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The replica method on and off equilibrium

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Abstract. — In this paper we show that the investigation of all thermodynamically relevant equilibrium configurations and some non equilibrium ones in a SK spin glass model can be studied using the replica method applied on a system composed of \(R\) real replicas constrained to have fixed values of the overlaps between themselves. Most of the results presented here are restricted to the case \(R = 2\).

1. Introduction.

In the infinite range spin glass at low temperature, replica symmetry is broken in a hierarchical fashion. This breaking implies the existence of an infinity of pure (equilibrium) states with properties described by the form of the matrix \(Q_{ab}\), the order parameter that characterizes the breaking of the replica symmetry [1].

The probability of each state at equilibrium is usually denoted by \(w_\alpha\). Most of the results presented in the literature deal with states which have a finite \(w\) in the infinite volume limit. However from the thermodynamic point of view all states which have the same free energy density should be considered. Furthermore one is often interested in states which differ from the equilibrium Gibbs states (where \(P \propto \exp(-\beta H)\)) by the addition of a small term in the Hamiltonian density. In other words one tries to control the properties of all the (equilibrium) states such that \(\delta_\alpha = -\lim_N w_\alpha\) is equal to zero, but one would also like to have information on those non-equilibrium, metastable states for which \(\delta_\alpha\) is not zero but small. In particular if we find that all the pure states for \(\delta_\alpha = 0\) satisfy a given property, it is interesting to know which is the minimum value of \(\delta_\alpha\) at which such property is violated.

In a normal system solved in the Mean Field Approximation the answer to some of these questions is directly contained in the free energy function, when considered as a function of the order parameter at values different from the minimum. When the Replica method is involved
this is not in general possible: the free energy that comes out has no physical meaning for values other than the saddle point.

We show that in the latter case the answer to those questions requires the study of a system composed by $R$ real replicas interacting among themselves. If we concentrate our attention to the probability distribution of the overlap of two states $\alpha$ and $\gamma$ defined as:

$$q_{\alpha \gamma} = \frac{1}{N} \sum_i S_i^\alpha S_i^\gamma,$$

we find that the appropriate interaction consists in a constraint on the overlap between replicas.

It is known that the probability distribution of the overlap $P(q)$ has support in the interval $[q_{\min}, q_{\max}]$. In other words the overlaps of all the states with non vanishing $w$ belong to this interval. Here we show that this is true even if we consider states with vanishing $\delta$ and compute the exponentially small probability for finding configurations with $q$ outside that interval. In a future paper we plan to discuss the problem of the distribution probability of three replicas using the same techniques. The very interesting case of configurations that violate ultrametricity will be discussed there.

2. The model.

Let us consider a system composed of $R$ real replicas of a Sherrington Kirkpatrick (SK) spin glass model constrained to have fixed values of their mutual overlaps. Denoting by $S_i^r$ the $i$-th spin of the $r$-th replica, we fix a constraint matrix

$$q_{rs}^C = \frac{1}{N} \sum_{i=1}^N S_i^r S_i^s,$$

where $N$ is the total number of spins. The Hamiltonian of the system is

$$H = -\sum_{i<j}^R J_{ij} S_i^r S_j^s + h \sum_{r=1}^R \sum_i S_i^r.$$

We take for each real replica the same realization of the quenched $\{J_{ij}\}$ chosen with Gaussian probability, zero mean and variance $1/N$, as well as the same magnetic field $h$. The partition sum is restricted to those spin configurations that satisfy (2). Practically we implement the constraint (2) introducing a set of Lagrange multipliers $\epsilon_{rs}$ in such a way that

$$Z = \sum_{\{S\}} \int_{-i\infty}^{i\infty} \frac{d\epsilon_{rs}}{2\pi} \exp \left( -\beta H_{\text{eff}}(\{S\}, \{\epsilon\}) \right),$$

$$H_{\text{eff}}(\{S\}, \{\epsilon\}) = H(\{S\}) - \frac{1}{\beta} \sum_{r<s} \epsilon_{rs} \left( \sum_i S_i^r S_i^s - N q_{rs}^C \right).$$

Instead of fixing the matrix $q_{rs}^C$, we can equivalently consider the partition function corresponding to the Hamiltonian (4) for fixed $\epsilon_{rs}$. This corresponds to systems coupled by a forcing term. The two description are obtained one from the other in the thermodynamic limit by a Legendre transformation. In the following we will adopt the point of view of fixing the matrix $q_{rs}^C$, but we will make some comments on the result obtained from the other point of view.

Different choices for the matrix $q_{rs}^C$ will have different effects on the system. Let us consider an unconstrained system composed of $R$ real replicas. Below $T_c$ ergodicity is broken, several
pure states are present. The values taken by the overlap matrix in an experiment are subject to a probability law \( P_{eq}(\{q_{rs}\}) \). As the multiplicity of pure states does not contribute to the entropy (their number grows less then exponentially with \( N \)), we expect that if we choose a constrain matrix \( q_{rs}^c \) with non-zero \( P_{eq}(\{q_{rs}\}) \), the only effect will be to select those pure states that respect the imposed relationships, without changing the density of free-energy or other extensive quantities. Conversely if we choose a constraint forbidden by the \( P_{eq}(\{q_{rs}\}) \), the relevant contributions to the partition sum will come from non-equilibrium configurations, and the free energy could increase.

Introducing replicas to average over the disorder, we derive the average partition function to the power \( n \)

\[
\overline{Z}^n = \sum_{\{S_{rs}^\alpha\}} \exp \left( \frac{\beta^2}{2N} \sum_{i<j} \left( \sum_r \sum_a S_i^r a S_j^r a \right)^2 + \sum_{r<s} \sum_a \epsilon_{rs}^a \left( \sum_i S_i^r a S_i^r a - N q_{rs}^c \right) + \beta h \sum_{i,r,a} S_i^r a \right) .
\]

(5)

Any replica is labelled by the two indices \((a, r)\).

For certain values of the matrix \( q_{rs}^c \), (5) may be invariant under a replica permutation group larger than the usual one of permutations of the indices \( a, P_n \). For instance if \( q_{rs}^c = q_{cs}^C \) for all \( r \neq s \), then the resulting group of invariance is \( P_n \otimes P_R^\infty \). A small difference in the magnetic field acting on the real replicas, could remove this symmetry. Standard manipulations on \( \overline{Z}^n \) lead to:

\[
\text{S.P.} \exp \left( \frac{nN \beta^2}{2} - \frac{N \beta^2}{2} \sum_{s<s'} Q_{ss'}^2 - N \sum_{s<s',a} \epsilon_{rs}^a q_{rs}^c - \frac{N \beta^2}{2} \sum_{s<s',a} \epsilon_{rs}^a \left( \frac{\epsilon_{rs}^a}{\beta^2} - 2Q_{aa}^r \epsilon_{rs}^a \right) \right)
\]

\[
\left[ \sum_{\{S_{rs}^\alpha\}} \exp \left( \beta^2 \sum_{s<s',a} Q_{ss'}^2 S_{ss'}^\alpha + \beta h \sum_{\alpha} S_{ss'}^\alpha \right) \right]^N,
\]

(6)

where by S.P. we denote the value computed at the saddle point and \( \alpha \) and \( \beta \) are the couples of indices \((r, a), (s, b)\) ordered in the following way:

\[
\begin{align*}
(r) & < (s) \quad \text{if} \ r < s \quad \text{when} \ r \neq s, \\
(r) & < (s) \quad \text{if} \ a < b \quad \text{when} \ r = s.
\end{align*}
\]

(7)

The \( R_n \times R_n \) matrix \( Q_{s:b} \) has the following meaning

\[
Q_{s:b} = Q_{ss}^b = \sum_i (S_i^r a S_i^r b) \quad a \neq b;
\]

(8)

\[
Q_{s:s} = Q_{ss}^s = \sum_i (S_i^r a S_i^r a) + \frac{1}{\beta} \epsilon_{rs}^a \quad a = b.
\]

(9)

The unusual term in the element \( Q_{s:s}^s \) is introduced in the matrix for convenience.

We eliminate at this point the Lagrange multipliers \( \epsilon_{rs}^a \), in (6) replacing their saddle point values. This gives, for the \( \epsilon \) dependent term of \( \overline{Z}^n \)

\[
- N \sum_{r<s,a} \epsilon_{rs}^a q_{rs}^c - \frac{N}{2} \sum_{r<s,a} \left( \frac{\epsilon_{rs}^a}{\beta^2} - 2Q_{aa}^r \epsilon_{rs}^a \right) = N \frac{\beta^2}{2} \sum_{r<s} (Q_{aa}^r - q_{rs}^c)^2.
\]

(10)
To solve the model we need a variational ansatz for the matrix $Q_{\alpha\beta}$. We choose each of the $n \times n$ blocks, (labelled by $r, s$) to be a Parisi hierarchical matrix, parametrized in terms of a diagonal term $Q_{rr}^{rs} = \tilde{q}_{rs}$ and a function $q_{rs}(x)$ of the interval $[0, 1]$. The symmetry of the overlap matrix implies $\tilde{q}_{rs} = \tilde{q}_{sr}$ and $q_{rs}(x) = q_{sr}(x)$.

We now assume a finite number of steps of RSB

$$ q^{rs}(x) = q_{i}^{rs}, \quad m_i \leq x \leq m_{i+1} \quad (11) $$

The parameters $m_i$ are equal for all the $r, s$. The matrices of this form close in an algebra similar to that of reference [2]. Non constant $q^{rs}(x)$ correspond to the usual scheme of breaking of $P_n$. Below $T_c$ replica symmetry is broken. An analytical evaluation of the free energy and of the order parameter functions appears hopeless, although approximations with a finite number of steps of RSB are feasible. The situation is different near $T_c$, where the $Q_{\alpha\beta}$ are small parameters and the free energy functional can be expanded in powers. The expansion reads:

$$ FR = -\frac{1}{nR} \left\{ \tau \Tr Q^2 + \frac{1}{3} \Tr Q^3 + \frac{y}{4} \sum_{\alpha\beta} Q_{\alpha\beta}^4 + \hbar^2 \sum_{\alpha\beta} Q_{\alpha\beta} \right\} - \frac{1}{2R} \sum_{r<s} (\tilde{q}^{rs} - q_{rs}^C)^2, \quad (12) $$

with $\tau = T_c - T$ and $y = 2/3$ in the case of SK model. We have truncated the model as usual by including all the terms up to the third power in $Q$ and a fourth order term that is responsible for replica symmetry breaking [2].

In the following section we will study the saddle point equations for the truncated model for $R = 2$.

3. The Saddle Point equations and their solutions.

For the truncated model with $R = 2$ the matrix (9) takes the form

$$ Q_{11}^{11} = Q_{22}^{22} = Q_{ab} $$
$$ Q_{12}^{21} = Q_{21}^{21} = P_{ab} \quad (13) $$

where $Q$ and $P$ are $n \times n$ matrices of the usual hierarchical form, parametrized respectively as

$$ Q_{ab} \rightarrow (\tilde{q} = 0, q(x)) $$
$$ P_{ab} \rightarrow (\tilde{p} = p_d, p(x)). \quad (14) $$

In terms of this parametrization the variational free-energy can be written as

$$ F_2 = \tau [(q^2) + (p^2) - p_d^2] $$
$$ -\frac{1}{3} [2(q)(q^2) + \int_0^1 dxq(x) \int_0^x dy(q(x) - q(y))^2 + 6pq(\langle p \rangle - p_d) + $$
$$ 3 \int_0^1 dxq(x) \int_0^x dy(p(x) - p(y))^2] + $$
$$ \frac{y}{4} [(q^4) + (p^4) - p_d^4] + \hbar^2 [(q) + (p) - p_d] - \frac{1}{4} (p_d - q^C)^2, \quad (15) $$

having denoted $< f > = \int_0^1 dx f(x)$. 

Our task now is to evaluate the value of the free energy at the saddle point. Variations of (15) lead to:

\[
\frac{\delta F_2}{\delta q(x)} = 2(\tau - \langle q \rangle)q(x) + 2(p_d - \langle p \rangle)p(x) - \int_0^x dy(q(x) - q(y))^2 \\
- \int_0^x dy(p(x) - p(y))^2 + yp^3(x) + h^2 = 0,
\]

(16)

\[
\frac{\delta F_2}{\delta p(x)} = 2(\tau - \langle q \rangle)p(x) + 2(p_d - \langle p \rangle)q(x) \\
- 2 \int_0^x dy(q(x) - q(y))(p(x) - p(y)) + yp^3(x) + h^2 = 0,
\]

(17)

\[
\frac{\delta F_2}{\delta p_d} = -[2\tau p_d - 2(pq) + yp^3 + h^2] - \frac{1}{2}(p_d - q_i) = 0,
\]

(18)

For future reference we substitute (17) with \( x = 1 \) into (18) simplifying the latter to

\[
(p(1) - p_d)[2(\tau - q(1)) + y(p^2(1) + p_d^3 + p(1)p_d)] - \frac{1}{2}(p_d - q^C) = 0.
\]

(19)

Equation (10) reads in this case

\[
\epsilon = 2(p(1) - p_d)[2(\tau - q(1)) + y(p^2(1) + p_d^3 + p(1)p_d)].
\]

(20)

Note that \( \epsilon \) is proportional to the difference between \( p(1) \) and \( p_d \).

The structure of the saddle point equation is very similar to the one found in [2] for the unconstrained problem. Let us remind ourselves briefly what are the results for this case:

The free saddle point equation is

\[
\frac{\delta F_{\text{free}}}{\delta q(x)} = 2(\tau - \langle q \rangle)q_F(x) - \int_0^x dy(q_F(x) - q_F(y))^2 \\
+ yq_F^3(x) + h^2 = 0.
\]

(21)

Depending on the values of the temperature and the magnetic field, RS is broken or not; above the deAlmeida-Thouless (dAT) line, \( h^2 = \frac{\tau^3}{2y} \), RS holds, while below the solution of (21) that maximizes \( F \) is the RSB

\[
q_F(x) = \begin{cases} 
q_{\text{min}} & 0 \leq x \leq x_{\text{min}} \\
\frac{x}{3y} & x_{\text{min}} \leq x \leq x_{\text{max}} \\
q_{\text{max}} & x_{\text{max}} \leq x \leq 1
\end{cases}
\]

(22)

where \( q_{\text{min}} = (h^2/2y)^{\frac{1}{2}}, \) \( x_{\text{min}} = 3yq_{\text{min}}, \) \( q_{\text{max}} = \frac{1 - \sqrt{1 - 6y\tau}}{3y}, \) \( x_{\text{max}} = 3yq_{\text{max}}. \) The possible values of the overlap between pure states found in an ideal experiment are restricted to the interval \([q_{\text{min}}, q_{\text{max}}]\).

Several solutions with different symmetries can be envisaged for equations (16, 17). A first distinction can be made between solutions symmetric or not under \( P_2^n \). In the first case

\[
q(x) = p(x) \quad \text{for all} \ x
\]

(23)
while in the second the two functions differ for same value of \( x \). Secondly we can distinguish solutions symmetric or not under \( P_n \) corresponding respectively to constant or variating functions of \( x \).

For \( q(x) = p(x) \), equations (16) and (17) coincide with eq. (21) for a free system with parameters \( \tau' = \frac{\tau + p_d}{2}, \ y' = y/2 \ h' = \frac{h}{\sqrt{2}} \). We know therefore its solution as a function of \( p_d \). The dAT line of the \( p(x) = q(x) \) solution, above which Replica Symmetry is restored is \( y h^2 = \left( \frac{\tau + p_d}{2} \right)^3 \). By direct inspection, we can verify that the value of the function \( q(x) \) in 1

\[
q(1) = \frac{1 - \sqrt{1 - \frac{3}{2} y (\tau + p_d)}}{\frac{3}{2} y}
\]

coincides with \( p_d \) for

\[
p_d = \frac{1 - \sqrt{1 - 6 y \tau}}{3 y},
\]

i.e. for \( p_d = q_{\text{max}} \). In this case \( p_d - q^C = \epsilon = \frac{\partial F}{\partial q_{s}} = 0 \) and it can be easily verified that the corresponding free energy coincides with that of the free system (with parameters \( \tau, y, h \)). For \( p_d \neq q_{\text{max}} \), and \( q^C \) fixed, \( \epsilon \) is given, to the lowest order in \( \tau \) by

\[
\epsilon = \frac{(\tau - q^C)^2}{2}
\]

(to that order \( q_{\text{max}} = \tau \).

We see that within the frame of this solution \( \epsilon \) is always positive except for \( q^C = \tau \) (more precisely we could write \( q^C = q_{\text{max}} \)). The free energy of the solution is an increasing function of \( q^C \), equal to \( F_{\text{free}} \) for \( q^C = \tau \). While it is perfectly reasonable that for \( q^C > q_{\text{max}} \) the free energy is bigger than \( F_{\text{free}} \), the result for \( q^C \leq q_{\text{max}} \) is unphysical. It is not possible that a constrained system has a free energy smaller than the corresponding unconstrained one. This leads us directly to the possibility of breaking the \( P_2^{\otimes n} \) invariance, and to look for solutions to (16), (17) with \( q(x) \neq p(x) \) for some \( x \).

Assuming polynomial solutions \( q(x), p(x) \) of (16) and (17) we note that the degree of \( p(x) \) must be equal to that of \( q(x) \). Moreover simple power counting shows that only piecewise linear or constant solutions are possible. Indeed in case of a positive degree of \( q \) (i.e. \( d \)), the degree of \( q^3(x) \) (i.e. 3d) must be compensated by the degree of \( \int_0^x (q(x) - q(y))^2 \), i.e. 2d+1. The solution can be obtained derivating the saddle point equation with respect to \( x \). For \( q^C > q_{\text{max}} \), we did not find any \( P_2^{\otimes n} \) breaking solution, while for \( q_{\text{min}} \leq q^C \leq q_{\text{max}} \) such a solution was found. Let us define \( x_0 \) the point where \( q_F(x) = q^C \). The following functions are solutions of the saddle point equations:

\[
q(x) = \begin{cases} 
q_F(2x) & 0 \leq x \leq x_0/2 \\
p_d & x_0/2 \leq x \leq x_0 \\
q_F(x) & x_0 \leq x \leq 1.
\end{cases}
\]

\[
p(x) = \begin{cases} 
q_F(x) & 0 \leq x \leq x_0 \\
p_d & x_0 \leq x \leq 1.
\end{cases}
\]

Equation (18) is verified by \( p_d = q^C \), as can by verified observing that \( p(1) = p_d \). In this situation, the free energy of this solution is equal to that of the free problem and \( \epsilon = 0 \).
This fact is not surprising because, as explained in section 1 the effect of the constraint is to select particular equilibrium states among a total number of pure states that grows less than exponentially with the size of the system. We notice that this solution has a larger free energy than the one with \( q(x) = p(x) \) and therefore the choice of it agrees with the usual criterion. In section 5 we will discuss the probabilistic interpretation of these solutions. Summarizing the results of this section we have found the solution to the saddle point equations for \( q^C \geq q_{\text{min}} \). For \( q_{\text{min}} \leq q^C \leq q_{\text{max}} \) the solution is such that \( q(x) \neq p(x) \) and the free-energy is equal to that of a free system with the same parameters, in all this range \( \epsilon = 0 \). For \( q^C > q_{\text{max}} \), the solution is such that \( q(x) = p(x) \), with a free energy bigger than in the free case. The free energy variation is proportional to \((q^C - q_{\text{max}})^2\), or substituting in (26) to \( \epsilon^2 \) or \( \epsilon (q^C - q_{\text{max}}) \).

We note that the computation shows that the overlap between two coupled real replicas tends to \( q_{\text{max}} \) when \( \epsilon \to 0^+ \).

4. Solution for \( p_d < q_{\text{min}} \).

In this case we expect again a positive free energy increment after we impose the constraint. We have searched for a maximum of the free energy both in the region \( p_d \approx q_{\text{min}} \) and for \( p_d = 0 \). In both cases we have searched solutions with discontinuities in the region of the plateaus i.e.:

\[
0 \leq x_1 \leq 3yq_{\text{min}}
\]

\[
3yq_{\text{max}} \leq x_4 \leq 1
\]

\((29)\)

For \( p_d = 0 \) we explored this space numerically. We restricted the search to solutions such that \( q(x) \) is non-decreasing and found out in all cases that the maximum of the free energy corresponded to a non-increasing \( p(x) \). The requirement that \( q(x) \) is non-decreasing is crucial in order to find a solution. Indeed also in the usual \((R = 1)\) case, the variational problem has a reasonable solution only if we restrict ourselves to the subspace of non-decreasing functions.

For instance for:

\[
q_{\text{min}} = \left(\frac{h^2}{2y}\right)^{1/3} = 0.15
\]

\[
q_{\text{max}} = \frac{1 - \sqrt{1 - 6y\tau}}{3y} = 0.25
\]

\((30)\)

we obtained:

\[
q = 0.1074; p = 0.04396 \text{ in the region } 0 \leq x \leq 0.1675
\]

\[
q = 0.1709; p = 0.01493 \text{ in the region } 0.1675 \leq x \leq 0.3957
\]

\[
q = 0.2480; p = 0.00416 \text{ in the region } 0.3957 \leq x \leq 1
\]

with a free energy \( 3.4056 \times 10^{-3} \) to be compared with the unconstrained value \( 3.3785 \times 10^{-3} \). In this case the linear part has disappeared. We have also checked the parametrization with an additional discontinuity. The new saddle point corresponded to a free energy difference of \( O(10^{-8}) \).

In the region \( p_d \approx q_{\text{min}} \) we are interested in the power dependence of the free energy on \( \delta = q_{\text{min}} - p_d \). We treat the system perturbatively assuming a fixed value for \( x_1 \) and \( x_4 \) and expanding the parameters of the solution in power series of \( \delta \).

We have checked that

\[
\Delta f = \lambda (p_d - q_{\text{min}})^3 + O((p_d - q_{\text{min}})^4)
\]

\((31)\)

The quadratic contribution vanishes. The order parameters \( q(x) \) and \( p(x) \) are parametrized as follows:
\[ q(x) = q_1; p(x) = p_1 \text{ for } 0 \leq x \leq x_1 \]
\[ q(x) = q_2; p(x) = p_2 \text{ for } x_1 \leq x \leq x_2 \]
\[ q(x) = \frac{x}{3}; p(x) = p_2 \text{ for } x_2 \leq x \leq x_3 \]
\[ q(x) = q_3; p(x) = p_2 \text{ for } x_3 \leq x \leq x_4 \]
\[ q(x) = q_4; p(x) = p_4 \text{ for } x_4 \leq x \leq 1 \]

with \( x_2 = 3yq_2 \) and \( x_3 = 3yq_3 \). We define the vector:

\[ \text{var}(\delta) = (p_1, p_2, p_4, q_1, q_2, q_3, q_4) \] (32)

For \( \delta = 0 \) we know that:

\[ \text{var}(0) = (q_{\text{min}}, q_{\text{min}}, q_{\text{min}}, q_{\text{min}}, q_{\text{max}}, q_{\text{max}}) \] (33)

The free energy can be expanded in powers of \( \text{var}(\delta) - \text{var}(0) \) and \( \delta \):

\[ f = f_0 + f_2 + f_3 + f_4 + \delta(g_1 + g_2 + g_3 + g_4) + r_0(\delta) \] (34)

The subindex denotes the power of \( \text{var}(\delta) - \text{var}(0) \). \( f_2 \) is for instance the unperturbed quadratic form and has both zero and negative eigenvalues (corresponding to the well known fact that the saddle point is a maximum of the free energy). The \( g \)'s are the forcing while \( r \) is the only term that depends on higher powers of \( \delta \) but is independent of \( \text{var} \). \( f \) is a polynomial function of 7 variables and several parameters. Fully expanded it has more than 500 terms. The analysis was done using special software (Mathematica). We first assumed that the new discontinuities were located in

\[ x_1 = \frac{x_2}{2}; x_4 = \frac{1 + x_3}{2} \] (35)

In order to discuss the zero modes we found it more convenient to express the variables in a different way:

\[ \text{var}(\delta) - \text{var}(0) = (s_1 - z_1 - z_2, d_2, d_4, s_1 + z_1 - z_2, s_1 + 2z_2, s_3 - z_3, s_3 + z_3) \] (36)

With this choice of variables it can be shown that both \( f_2 \) and \( g_1 \) depend only on \( d_2, d_4, s_1, s_3 \) so that maximizing:

\[ f_2 + \delta g_1 \] (37)

we obtain:

\[ (d_2, d_4, s_1, s_3) = -\delta(1, 1, 1/3, 0) \] (38)

The other variables \( z_3, z_1, z_2 \) are determined by the higher order terms in the free energy. We remark that they will be of the same order of magnitude in \( \delta \) but their contribution to the free energy is of a higher order. In fact from equations (37) and (38) we can already calculate exactly the 2nd order term in the free energy to prove that it is zero. This result is independent of the position of the discontinuities. To the same leading order it can be proved that (9) is a solution of the S.P. full equations. We therefore safely conclude that the free energy increment leading contribution goes like the third power of \( \delta \). The variables \( (z_3, z_2, z_1) \) can then be derived maximizing:

\[ f_3 + \delta \cdot g_2 |_{(d_2, d_4, s_1, s_3)} = -\delta(1, 1, 1/3, 0) \] (39)
There are three SP solutions to this equation:

$$\begin{cases}
(z_1, z_2, z_3) = \left( \frac{\delta}{3}, 0, 0 \right) \\
(0, \delta/6, 0) \\
(0, -\delta/3, 0)
\end{cases}$$

and correspondingly three values for the free energy contribution:

$$q_{\min}^2 \delta^3 (8/27, 1/3, 0)$$

The criteria of maximizing the free energy or imposing that \(q(z)\) be non-decreasing lead to the choice of the second solution. This result proves that there is a cost in free energy when one wants configurations with mutual overlap less than \(q_{\min}\). The actual value depends on the location of the discontinuity \(x_1\). A calculation of the derivative with respect to this parameter shows that it is positive in the region \(0 \leq x_1 \leq 3yq_{\min}\). In all this interval the variables \(d_2, d_4, s_3\) and 

$$\left(2 + \frac{x_1}{q_{\min}}\right) s_1 + 4 \left(1 - \frac{x_1}{q_{\min}}\right) z_2$$

are determined by the 2nd order terms while \(z_1, z_3\) and the orthogonal combination of \(s_1\) and \(z_2\) require the consideration of the higher order terms.

The largest free energy corresponds to the boundary of the interval \(x_1 = 3yq_{\min}\) and equals:

$$\frac{5}{12} q_{\min}^2 \delta^3$$

For every choice of \(x_1\) the solution corresponding to the maximum free energy satisfies

$$p_d \leq p_4 \leq p_2 \leq p_1 \leq q_1 \leq q_2 \leq q_3 \leq q_4$$

5. Interpretation of the \(P, Q\) order parameters.

Let us imagine real replicas for our system. Two real replicas will generate 4 systems, two left ones and two right ones. We can ask about the joint probability of measuring all possible overlaps. For instance we may want to compute the following Gibbs-Boltzmann average:

$$\int dP(q_{L1,L2,R1,R2,PL1,R2,PR1,L2}) q_{L1,L2}^{m} q_{R1,R2}^{m} p_{L1,R2}^{p} p_{R1,L2}^{p} = \langle Q_{12}^{m} q_{12}^{p} F_{12}^{p} F_{21}^{p} \rangle$$

where, without assuming any particular form for the \(Q_{ab}^{rs}\) we have denoted

$$Q_{ab}^{LL} = Q_{ab}$$
$$Q_{ab}^{RR} = Q_{ab}^{LR}$$
$$Q_{ab}^{LR} = Q_{ab}^{RL} = P_{ab}$$

In the Replica Approach the RHS is calculated by averaging over all possible saddle point matrices of the n-replicated system, 1,2 denote two distinct replica labels and in the end \(n \to 0\). Different saddle point matrices are usually related through replica permutations. It is then possible to average the RHS over the relevant permutations so that at the end one has to consider a single saddle point solution. In our case there are 2n replicas with the diagonal of the \(P\) matrix obeying the constraint. There is a symmetry group \(P_n\) that permutes
Ra, Lb \rightarrow RP(a), LP(b) and maps Saddle Points into Saddle Points. In addition as pointed out in Section 2 the fact that \( q_{C}^{2} = q^{C} \) implies a new symmetry:

\[
Ra, La \rightarrow La, Ra \text{ for each } a
\]  

(47)

Therefore:

\[
\langle Q_{12}^{m} Q_{12}^{p} P_{12}^{r} P_{21}^{s} \rangle = \frac{1}{2n(n-1)} \left( \sum_{a,b} \langle Q_{ab}^{m} Q_{ab}^{p} P_{ab}^{r} P_{ab}^{s} \rangle + \sum_{a,b} \langle Q_{ab}^{m} Q_{ab}^{p} P_{ab}^{m} P_{ab}^{s} \rangle \right)
\]

(48)

This is all the symmetry there is in the Hamiltonian. We conjecture that when the constraint costs energy there are no other saddle point matrices because then \( p_d \) is different from any other term either in \( Q_{ab} \) or in \( P_{ab} \). Therefore, taking for the matrices the Parisi form, as a function of the \( q(x), q'(x), p(x) \) we obtain:

\[
\int dP(q_{L1,L2}, q_{R1,R2}, p_{L1,R2}, p_{R1,L2}) q_{L1,L2}^{m} q_{R1,R2}^{p} p_{L1,R2}^{r} p_{R1,L2}^{s} = \frac{1}{2} \int_{0}^{1} (q^{m}(x) q^{p}(x) p^{r}(x) p^{s}(x) + q^{p}(x) q^{s}(x) p^{m}(x) p^{r}(x)) dx
\]

(49)

The reconstruction is trivial and yields:

\[
dP(q_{L1,L2}, q_{R1,R2}, p_{L1,R2}, p_{R1,L2}) = \int_{0}^{1} \frac{1}{2} \delta(q_{L1,L2} - q(x)) \delta(q_{R1,R2} - q(x)) \delta(p_{L1,R2} - p(x)) \delta(p_{R1,L2} - p(x)) + \delta(q_{L1,L2} - p(x)) \delta(q_{R1,R2} - p(x)) \delta(p_{L1,R2} - q(x)) \delta(p_{R1,L2} - q(x)) \ dx
\]

(50)

It may surprise at first that according to this equation fixing one of the four overlaps (at least far from the plateaus) fixes automatically all the others. A bit of reflection suggests that the reason lies in the scarcity of configurations satisfying the constraint. It is worth noticing that in this situation the probability that any overlap be equal to the value fixed by the constraint is strictly zero.

The latter argument shows that such a result would be unacceptable if the constraint is soft (i.e.: \( q_{\text{min}} \leq p_{d} \leq q_{\text{max}} \)). In fact in this case there are additional saddle points to be considered because block matrices of size \( m \) along the diagonal of the \( P \) matrix have all their terms equal to \( p_{d} \). Permutations of these \( m \) replicas independently of the Right and Left systems will generate new saddle points. In this way one generates \( (m!)^{n} \) new solutions, although many of them will not change the value of any one term in the sum in the RHS of (48).

Still there are additional solutions due to the specific form of our ansatz. To see them it is convenient to rearrange the \( 2n \times 2n \) matrix into a manifestly ultrametric form. In the \( Q \) matrix we first identify the block matrices \( Q^{(m)} \) along the diagonal whose elements are all strictly larger than \( p_{d} \). \( m \) is its dimension. There will be another set of matrices with corresponding dimension \( m' \), such that their elements are larger or equal to \( p_{d} \). We now permute the replicas...
in such a way that the constrained diagonal of the \( P \) matrix appears immediately besides the \( Q^{(m)} \). In this way we generate a matrix that along the diagonal will have the following blocks (of dimension \( 2m' \times 2m' \)):

\[
\begin{pmatrix}
Q^{(m)} & \hat{P}_d & P_d & P_d & P_d \\
\hat{P}_d & Q^{(m)} & P_d & P_d & P_d \\
P_d & P_d & Q^{(m)} & \hat{P}_d & P_d \\
P_d & P_d & P_d & P_d & Q^{(m)} \\
\end{pmatrix}
\]

(51)

The matrices \( P_d \) and \( \hat{P}_d \) are identical in the SP solution but the constraint applies only to the diagonal of the latter. The rest of the matrix from \( 2m' \) to \( 2n \) is identical to the corresponding part of the \( Q \) but simply doubled. From this form of the matrix it is obvious that transposing one replica in \( \hat{P}_d \) with one in \( P_d \) may leave the constrained matrix element invariant and therefore lead to a new SP. But the counting is highly non trivial because one transposition changes the elements of one \( P_d \) and conditions the successive transpositions. We will discuss this counting in a future paper.

6. Conclusions.

We have shown that the replica method can give information on the equilibrium and near equilibrium configurations if we couple two or more replicas in an appropriate way. The coupled model can be solved using a generalised hierarchical matrix.

Explicit computations have been presented in the two-replica case (we hope to report soon on the three-replica case). The main results show that the free energy density of a system composed by two replicas increase if we force the overlap between the replicas to stay outside the support of the function \( P(q) \).

In order to understand this result it may be useful to imagine what would be the implications of just the opposite results. In this hypothetical case the free energy would not increase when \( q \) goes outside the support of the function \( P(q) \). Therefore a small perturbation in the Hamiltonian (small in the sense that the variation of the energy density, not of the total energy, is small) will generate states with high probability and a value of \( q \) outside the interval \([q_{\text{min}}, q_{\text{max}}]\). The fact that the free energy does increase implies that the results obtained on the support of the function \( P(q) \) are sound from the thermodynamic point of view, i.e. they do not change discontinuously when a small perturbation is applied to the system. It is possible that the same conclusions could be obtained as far as ultrametricity is concerned; we are actually trying to verify this point by extending our treatment to the case \( R = 3 \) and hope to have definite results quite soon.

A very interesting question is the behaviour of the function \( P(q) \), for \( q \) slightly off the support. Let us consider the case of \( q \) slightly larger than \( q_{\text{max}} \). Our computation implies that in this case

\[
P(q) \propto \exp(-AN(q - q_{\text{max}})^3)
\]

(52)

this result should be written (if we want to be precise) as

\[
\lim_{N \to \infty} \frac{1}{N} \ln(P(q)) = A(q - q_{\text{max}})^3 + O((q - q_{\text{max}})^4)
\]

(53)

for \( q > q_{\text{max}} \).
Our results apply in the region where \( N(q - q_{\text{max}})^3 \) is large. It is interesting to conjecture what happens in the region where \( N \) is large but \( N(q - q_{\text{max}})^3 \) is finite (the crossover region). It is natural to assume that in this case the function \( \delta(q - q_{\text{max}}) \), which appears in the infinite volume limit is replaced by

\[
N^{1/3} g(N(q - q_{\text{max}})^3),
\]

where \( g(z) \) is an appropriate function that goes like \( \exp(-Az) \) for large \( z \). In other words we would predict that the width of the pick of the function \( P(q) \) at \( q = q_{\text{max}} \) scales as \( N^{-1/3} \). Unfortunately it is not clear how to prove our conjecture about the function \( g(z) \) in the crossover region.

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References