Non trivial overlap distributions at zero temperature

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We explore the consequences of Replica Symmetry Breaking at zero temperature. We introduce a repulsive coupling between a system and its unperturbed ground state. In the Replica Symmetry Breaking scenario a finite coupling induces a non trivial overlap probability distribution among the unperturbed ground state and the one in presence of the coupling. We find a closed formula for this probability for arbitrary ultrametric trees, in terms of the parameters defining the tree. The same probability is computed in numerical simulations of a simple model with many ground states, but no ultrametricity: polymers in random media in 1+1 dimension. This gives us an idea of what violation of our formula can be expected in cases when ultrametricity does not hold.

I. INTRODUCTION

In recent times there has been a wide interest in the behavior spin glasses with Gaussian couplings at zero temperature.

Some of the reasons for this interest are the following:

- The energies are continuous variables and the ground state is unique. It is also natural to suppose (although it is far from being proved) that the limits $T \to 0$ and $N \to \infty$ do commute and therefore the shape of the energy landscape is similar to that of the free energy landscape at non-zero temperature (for a discussion of this point see \cite{1}).

- Working at zero temperature avoids completely the possibility that the temperature used is too near to the critical point.

- Technical progresses has been done in the algorithm for finding the ground state \cite{2,4,5,6} and it is now possible to studies three dimensional systems up to $14^3$ spins \cite{7}.

In this framework it has been suggested that a possible test of the applicability of the Replica Symmetry Breaking (RSB) scenario is the study of the overlap of the ground state of two systems whose total Hamiltonian differs by a quantity of order 1 \cite{3,5}.

Let us consider a simple case. We have a first system with Hamiltonian $H_0(\sigma)$ and its ground state is given by $\tau_i$. We now consider a second system whose Hamiltonian is

$$H_1(\sigma) = H_0(\sigma) + \epsilon H_\tau(\sigma) .$$

Three quite simple choices of $H_\tau(\sigma)$ are:

$$H_\tau(\sigma) = q(\sigma, \tau), \quad H_\tau(\sigma) = q^2(\sigma, \tau), \quad H_\tau(\sigma) = q_l(\sigma, \tau) ,$$

where the overlap $q$ and the link overlap $q_l$ are given by

$$q(\sigma, \tau) = N^{-1} \sum_i \sigma_i \tau_i ,$$

$$q_l(\sigma, \tau) = N^{-1} \sum_{i,k} \sigma_{i\tau_i} \sigma_{k\tau_k} ,$$
where the sum is done over all the nearest neighbor pairs \((i, k)\) in a short range model or over all the pairs in the SK model \((N_l\) being the total number of pairs in this sum). The third possibility has been actually used by [3].

In presence of quenched disorder, the the value of the overlap among the ground states of \(H_0\) and \(H_1\) can be sample dependent. This observation can be used to the starting point for investigating possible RSB in the three dimensional Edwards-Anderson model. The question we address in this paper, is the computation of the probability distribution induced by the random couplings of \(q\) or of \(q_l\) among the two ground states, in the hierarchical RSB scenario.

Obviously the choice \(H_q(\sigma) = q\) is interesting only in presence of a magnetic field which breaks the symmetry \(\sigma(i) \rightarrow -\sigma(i)\), otherwise we would get that \(\sigma(i) = -\tau(i)\) for positive non zero \(\epsilon\) and \(q = -1\). The second choice is more interesting at zero magnetic field, but it is slightly harder to implement numerically, because its non local nature. The third choice is however equivalent to the first one in the SK model, where is known that \(q_l = q^2\) apart from corrections that vanishes when the number of spins goes to infinity. In short range models, it is possible (as suggested by the principle of replica equivalence [8]) that with probability one when the volume goes to infinity \(q_l = f(q^2)\), where \(f\) is a function that can be determined numerically and which should be not too far from

\[
f(q^2) = A + (1 - A)q^2.
\]

It is evident that for finite \(\epsilon\) the perturbation is of order 1 and it quite interesting that if replica symmetry is broken the function \(P(q)\) is non trivial at \(\epsilon \neq 0\). Let us define as \(E_{gs}(0) + \Delta(q)\) the energy of the first excited state of the Hamiltonian \(H_0\) with an overlap \(q\) with the ground state. The ground state of the Hamiltonian \(H_1\) is

\[
E_{gs}(\epsilon) = E_{gs}(0) + \min_{0 \leq q \leq 1} \{\Delta(q) + \epsilon g(q)\}
\]

where \(g(q) = q, q^2, q_l\). The main achievement of this paper will be the computation in section II and III of the joint probability distribution of \(\Delta\) and \(q\) for which the minimum is attained, for arbitrary RSB trees. In section IV we will give some example in mean field models, while in section V we show the result of a numerical computation for directed polymers in random media in 1+1 dimension.

II. REPLICA SYMMETRY BREAKING

The computation presented in this note could be done in two different ways:

- Using the replica formalism [9] to compute the partition function of the perturbed Hamiltonian \(H_1\).
- Exploiting directly the information coming from replica symmetry breaking on the probability distribution of the lowest lying states and doing a pure probabilistic computation.

The first alternative leads to some apparently messy combinatorial analysis so that we have decided to follow the second alternative. In this case the computation is physically instructive.

In this section we will recall, without proof, some known results about replica symmetry breaking and also find some new consequences of those results. Let us assume that replica symmetry is broken in the system we consider and its breaking is characterized by a function \(x(q, T)\) such that in the low temperature limit

\[
x(q, T) = Ty(q) + O(T^2),
\]

where the function \(y(q)\) may be singular at \(q = 1\) (in the SK model it diverges as \((1 - q)^{-1/2}\) near \(q = 1\)).

The space of lower lying configurations is organized in a rather complex way.

A. One step replica symmetry breaking

In this case only two values of the overlap are allowed \((q_0 \text{ and } 1)\), i.e. all different minima have a mutual overlap equal to \(q_0\). If we call \(R\) a reference total energy, which depends on the choice of the systems, i.e. on the variables \(J\), the probability to find a configuration in the interval \((E, E + dE)\) is given by
\[ \nu_0(E|R) \equiv \exp(y_0(E - R)) . \]  

We notice that configurations which differ by a number of spin flips which remains finite when the volume goes to infinity are identified.

This well known results has the consequence that the probability distribution of the ground state energy \( E_0 \) is given by the Gumbel law

\[ \mu_0(E_0|R) = \exp(y_0(E_0 - R)) \exp(-A_0 \exp(y_0(E_0 - R)) . \]

with \( A_0 = 1/y_0 \). This formula is easily understood noticing that the probability that there are no configurations for \( E' < E \) is given by

\[ \exp \left( -\int_{-\infty}^{E} dE' \exp(y_0(E' - R)) \right) = \exp(-y_0^{-1} \exp(y_0(E - R)) . \]

In the same way we obtaining that the probability of having a ground state at \( E_0 \) and the first excited configuration at \( E_1 \) is given by:

\[ P(E_0, E_1|R) = \nu_0(E_0|R) \mu_0(E_1|R) , \]

\[ = \exp(y_0(E_0 - R)) \exp(y_0(E_1 - R)) \exp(-y_0^{-1} \exp(y_0(E_1 - R)) . \]

Finally if we define \( \Delta_0 = E_1 - E_0 \), the probability distribution of \( \Delta_0 \), integrated over \( E_0 \) and \( E_1 \), one finds the simple result

\[ P(\Delta_0) = y_0^{-1} \exp(-y_0 \Delta_0) , \]

for positive \( \Delta_0 \), the probability being obviously zero for negative \( \Delta_0 \).

**B. Many level replica symmetry breaking**

Let us in this section generalize the computation for an arbitrary RSB tree (see figure). As customary, we will first consider a tree with \( k \) levels and at the end we will generalize the result to the continuous branching limit. The construction of the tree has been described many times, and we only repeat it briefly to fix the notation. At each node of the tree at the level \( l \) it is assigned an energy \( E_l \), which is chosen in such a way that the number of nodes with energy in the interval \( (E_l, E_l + dE_l) \) branching from a node with energy \( E_{l-1} \) is a Poisson variable with average equal to \( \exp(y_l(E_l - E_{l-1}))dE_l \). We will consider the case in which for all \( l \), \( y_{l+1} > y_l \), which will be a necessary condition of convergence of the integrals that appear in the computation. The root energy \( E_0 = R \) is the reference energy of the previous section. We call \( l \)-clusters, the set of branches which coincide at the \( l \)-th level of the tree.
Let us define for any \( l = k - 1, \ldots, 1 \) the first \( l \)-excited state, as the first excited state which is in the same \( l \)-cluster as the ground state, but in a different \( l + 1 \)-cluster, and denote its energy \( E_{gs} + \Delta_l \). In this section we compute the joint probability distribution of all the \( l \)-gaps \( \Delta_l \). We will get this quantity by first computing \( P_k(E_{gs}, E_{gs} + \Delta_k, \ldots, E_{gs} + \Delta_1|E_0) \) and then integrating over \( E_{gs} \). In that computation we make use of the following properties:

1. The probability of a ground state \( \mu_1(E|E_0) \) of an \( l \)-cluster (we call it an \( l \) ground state) is given by
   \[
   \mu_1(E|E_0) = \exp \left(y_{l+1}(E - E_l) + A_1 e^{y_{l+1}(E - E_l)} \right). \tag{12}
   \]
   where the \( A_i \) are positive constants whose value could be easily compute, but we will not need. For \( l = k \) the formula was derived in the previous section. Let us now proceed by induction supposing that the formula holds for \( l + 1 \) and show that it holds for \( l \). Under the induction hypothesis, we find that the number of \( l + 1 \)-ground states with energy \( E \) in an \( l \) cluster is given by
   \[
   \nu_{l+1}(E|E_0)dE_l = \int_0^E dE_{l+1} \ e^{y_{l+1}(E_{l+1} - E_l)} \ \mu_{l+1}(E|E_{l+1})
   \]
   from which we immediately find that the distribution of the \( l \) ground state is given by \([12]\) exploiting the reasonings of the previous sub-section.

2. The joint probability \( P_k(E_{gs}, E_{gs} + \Delta_k, \ldots, E_{gs} + \Delta_1|E_k, E_{k-1}, \ldots, E_0) \) can be written as:
   \[
   P_k(E_{gs}, E_{gs} + \Delta_k, \ldots, E_{gs} + \Delta_0|E_k, E_{k-1}, \ldots, E_0) = \nu_k(E_{gs}|E_{k-1}) \mu_k(E_{gs} + \Delta_k|E_{k-1}) \mu_{k-1}(E_{gs} + \Delta_{k-1}|E_{k-2}) \times \ldots \times \mu_1(E_{gs} + \Delta_0|E_0) \tag{14}
   \]
   from which we get:
   \[
   P_k(E_{gs}, E_{gs} + \Delta_k, \ldots, E_{gs} + \Delta_0|E_0) = \notag
   \]
   \[
   \int_0^E dE_{k-1} \ldots dE_1 \ \nu_k(E_{gs}|E_{k-1}) \mu_k(E_{gs} + \Delta_k|E_{k-1}) e^{y_{k-1}(E_{k-1} - E_k)} \mu_{k-1}(E_{gs} + \Delta_{k-1}|E_{k-2}) \times \ldots \times \mu_2(E_{gs} + \Delta_2|E_1) e^{y_1(E_1 - E_0)} \mu_1(E_{gs} + \Delta_1|E_0) \tag{15}
   \]

3. A detailed computation shows that
   \[
   \int_0^E \nu_k(E_{gs}|E_{k-1}) \mu_k(E_{gs} + \Delta_k|E_{k-1}) e^{y_{k-1}(E_{k-1} - E_k)} = (y_k - y_{k-1}) e^{-(y_k - y_{k-1})\Delta_k} \nu_{k-1}(E_{gs}|E_{k-2}). \tag{16}
   \]
   This allows to integrate all the \( E_l \) \( (l = k - 1, \ldots, 1) \) telescopically, and obtain
   \[
   P_k(E_{gs}, E_{gs} + \Delta_k, \ldots, E_{gs} + \Delta_1|E_0) = \prod_{i=2}^k \left((y_i - y_{i-1}) e^{-(y_i - y_{i-1})\Delta_i} \right) \nu_1(E_{gs}|E_0) \mu_1(E_{gs} + \Delta_1|E_0) \tag{17}
   \]

4. We can finally integrate \( E_{gs} \) as in the previous section and get that the gaps’ probability distribution is:
   \[
   P(\Delta_k, \ldots, \Delta_1) = \prod_{i=1}^k \left((y_i - y_{i-1}) e^{-(y_i - y_{i-1})\Delta_i} \right) \tag{18}
   \]
   having defined \( y_0 = 0 \).

We can now consider the continuum branching limit, in which the branches can be indexed by the value of \( q \), or by any monotonically increasing function of \( q \). \( y_i \to y(q) \), \( y_i - y_{i-1} \to y'(q) dq \) where the previous formula reduces to

\[
P(\{\Delta(q)\}) = \exp \left(- \int_0^1 dq y'(q)\Delta(q) \right) \prod_{q=0}^1 y'(q) dq \tag{19}
\]
where, if \( y_1 \to y(0) \neq 0 \), we make the convention that \( y'(0) = y(0)\delta(q) \).
III. THE OVERLAP PROBABILITY DISTRIBUTION

We are finally in the position to compute the joint distribution of the gap and of the overlap. For a given sample, as we said, the difference among the ground state energy of the Hamiltonians \( H_1 \) and \( H_0 \) is given by the

\[
E_{gs}(\epsilon) - E_{gs}(0) = \min_{0 \leq q \leq 1} \Delta(q) + \epsilon g(q). \tag{20}
\]

Noticing that the indexing of the tree could be done by the function \( g(q) \) itself, we can concentrate here to case \( g(q) = |q| \), and consider only positive overlaps. All the other cases can be obtained by this one via a simple change of variable. Let us call \( \Delta \) or \( \chi \) where we defined \( \chi = y(0) + \int_{0}^{1} dq \, y(q) \). The factor \( y'(q) \) that multiply the exponential comes from the only \( \Delta \) which has remained unintegrated.

Let us notice that the formula depends on \( \Delta \) only in the combination \( \Delta/\epsilon + q \).

Integrating over \( \Delta \) we get, for the overlap probability

\[
P(q) = \delta(q-1) \exp(-\epsilon \chi) + \epsilon y'(q) \int_{q}^{1} dq' \exp\left(-\epsilon \int_{q}^{q'} dq'' (y(q'') - y(0))\right) + \delta(q-1) \exp(-\epsilon \chi), \tag{21}
\]

where we defined \( \chi = y(0) + \int_{0}^{1} dq \, y(q) \). The factor \( y'(q) \) that multiply the exponential comes from the only \( \Delta \) which has remained unintegrated.

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\]

It is also interesting to study the probability distribution of \( w = \Delta/\epsilon + q \). Integrating over \( \Delta \) and \( q \) for fixed \( w \) with the condition \( 0 \leq q \leq w \) we find the remarkable formula:

\[
P(w) = \theta(1-w)\epsilon(y(w) - y(0)) \exp\left(-\epsilon \int_{0}^{w} dq \, (y(q') - y(0))\right) + \delta(w-1) \exp(-\epsilon \chi). \tag{23}
\]

The primitive of this function has a very simple dependence on \( y \) and \( \epsilon \). If we define \( Q(w) = \int_{w}^{1} dw' \, P(w') \) we find:

\[
Q(w) = \exp\left(-\epsilon \int_{0}^{w} dq \, (y(q') - y(0))\right) \tag{24}
\]

which is particularly well suited for the extraction of the function \( y(q) \) from numerical simulations. Notice that eq. (24) implies that \( \epsilon^{-1}\ln(Q(w)) \) is \( \epsilon \)-independent, which is a non-trivial result.

IV. EXAMPLES

In this section we show how our formula looks like in some cases. The first example we make is the one of spherical models. These models are defined by a random Gaussian Hamiltonian \( \bar{H}(\sigma) \) \( (\sigma = \{\sigma_1, ..., \sigma_N\}) \), which have correlation function

\[
\bar{H}(\sigma)\bar{H}(\tau) = N f(g(\sigma, \tau)) \tag{25}
\]

and the spins are subject to the spherical constraint \( \sum_i \sigma_i^2 = N \). In these models, the function \( y(q) \) is temperature independent and equal to \( 1 \)

\[
y(q) = 1/2 f'''(q)/(f''(q)^{3/2}) \tag{26}
\]
This last equation makes sense only if the resulting function $y(q)$ is an increasing function of $q$. This in particular happens for $f(q) = 1/2(q^2 + aq^p)$ if $p \geq 4$ and $a$ small enough, where we find

$$y(q) = \frac{a}{\sqrt{2}} \frac{1}{(p-3)!} \left( \frac{q^{p-3}}{2 + \frac{a}{(p-2)!} q^{p-2}} \right)^{3/2},$$

(27)

while

$$Y(w) \equiv \int_0^w dq y(q) = 1 - \frac{1}{\sqrt{1 + \frac{aq^{p-2}}{2(p-2)!}}}.$$  

(28)

In figure 2 we show the function $Y(w)$ and the function $Q(w)$ for various values of $\epsilon$ in the case $p = 5$, $a = 0.3$. In figure 3 we show the function $P(q)$ for the same values of the parameters.

In the case of the SK model the function $y(q)$ at low temperature, has been estimated in [10] using the so-called PaT approximation, and displays a square root divergence at $q = 1$, while starting linearly at $q = 0$ (a best fit of the form $y(q) = \frac{aq + bq^2}{\sqrt{1-q}}$ gives $a = 1.309$, $b = -0.695$).

Using that estimate we immediately compute the function $Q(w)$ which is plotted in figure 4 for various values of $\epsilon$. 

**FIG. 2.** The function $Y(w)$ in the spherical model with $p = 5$ $a = 0.3$. In the inset, the function $Q(w)$ for $\epsilon = 2^k$, from top to bottom $k = 4, 7, 10, 13, 16$. 

**FIG. 3.** The function $P(q)$ for the same model and parameters of figure 2.
FIG. 4. The function \( Y(w) \) for the SK model in the PaT approximation. In the inset, the function \( Q(w) \) computed by \(^{24}\) for \( \epsilon = 0.01 \times 2^k \) with (from top to bottom) \( k = 3, 5, 7, 9, 11, 13 \).

It is interesting to study the limit \( \epsilon \to \infty \) of our formula. Let us suppose that \( y \) behaves as \( y(q) = a q^{\alpha} + ... \) for \( \alpha > 1 \) for low \( q \). In this case \( P(q) \) will be dominates by the behavior of \( y \) close to \( q = 0 \). We can introduce a cut-off \( \Lambda \) such that \( \Lambda \to 0 \) and \( \Lambda^{1+\alpha} \epsilon \to \infty \).

\[
P(q) \simeq \epsilon a q^{\alpha-1} \int_q^\Lambda \exp \left( - \frac{\epsilon}{\alpha+1} q^{\alpha+1} \right)
\]  \( \text{(29)} \)

which, rescaling the integration variable and sending the cut-off to zero becomes:

\[
P(q) = \frac{1}{q} \left( \frac{\epsilon a q^{\alpha+1}}{1+\alpha} \right)^{1+\alpha} \Gamma(1+\alpha, \frac{\epsilon a}{\alpha+1} q^{\alpha+1})
\]  \( \text{(30)} \)

where the incomplete gamma function is

\[
\Gamma(n, x) = \int_x^\infty dy \, y^{n-1} e^{-y}.
\]  \( \text{(31)} \)

This case is relevant in the spherical models where \( y(q) \sim a q^4 \) (for a polymer of total length \( L \)) and for the SK model where \( y(q) \sim a q^\varphi \).

V. DIRECTED POLYMERS IN 1 + 1 DIMENSION

The natural playground of the exposed theory are finite dimensional spin glasses. Our analysis predicts a very peculiar dependence of the probability of \( q \) and \( w \) on \( \epsilon \). Formulae \(^{22,24}\) has been derived assuming that the low lying states verify ultrametricity. It is therefore interesting understand what violations of the scaling forms \(^{22,24}\) can be expected when the ground states structure is nontrivial, but ultrametricity does not hold.

In this paper we study numerically the simple case of directed polymers in random media in 1+1 dimension. The model we use is defined on the square lattice, where the polymer can perform a random walk starting from the origin. On each site of the lattice is defined an passage energy cost which is a Gaussian variable with unit variance, and independent of all the other energies. The properties of this sort of models have been studied extensively \(^{12}\), and it is well known that while the low temperature thermodynamics is dominated by a single ground state, there exist many “pure states” (i.e. metastable states separated by growing barriers) with typical energy gap with the ground state scaling as \( L^{1/3} \) (for a polymer of total length \( L \)). The overlap for two polymers of length \( L \) with a common source in the origin is often defined as the fraction of the monomers passing in the same sites of the lattice in the two polymers. Given the previously mentioned scaling of the energy gap it is natural that the scaling of the coupling in order to have a non trivial \( P(q) \) as defined in the previous section is

\[
\epsilon = \eta L^{1/3}.
\]  \( \text{(32)} \)

If we had to suppose the validity of the formula \(^{24}\) we would conclude that the function \( y(q) \) for samples of length \( L \) depends on \( L \) and scales as \( L^{-1/3} \).
As we stressed, ultrametricity does not hold in this model. Although we did not make a systematic study, we can easily show the lack of ultrametricity generalizing the coupling procedure to a third “replica”, which has a repulsion both with the unperturbed ground state, and with the one obtained with the coupling. For simplicity, we look at the case in which all couplings are equal. In figure 5 we show the overlap between the second and the third replica as a function of the overlap between the first and the third, fixing the overlap between the first and the second to 0.8, and we see no sign of ultrametricity.

In figure 5 we show the function \( Q(w) \) for various values of \( L \) and \( \epsilon \) of the form (32). We see that for values of \( L \approx 200 \) the expected independence of \( Q(w) \) of \( L \) is reasonably obeyed. A close inspection to \( Q(1) \) however, which represents the probability of \( q = 1 \) reveals that this quantity behaves as \( Q(1) = \exp(-\eta \chi L^{2/3}) \), with \( \chi = 0.85 \pm 0.02 \), and that the scaling is violated in proximity of \( w = 1 \).

We next try to scale the data with \( \epsilon \) according to the formula (24). In figure 7 we see that the works quite well for small values of \( \epsilon \), while we show in figure 8 that there are important violations for large values of \( \epsilon \).
FIG. 7. The cumulative probability $-1/\epsilon \log(Q(w))$ and 7 different values of $\eta = 0.1 \times 1.4^n$, $n = 1, \ldots, 7$ and $L = 400$. The data are obtained on sets of 10000 different samples. We see that for these low values of $\epsilon$ the scaling is reasonably obeyed. In the inset we plot $Q(w)$ for the same values of the parameters.

FIG. 8. The cumulative probability $-\epsilon^{-1} \ln(Q(w))$ and 5 different values of $\eta = 0.1 \times 1.4^n$, $n = 15, \ldots, 20$ and $L = 400$. The data are obtained on sets of 10000 different samples. In the inset the function $Q(w)$. For these values of $\epsilon$ the scaling form of the function $Q(w)$ is violated.

VI. CONCLUSIONS

Monte-Carlo simulations of finite dimensional spin glasses, show a behavior in agreement with RSB. However, the use of Monte-Carlo has been criticized on the ground that one can only equilibrate the system too close to the critical point, where finite size effects are large and could spoil the conclusions about ergodicity breaking in the thermodynamic limit (see however [13,14]). It is important therefore to find consequences of RSB at zero temperature. In this paper we have devised some of them.

We have found that a universal formula holds for the probability of the overlap among the uncoupled ground state and the coupled one. The investigation of the validity of that formula in three dimensional systems is not beyond reach with the present technology, and will furnish an important test to understanding the nature of the spin-glass phase of three dimensional systems.

Two main ingredient will be involved in the calculation: the exponential distribution of the states and their ultrametric organization. This implies that the tree of states is described by a single function $y(q)$. The function $y(q)$ may in principle depend on $N$. Mean field theory predicts that $y(q)$ remains finite in the thermodynamic limit implying that the energy differences between pure states remain finite in the thermodynamic limit. However, one could envisage systems where both exponential distribution and ultrametricity are valid, but the typical energy differences scale as $L^\theta$. In this case, one still have a function $y(q)$ which scales as $L^{-\theta}$ and in order to measure a nontrivial overlap distribution one needs a coupling of order $L^\theta$. The numerical study of the overlap and gap distribution, and the comparison with the formulae found in this paper will give important information about the organization of the states in short range models.
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