,42}(q, q_1, q_2, q_3, q_4) = \delta(q_1 - q_3) \delta(q_2 - q_4) P_{12,23,31}(q, q_1, q_2)
+ 2 \int \frac{P_{12,23,31}(q, q_1, q_2) P_{12,23,31}(q, q_3, q_4)}{P(q)}. \quad (59)
$$

Similar results can be obtained for other probability distributions.

Equation (59) is particular interesting because integrating over $q$ it implies that

$$
3 P_{13,32,14,42}(q_1, q_2, q_3, q_4) = \delta(q_1 - q_3) \delta(q_2 - q_4) (P(q_1) P(q_2) + \delta(q_1 - q_2) P(q_2))
+ 2 \int dq \frac{P_{12,23,31}(q, q_1, q_2) P_{12,23,31}(q, q_3, q_4)}{P(q)}. \quad (60)
$$

This equation can also written in more suggestive form as

$$
3 P_{13,32,14,42}(q_1, q_2, q_3, q_4) = \delta(q_1 - q_3) \delta(q_2 - q_4) (P(q_1) P(q_2) + \delta(q_1 - q_2) P(q_2))
+ 2 \int dq P_{12,23,31}(q, q_1, q_2) P_{23,31,12}(q_3, q_4 | q), \quad (62)
$$

where $P_{23,31,12}(q_3, q_4 | q)$ is a conditional probability.

Now the l.h.s of eq. (61) is by definition invariant under cyclic permutation of the $q$’s, while the r.h.s in not invariant for a generic choice of the function $P_{12,23,31}$. A boring computation is needed to verify that if we insert the ultrametric result of the previous section, we find a symmetric result (as we should) for $P_{13,32,14,42}$. It not clear which is the most general form of the of the probability $P_{12,23,31}$, which gives is compatible with separability. We have checked what happens in the case of two or three possible values of the overlaps, discussed in the previous section.

- In the case of two possible values of the overlap, the only non trivial relation is

$$
P_{13,32,14,42}(q_0, q_1, q_0, q_1) = P_{13,32,14,42}(q_1, q_1, q_0, q_0).
$$

An explicit computation shows that this relation is identically satisfied.
• In the case of two possible values of the same relation would is not identically satisfied, however it is satisfied for $a = b = c$ with arbitrary $d$.

The previous examples shows that separability does not imply ultrametricity in the general case, but impose rather strong constraints on the distributions functions $P$.

This relations coming from separability are quite powerful in imposing further constraint on the probability distribution beyond replica equivalence. Their origins can be well understood in an algebraic framework, however it is not clear if they can be derived in a more general setting. It would be extremely interesting to check if they are satisfied in numerical simulations.

Acknowledgments

It is a pleasure to thank Francesco Guerra and Imre Kondor for illuminating discussions. I am also grateful to M. Aizenman and F. Contucci for communicating to me (prior to publications) their work [8], which strongly overlaps with this one and for further correspondence.

References

[1] M. Mézard, G. Parisi and M. A. Virasoro, *Spin Glass Theory and Beyond*, World Scientific, (Singapore 1987).

[2] G. Parisi, *Field Theory, Disorder and Simulations*, World Scientific, (Singapore 1992).

[3] G. Parisi, J. Stat. Phys. 51, 51 (1993).

[4] S. F. Edwards and P. W. Anderson, J. Phys. F 5, 965 (1975).

[5] C. M. Newman and D. L. Stein, Phys. Rev. B 46 973 (1992).

[6] G. Parisi, in *Disordered Systems and Localization*, C. Castellani, C. Di Castro and L. Peliti eds, Springer-Verlag, Berlin (1981); G. Parisi and M. A. Virasoro, J. Phys. 50, 3317 (1989); S. Caracciolo, G. Parisi, S. Patarnello and N. Sourlas, J. Phys. I (France) 51, 1877 (1990); S. Franz, G. Parisi and M. A. Virasoro, J. Phys. I France 2, 1869 (1992); A. Cavagna, I. Giardina and G. Parisi, J. Phys. A: Math. Gen. 30, 7021 (1997).

[7] F. Guerra, Int. J. Phys. B 10 1675 (1997).

[8] M. Aizenman and P. Contucci, *On the stability of the quenched state in mean field spin glass models*, [cond-mat 9712129](https://arxiv.org/abs/cond-mat/9712129).

[9] D. E. Knuth, *Combinatorial Matrices*, Institut Mittag-Leffler preprint, unpublished (1991).

[10] B. Lautrup, *Uniqueness of Parisi’s Scheme for Replica Symmetry Breaking*, Niels Bohr preprint, unpublished (1991).

[11] I. Kondor A note on replica symmetry breaking, Frankfort University preprint, unpublished (1982).

[12] N. Sourlas (unpublished).
[13] G. Parisi and N. Sourlas, in preparation.

[14] C. De Dominicis, D. M. Carlucci and T. Temesvari, J. Phys. I France 7, 105 (1997) D. M. Carlucci and C. De Dominicis *On the Replica Fourier Transform* cond-mat/9709200

[15] D. Iniguez, G. Parisi and J.J. Ruiz-Lorenzo, J.Phys. A29 (1996) 4337.