Journal of Statistical Physics, Vol. 103, Nos. 5/6, 2001

The K-SAT Problem in a Simple Limit

Luca Leuzzi[1] **and Giorgio Parisi**[2]

Received July 26, 2000; revised December 12, 2000

In this work we compute the thermodynamic properties of the 3-satisfiability problem in the infinite connectivity limit. In this limit the computation can be strongly simplified and the thermodynamic properties can be obtained with a high accuracy. We find evidence for a continuous replica symmetry breaking in the region of high number of clauses, $\alpha > \alpha_c$.

KEY WORDS: NP complete; K-SAT; Replica Symmetry Breaking.

1. INTRODUCTION

The statistical mechanics of the random K-satisfiability (K-SAT) problem has been the object of many studies in the last years.[1–3] The K-SAT was the first problem to be shown to be Non-deterministic Polynomial (NP) complete.[4] This model is important because it provides a simple prototype for all the NP complete problems in complexity theory of computer science as well as in statistical mechanics of disordered and glassy systems, in computational biology and in other fields.

It is usually believed that the solutions of NP complete problems, or the certainty that they have no solutions, can only be found, in the worst case, by algorithms with a running time of computation that grows faster than polynomially (namely exponentially) with the number of variables N of the system.

[1] Instituut voor Theoretische Fysica, FOM, Universiteit van Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands. e-mail: leuzzi@wins.uva.nl

[2] Dipartimento di Fisica, INFM and INFN, Università di Roma *La Sapienza*, P. A. Moro 2, 00185 Roma, Italy. e-mail: giorgio.parisi@roma1.infn.it

0022-4715/01/0600-0679$19.50/0

Generally speaking, in the statistical mechanics approach, for each given instance of the problem, one introduces a Hamiltonian $\mathscr{H}(C)$, constructed in such a way that the configuration C^*, which minimize $\mathscr{H}(C)$, is the solution of the problem if $\mathscr{H}(C^*)=0$. On the contrary, if $\mathscr{H}(C) > 0$ for any C, the problem does not have a solution. In this framework one consider for each problem the partition function

$$Z(\beta)=\sum_C \exp(-\beta\mathscr{H}(C)), \tag{1}$$

where $\beta=T^{-1}$, T being the temperature of the system. In the same way one introduces the usual thermodynamic quantities, e.g. the internal energy

$$\mathscr{E}(\beta)= -\frac{\partial \ln(Z(\beta))}{\partial\beta} \tag{2}$$

It can be argued that quantities like the internal energy density (i.e. $E\equiv\mathscr{E}/N$) do not depend on N in the infinite N limit, so that a computation of their average over the different instances of the problem is sufficient for obtain interesting information in this limit.

When one studies the behaviour of the K-SAT model at finite temperature, one finds a rich structure of phase transitions.[1] In certain region of the parameter space, replica symmetry is broken (in other words there are many equilibrium states in the large volume limit)[5]. Explicit computation shows that it may be possible to obtain a basic understanding of the connection between the SAT/UNSAT phase transition in random combinatorial structures[1, 2] and the transition between a Replica Symmetric (RS) structure and a structure where the replica symmetry is broken in the frame of spin-glasses.[5] Recent results[6] suggest that the SAT/UNSAT transition seems to take place into the phase of broken replica symmetry. Yet the question stays open of how exactly the typical-case complexity theory of computer science and the Replica Symmetry Breaking (RSB) transition are related.

One of the main aim of the recent research on this model has been to understand better the structure of solutions, especially at the borderline between the region of the phase diagram where the problem has solution and the region where no solution is possible. Indeed this is the zone where the most unlikely (hardest) solutions are.

We will concentrate our attention on the case $K=3$ (3-SAT), that is known to be the first and simplest NP complete instance of K-SAT. The 2-SAT model is, in fact, already solvable in a time increasing polynomially (actually even linearly)[7] with the number of variables.

The basic boolean variables of the problem, $s(i)$, are defined on the sites i with $i=1, ..., N$. For technical reasons we prefer to use variables $\sigma(i)$ which take the values ± 1. Our problem is then related to the original one through the variables transformation $s(i)=(1+\sigma(i))/2$.

We consider an ensemble of randomly generated 3-SAT formulae. The Hamiltonian corresponding to a given formula is

$$\mathscr{H} = \sum_{i_1 < i_2 < i_3} r_{i_1, i_2, i_3} \frac{1-\epsilon_1^{(i_1, i_2, i_3)}\sigma(i_1)}{2} \frac{1-\epsilon_2^{(i_1, i_2, i_3)}\sigma(i_2)}{2} \frac{1-\epsilon_3^{(i_1, i_2, i_3)}\sigma(i_3)}{2}. \qquad (3)$$

For each instance of the problem we generate αN clauses, where each clause is determined by randomly selecting three of the N sites and assigning to them a random ± 1 variable. The terns of randomly chosen sites $\{i_1, i_2, i_3\}$ are given by the variables r_{i_1, i_2, i_3} that take the value 1 with probability $p \equiv \alpha N^{-2}$ and the value 0 with probability $1-p$. For finite N there are approximately αN variables r which are different from zero and they become exactly equal to αN in the limit $N \to \infty$. Given a tern $\{i_1, i_2, i_3\}$, a set of three variables ϵ are drawn, taking the value $+1$ or -1 with probability 1/2. The function (3) depends only on those variables $\epsilon^{(i_1, i_2, i_3)}$ such that $r_{i_1, i_2, i_3}=1$ and all the terms are non-negative: $\mathscr{H}$ just counts the number of clauses that are not satisfied. Obviously $\mathscr{H}=0$ if and only if all the clauses are satisfied.

As we have already explained we are going to consider $\mathscr{H}$ as the Hamiltonian of a disordered system, in order to apply to the K-SAT model the statistical mechanics techniques and to compute all the mathematical expressions in this framework. We will introduce the fictive temperature $T \equiv 1/\beta$ and at the end we will then send $\beta \to \infty$ to compute the ground state properties.

In the large N limit we can write the equivalent Hamiltonian, in which the number of terms in the interaction is fixed and equal to αN, as:

$$\mathscr{H} = \sum_{l=1, \alpha N} \frac{1-\epsilon_1^{(l)}\sigma(i_1^{(l)})}{2} \frac{1-\epsilon_2^{(l)}\sigma(i_2^{(l)})}{2} \frac{1-\epsilon_3^{(l)}\sigma(i_3^{(l)})}{2} \qquad (4)$$

where the sites $i_t^{(j)}$ $(t=1, 2, 3)$ are randomly chosen for each one of the αN triplets.

For reasons that are discussed in refs. 1 and 2, one is interested to study the statistical properties of the system in the thermodynamic limit $N \to \infty$. It is interesting to consider the zero temperature energy density $E_0(\alpha)$ (i.e. the average over the distribution of clauses of the number of clauses that are not satisfied by the formula corresponding to the Hamiltonian in equation (3)) as a function of the ratio α between the number of clauses and the number of variables. We are eventually interested in the zero temperature entropy density $S_0(\alpha)$. The number of solutions satisfying the formula is asymptotically given by $\exp(NS_0(\alpha))$. It has been conjectured[1] that

$$\begin{aligned} E_0(\alpha)=0, \qquad & S_0(\alpha) > 0, \qquad \text{for} \quad \alpha < \alpha_c, \\ S_0(\alpha)=0, \qquad & E_0(\alpha) > 0, \qquad \text{for} \quad \alpha > \alpha_c, \end{aligned} \tag{5}$$

where the value of α_c is estimated to be around 4.2.[3]

Below α_c we have solutions (with probability going to 1 for N going to infinity), while above α_c the problem does not have solutions (i.e. it is UNSAT). At $\alpha \ll \alpha_c$ the problem is quite underconstrained and it is relatively easy to find an assignment of variables $\{\sigma_i\}$ satisfying the clauses. For $\alpha \gg \alpha_c$, though in general still hard, to prove unsatisfiability is easier than in the hardest cases near α_c. Around the density of clauses α_c it is indeed very difficult either to find a satisfying assignment or to show unsatisfiability, i.e. it is most difficult to discriminate whether the problem admit any solution or no solution at all. These are the cases where an exponential time may be needed.

Far from this critical value, anyway, things simplify and more insight over the structure of the phase space can be gained.

Indeed the exact evaluation of the free energy in the α-β plane is a rather complex computation. The aim of the present work is then to show that the computation strongly simplifies in the most overconstrained limit of $\alpha \to \infty$. Let us first introduce the reduced inverse temperature μ through the relation

$$\beta \equiv \frac{\mu}{\sqrt{\alpha}}. \tag{6}$$

and let us define the rescaled energy density

$$e(\mu, \alpha) \equiv \frac{1}{\sqrt{\alpha}}\left(E(\beta, \alpha) - \frac{\alpha}{8}\right), \tag{7}$$

A similar definition can be written for the other thermodynamic functions. In particular for the free energy we have the rescaled quantity $f(\mu, \alpha) = (F(\beta, \alpha) - \alpha/8)/\sqrt{\alpha}$. We shall also introduce the reduced temperature $\tau = \mu^{-1} = T\alpha^{1/2}$. We will show below that the function $e(\mu, \alpha)$ has a limit when α goes to infinity. We can thus define

$$e(\mu) = \lim_{\alpha \to \infty} e(\mu, \alpha). \tag{8}$$

In the following we will also compute the function $e(\mu)$ with high accuracy. In the conclusions we will implicitly assume that the limit $\alpha \to \infty$ of full connectivity and the zero temperature ($\mu \to \infty$) limit can be freely exchanged.

The interest for this computation is threefold:

- The limit where α goes to infinity plays the same role of the infinite connectivity model for spin glasses (finite connectivity/dilute models correspond to finite α) and most of our analytic understanding comes from the study of the infinite range models (Sherrington–Kirkpatrick like models)[8], where the analytic computations are much simpler.
- Replica symmetry is broken in a region of the α-β plane, for $\alpha > \alpha_c \simeq 4.2$[3] (or maybe for $\alpha > \alpha_s \simeq 3.9$ as recently derived in ref. 6 by means of a variational approach). It is reasonable to assume that in this whole region the way in which replica symmetry is broken is the same as in the limit $\alpha \to \infty$.
- If we neglect the dependence of $e_0(\alpha) \equiv \lim_{\mu \to \infty} e(\mu, \alpha)$ on α for $\alpha \geqslant \alpha_c$ (i.e. if we perform an asymptotic expansion in $1/\sqrt{\alpha}$ and we consider only the leading order), we get the following estimate for α_c:

$$\alpha_c \approx (8e_0)^2. \tag{9}$$

Where the estimate α_c depends from the order of the asymptotic expansion. In this work we will limit ourselves to the leading order in the μ^{-1} expansion. The precise value of e_0 will be given in the next section where we derive the thermodynamic observables using the replica tool.

2. THE REPLICA FORMALISM

In the replica formalism one computes

$$Z^{(n)} \equiv \overline{Z[\{\Delta\}]^n}, \tag{10}$$

where $\{\Delta\}$ denotes the random couplings, the bar is the average over the distribution of the random couplings and the partition function is defined as:

$$Z[\{\Delta\}] = \sum_{\{\sigma_i\}} \exp(-\beta H[\{\sigma_i\}, \{\Delta\}]). \tag{11}$$

In our case Δ represents the ensemble of random clauses, namely the ensemble of terns $\{i_1, i_2, i_3\}$ with associated ϵ's. The free energy density at finite n is defined as

$$F^{(n)} = -\lim_{N \to \infty} \frac{\ln(\overline{Z^{(n)}})}{\beta n N}. \tag{12}$$

where we firstly perform the thermodynamic limit keeping n fixed and only afterwards we send $n \to 0$ by an analytic continuation procedure.

We are eventually interested in computing the limit $n \to 0$ of $F^{(n)}$, which is the value of the free energy density of the generic system in the infinite volume limit:

$$F = \lim_{n \to 0} F^{(n)} = -\lim_{N \to \infty} \frac{\overline{\ln Z[\{\Delta\}]}}{\beta N}. \tag{13}$$

Starting from (3) and carrying out the average over the distribution of the r's we have

$$\overline{Z^{(n)}} = \overline{\sum_{\{\sigma_i^a\}} \prod_{i_1, i_2, i_3} \left(1 - p + p \exp\left(-\beta \sum_{a=1,n} \prod_{j=1,3} \frac{1 - \epsilon_j^{(i_1, i_2, i_3)} \sigma^a(i_j)}{2}\right)\right)}. \tag{14}$$

where here the $\overline{(...)}$ is now the average only over the ϵ's distribution. In the limit of large N we can write the previous expression in terms of the effective Hamiltonian $\mathcal{H}_{eff}$ and the temperature like parameter α:

$$\overline{Z^{(n)}} = \sum_{\{\sigma_i^a\}} \exp(-\alpha \mathcal{H}_{eff}), \tag{15}$$

where

$$\mathcal{H}_{eff} \equiv \frac{1}{N^2} \sum_{i_1 < i_2 < i_3} h_{eff}(\sigma(i_1), \sigma(i_2), \sigma(i_3) \,|\, \beta) \tag{16}$$

and

$$h_{eff} \equiv 1 - \overline{\exp\left(-\beta \sum_{a=1,n} \prod_{j=1,3} \frac{1 - \epsilon_j^{(i_1, i_2, i_3)} \sigma^a(i_j)}{2}\right)}. \tag{17}$$

For a given tern of sites $\{i_1, i_2, i_3\}$ the average is performed over the 2^3 possible values of the three variables ϵ.

Let us now consider the limit $\alpha \to \infty$ at fixed μ. The computation is long but straightforward. In this limit the inverse temperature β, defined as in (6), becomes a quantity of order $\alpha^{-1/2}$ so that we can freely expand the exponential in the previous expression (16):

$$\mathscr{H}_{eff} = \frac{1}{N^2} \sum_{i_1 < i_2 < i_3} \left(\frac{\mu}{\sqrt{\alpha}} \overline{\sum_{a=1,n} \prod_{j=1,3} \frac{1 - \epsilon_j^{(i_1,i_2,i_3)} \sigma^a(i_j)}{2}} \right.$$
$$\left. + \frac{\mu^2}{2\alpha} \overline{\left(\sum_{a=1,n} \prod_{j=1,3} \frac{1 - \epsilon_j^{(i_1,i_2,i_3)} \sigma^a(i_j)}{2} \right)^2} + \mathcal{O}\left(\frac{\mu^3}{\alpha^{3/2}} \right) \right), \tag{18}$$

where

$$\overline{\sum_{a=1,n} \prod_{j=1,3} \frac{1 - \epsilon_j^{(i_1,i_2,i_3)} \sigma^a(i_j)}{2}} = \frac{n}{8}, \tag{19}$$

$$\overline{\left(\sum_{a=1,n} \prod_{j=1,3} \frac{1 - \epsilon_j^{(i_1,i_2,i_3)} \sigma^a(i_j)}{2} \right)^2} = \frac{1}{8} \sum_{a,b} \prod_{j=1,3} \frac{1 + \sigma_{i_j}^a \sigma_{i_j}^b}{2}$$
$$= \frac{n}{8} + \frac{1}{32} \sum_{a<b} \prod_{j=1,3} (1 + \sigma_{i_j}^a \sigma_{i_j}^b) \tag{20}$$

Using standard manipulations, for large N and α, we easily get

$$Z^{(n)} = \exp\left(-\frac{Nn\mu\sqrt{\alpha}}{8} + \frac{Nn\mu^2}{16} \right)$$
$$\times \sum_{\{\sigma_i^a\}} \exp\left(\frac{N\mu^2}{64} \sum_{a<b} \left(1 + \frac{1}{N} \sum_i \sigma_i^a \sigma_i^b \right)^3 \right) \tag{21}$$
$$= \exp\left(-\frac{Nn\mu\sqrt{\alpha}}{8} + \frac{Nn\mu^2}{16} \right)$$
$$\times \sum_{\{\sigma_i^a\}} \int \prod_{a<b}^{1,n} dQ_{ab}\, \delta\left(\sum_i \sigma_i^a \sigma_i^b - NQ_{ab} \right) \exp\left(\frac{N\mu^2}{64} \sum_{a<b} (1 + Q_{ab})^3 \right)$$
$$\equiv \int \prod_{a<b}^{1,n} d\Lambda_{ab} \prod_{a<b}^{1,n} dQ_{ab} \exp(NnA[\{Q\}, \{\Lambda\}]), \tag{22}$$

where

$$A[\{Q\}, \{\Lambda\}] = -\frac{\mu\sqrt{\alpha}}{8} + \frac{\mu^2}{16} + \frac{\mu^2}{64n} \sum_{a<b} (1 + Q_{ab})^3$$
$$-\frac{1}{n} \sum_{a<b} \Lambda^{ab} Q_{ab} + \frac{1}{n} \log\left(\sum_{\{\sigma_i^a\}} \exp\left(\sum_{a<b} \Lambda^{ab} \sigma_a \sigma_b \right) \right). \tag{23}$$

In the infinite N limit we can use the saddle point method and we find that the free energy density is given by

$$F(\alpha) = -\frac{\sqrt{\alpha}}{\mu} A[\{Q^{sp}\}, \{\Lambda^{sp}\}] \tag{24}$$

and the expression of the internal energy comes out to be:

$$E(\mu, \alpha) = \frac{\alpha}{8} - \frac{\mu\sqrt{\alpha}}{8}\left(1 + \frac{1}{4n}\sum_{a<b}(1+Q_{ab})^3\right). \tag{25}$$

The elements $\{Q^{sp}\}$ and $\{\Lambda^{sp}\}$ satisfy the following consistency equations:

$$\Lambda^{sp}_{ab} = \frac{3\mu^2}{64}(1+Q^{sp}_{ab})^2, \qquad Q^{sp}_{ab} = \frac{\sum_{\{\sigma_a\}} \sigma_a\sigma_b \exp\{\sum_{a<b}\sigma_a\sigma_b\Lambda^{ab}\}}{\sum_{\{\sigma_a\}} \exp\{\sum_{a<b}\Lambda^{ab}\sigma_a\sigma_b\}}. \tag{26}$$

Our task is now to find the solution of these equations.

We notice that equation (25) implies that the exact definition of e_0 in (9) is

$$\lim_{\mu\to\infty} -\frac{\mu}{8}\left[1 + \frac{1}{4n}\sum_{a<b}(1+Q_{ab})^3\right] \tag{27}$$

3. THE REPLICA SYMMETRIC SOLUTION

The simplest possibility (which is correct at high temperature) consists in assuming that the off-diagonal elements of the matrix Q and Λ are constant and they are equal to q_0 and λ_0 respectively. A simple computation shows that

$$A(q_0, \lambda_0) = -\frac{\mu\sqrt{(\alpha)}}{8} + \frac{\mu^2}{16} - \frac{\mu^2}{128}(1+q_0)^3 - \frac{\lambda_0(1-q_0)}{2} + \int dp(z_0)\log(2\cosh z_0\sqrt{\lambda_0}) \tag{28}$$

and the final form of the rescaled free energy, as defined in (7), is given by

$$f(\mu, \alpha) = -\frac{\mu}{16}\left[1 - \frac{(1+q_0)^2(2-q_0)}{4}\right] + \frac{1}{\mu}\int dp(z_0)\log(2\cosh z_0\sqrt{\lambda_0}), \tag{29}$$

where the parameters q_0 and λ_0 satisfy the equations:

$$\lambda_0 = \frac{3}{64}\mu^2(1+q_0)^2, \qquad q_0 = \int \mathrm{d}p(z_0)(\tanh(z\sqrt{\lambda_0}))^2, \tag{30}$$

and we have used the following compact measure for the Gaussian measure:

$$dp(z) \equiv \frac{e^{-z^2/2}}{\sqrt{2\pi}}\, dz. \tag{31}$$

The solution of the equation (30) can be found by iterations. The parameter q_0 is an analytic function of τ (Fig. 3, full curve). No transition is present. The zero temperature value of the rescaled energy (7) is given by $e_0 = \sqrt{\frac{3}{8\pi}} \approx 0.345494$.

The corresponding value of α where the energy density $E(\mu, \alpha)$ goes to zero, i.e. the ratio of the number of variables and the number of clauses up to which all clauses are satisfied, turns out to be, following (9), $\alpha_c = 24/\pi = 7.6394373$ in this asymptotic approximation.

The value of the entropy corresponding to this solution is shown in Fig. 1. It becomes negative at low temperature signaling an inconsistency of the approach based on replica symmetry. In order to obtain reasonable results in the low temperature region we must break the replica symmetry as we will show in the next section.

4. THE REPLICA SYMMETRY BREAKING

4.1. One Step Replica Symmetry Breaking

If replica symmetry is broken, very often reasonable results are obtained in the framework of the one step replica symmetry breaking, where it is assumed that the elements of the matrix Q take only two values (for the physical interpretation of one step replica symmetry breaking see reference.)[(5)].

In the one step case one divides the indices a in n/m groups, each group having m components. We set $Q_{a,b}$ equal to q_1 if a and b belong to the same group, otherwise we set $Q_{a,b}$ equal to q_0. Similar relations are used for the matrix Λ. The free energy is now a function of three independent parameters: m, q_0 and q_1. The limit $n \to 0$ is obtained in this case by doing an analytic continuation also in m, that in such a process will not be integer anymore. In the 0 replicae limit m acquires non-integer values between 0 and 1.

After some simple computation we get

$$A(q_0, q_1; \lambda_0, \lambda_1, m)$$
$$= -\frac{\mu\sqrt{\alpha}}{8} + \frac{\mu^2}{16} - \frac{\mu^2}{128}\left[m(1+q_0)^3 + (1-m)(1+q_1)^3\right]$$
$$-\frac{\lambda_1}{2} + \frac{1}{2}\left[m\lambda_0 q_0 + (1-m)\,\lambda_1 q_1\right]$$
$$+\frac{1}{m}\int dp(z_0)\log\left(\int dp(z_1)(2\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^m\right), \quad (32)$$

$$f(\mu) = -\frac{\mu}{16}\left[1 - \frac{m}{8}\left((1+q_0)^2(1-2q_0) - (1+q_1)^2(1-2q_1)\right)\right.$$
$$\left. -\frac{(1+q_1)^2(2-q_1)}{4}\right]$$
$$-\frac{1}{m\mu}\int dp(z_0)\log\int dp(z_1)(2\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^m, \quad (33)$$

where the following equations are satisfied:

$$\lambda_i = \frac{3}{64}\mu^2(1+q_i)^2, \qquad i=0,1 \quad (34)$$

$$q_0 = \int dp(z_0)\left(\frac{1}{\int dp(z_1)(\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^m}\right.$$
$$\left.\times\int dp(z_1)\tanh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0})(\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^m\right)^2 \quad (35)$$

$$q_1 = \int dp(z_0)\frac{1}{\int dp(z_1)(\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^m}$$
$$\times\int dp(z_1)(\tanh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^2(\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0}))^m \quad (36)$$

and the parameter m is chosen in such a way to minimize the resulting free energy.

One finds that for $\mu > \mu_c = 4.55$ the previous equations have a non trivial solution (e.g. $m \neq 0$, $q_1 \neq q_0$). The corresponding values of m, q_0 and q_1 are shown in Figs. 3 and 4. It is evident that the value of m is different from the one at critical temperature and that the difference $q_1 - q_0$ vanishes

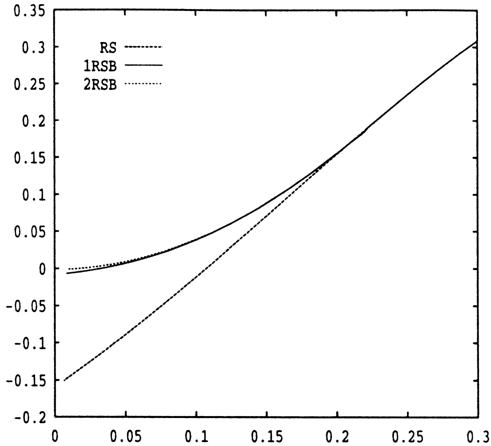

Fig. 1. Entropy as function of the reduced temperature τ in the replica symmetric case and in the broken symmetry case with one and two steps breaking.

at μ_c. This behaviour is similar to the one that is realized in the Sherrington–Kirkpatrick (SK) model in non-zero magnetic field.

In Figs. 1 and 2 we plot the entropy as function of the temperature. Also in this case the entropy becomes negative at sufficiently small temperature, but this happens in a rather smaller region above $\tau = 0$.

In the SK model for spin glasses, where this disaster happens at one step level, (we recall that the entropy cannot be negative), the correct value

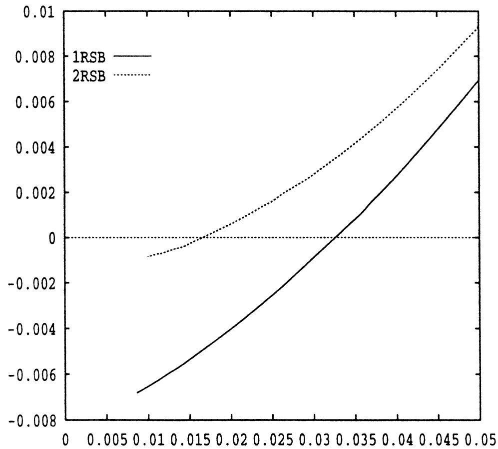

Fig. 2. Detail of the cases with broken replica symmetry, shown in Fig. 1, at low temperature.

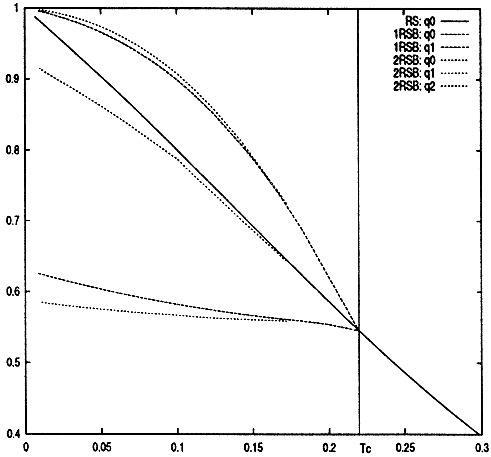

Fig. 3. Values of q_0 as function of the temperature τ in the replica symmetric case (full curve), of q_0 and q_1 in the broken symmetry case with one step breaking (dashed curves) and those of q_0, q_1 and q_2 in the two step replica symmetry breaking case (dotted curves).

of the entropy is proportional to τ^2. If a similar behaviour is present in this model the free energy should be given by $A+B\tau^3$ at small, but not too small τ. We show in Figs. 5 and 6 the free energy as function of τ^3. We see that in a wide range of τ^3 a linear behaviour is present supporting a quadratic dependence of the entropy on the the temperature. The extrapolated value of the zero temperature rescaled free energy obtained using

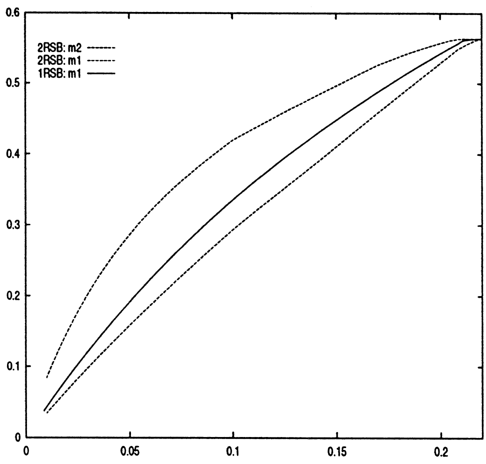

Fig. 4. Parameters m's as function of τ for one step (full curve) and two steps (dashed curves) replica symmetry breaking.

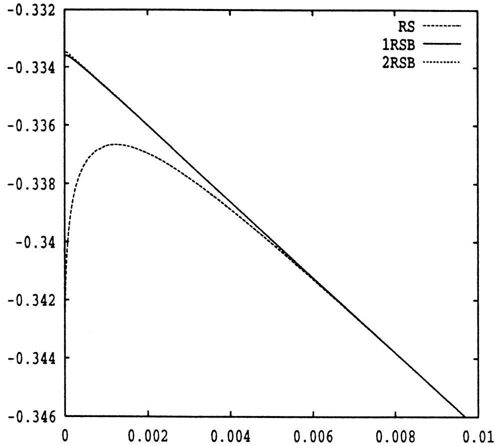

Fig. 5. Rescaled free energy versus the cube of the reduced temperature τ^3 in the replica symmetric case and in the broken symmetry cases with one and two steps breaking.

this method ($f_{ext}^{(1)} = A = -0.333412$) is slightly larger than the actual value at zero temperature ($f_{1RSB}(T=0) = -0.333740$), however this first value should be more reliable, because it is known that the errors in the free energy, if one makes the approximation of considering only a finite number of RSB steps, are negligible at higher temperature, but they become larger at low temperature. $f_{ext}^{(1)}$ gives an estimate (9) equal to $\alpha_c \simeq 7.114468$.

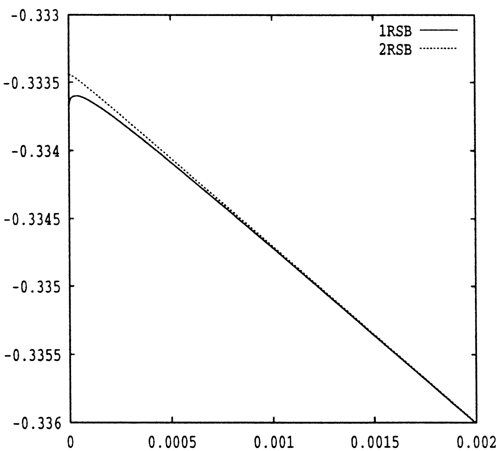

Fig. 6. Detail of Fig. 5 showing the one and two step symmetry breaking cases at low τ.

4.2. Two Steps Replica Symmetry Breaking

In we perform another step in breaking the replica symmetry and we let the elements of Q and Λ take three different values (q_0, q_1 and q_2 and λ_0, λ_1 and λ_2 respectively) the free energy will be a function of the five independent variables: q_0, q_1, q_2, m_1, m_2. In this case we have:

$$A(q_0, q_1, q_2; \lambda_0(q_0), \lambda_1(q_1), \lambda_2(q_2)) = -\frac{\mu\sqrt{\alpha}}{8} + \frac{\mu^2}{16}$$
$$-\frac{\mu^2}{128}[m_1(1+q_0)^3 + (m_2-m_1)(1+q_1)^3 + (1-m_2)(1+q_2)^3]$$
$$-\frac{\lambda_2}{2} + \frac{1}{2}[m_1\lambda_0 q_0 + (m_2-m_1)\,\lambda_1 q_1 + (1-m_2)\,\lambda_2 q_2]$$
$$+\frac{1}{m_1}\int \mathrm{d}p(z_0)\log\left(\int \mathrm{d}p(z_1)\right.$$
$$\left.\times\left[\int \mathrm{d}p(z_2)(2\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0} + z_2\sqrt{\lambda_2-\lambda_1}))^{m_2}\right]^{\frac{m_1}{m_2}}\right), \quad (37)$$

$$f(\mu) = -\frac{\mu}{16}\left[1 - \frac{1}{8}(m_1((1+q_0)^2(1-2q_0) - (1+q_1)^2(1-2q_1))\right.$$
$$\left. + m_2((1+q_1)^2(1-2q_1) - (1+q_2)^2(1-2q_2))) - \frac{(1+q_2)^2(2-q_2)}{4}\right]$$
$$-\frac{1}{m_1\mu}\int \mathrm{d}p(z_0)\log\left(\int \mathrm{d}p(z_1)\right.$$
$$\left.\times\left[\int \mathrm{d}p(z_2)(2\cosh(z_0\sqrt{\lambda_0} + z_1\sqrt{\lambda_1-\lambda_0} + z_2\sqrt{\lambda_2-\lambda_1}))^{m_2}\right]^{\frac{m_1}{m_2}}\right), \quad (38)$$

where the self consistency equations are:

$$\lambda_i = \frac{3}{64}\mu^2(1+q_i)^2, \qquad i = 0, 1, 2 \quad (39)$$

$$
\begin{aligned}
q_0 = \int \mathrm{d}p(z_0) \Bigg(& \frac{1}{\int \mathrm{d}p(z_1)[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2}]^{\frac{m_1}{m_2}}} \\
& \times \int \mathrm{d}p(z_1) \left[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2} \right]^{\frac{m_1}{m_2}-1} \\
& \times \int \mathrm{d}p(z_2) \tanh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}) \\
& \times (\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2} \Bigg)^2
\end{aligned}
\tag{40}
$$

$$
\begin{aligned}
q_1 = \int \mathrm{d}p(z_0) \Bigg(& \frac{1}{\int \mathrm{d}p(z_1)[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2}]^{\frac{m_1}{m_2}}} \\
& \times \int \mathrm{d}p(z_1) \left[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2} \right]^{\frac{m_1}{m_2}-2} \\
& \times \Bigg[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2} \\
& \times \tanh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}) \Bigg]^2 \Bigg)
\end{aligned}
\tag{41}
$$

$$
\begin{aligned}
q_2 = \int \mathrm{d}p(z_0) \Bigg(& \frac{1}{\int \mathrm{d}p(z_1)[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2}]^{\frac{m_1}{m_2}}} \\
& \times \int \mathrm{d}p(z_1) \left[\int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_2\sqrt{\lambda_1-\lambda_0}+z_1\sqrt{\lambda_2-\lambda_1}))^{m_2} \right]^{\frac{m_1}{m_2}-1} \\
& \times \int \mathrm{d}p(z_2)(\cosh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^{m_2} \\
& \times \tanh(z_0\sqrt{\lambda_0}+z_1\sqrt{\lambda_1-\lambda_0}+z_2\sqrt{\lambda_2-\lambda_1}))^2 \Bigg)
\end{aligned}
\tag{42}
$$

From Figs. 3 and 4 we see that the transition between the replica symmetric structure and the broken one at $\tau_c = 1/\mu_c = 0.21978$ is confirmed. In the two step computation the entropy (Fig. 2) still becomes negative but at a lower temperature than in the one step case and the zero temperature value is less negative than before. Even the τ^2 behaviour for small τ, or the equivalent $A + B\tau^3$ law for the free energy, is satisfied up to a smaller temperature. The extrapolated value of the zero temperature free energy is now $f_{ext}^{(2)} = A = -0.333401$, where the value given by the actual 2RSB free energy is $f_{2\mathrm{RSB}} = -0.333450$. Their difference is of an order of magnitude smaller than in the one step replica symmetry breaking case (we recall that in that case $f^{(1)}_{ext} = -0.333412$ and $f_{1\mathrm{RSB}}(T=0) = -0.333740$).

The pathologies here exhibited clearly show that the one step and the two steps solutions are still not exact, and it is natural to suppose that they will disappear when we break the replica symmetry in a continuous way.[5]

Using equation (9) once again, we find $\alpha_c \approx 7.1139985$. This value is not too far from the estimated result (i.e. 4.2)[3] if we consider how crude is our approximation.

5. CONCLUSIONS

We have seen that the transition from the replica symmetric case to the replica broken case is a smooth transition, which is quite different from the quasi first order transition of the p-spin model.[9] This difference is likely due to the fact that the self overlap q_0 is different from zero in the high temperature phase.

The one step approximation is not exact at low temperature and it is likely not to be exact in the whole replica symmetry broken phase. The two step replica symmetry breaking computation gives clear hints that the replica symmetry must be broken in a continuous way. In any case both approximations apparently give excellent approximations for the free energy at low temperature (the error on the value of the zero temperature free energy is $O(10^{-4})$ at one step and $O(10^{-5})$ at two steps RSB level respectively).

The model has a behaviour that is very similar to the one of the Sherrington–Kirkpatrick model in presence of a magnetic field. It is natural to conjecture that these properties hold in a quite large interval of values of α, for $\alpha \geqslant \alpha_c$, even far from the full connectivity limit $\alpha \to \infty$. It would be very interesting to check these predictions using numerical simulations and/or analytic tools.

ACKNOWLEDGMENTS

We wish to thank Enzo Marinari and Riccardo Zecchina for many useful discussions on the subject of this paper.

REFERENCES

1. R. Monasson and R. Zecchina, *Phys. Rev. Lett.* **76:** 3881 (1996); R. Monasson and R. Zecchina, *Phys. Rev. E* **56**:1357 (1997).
2. R. Monasson, R. Zecchina, S. Kirkpatrick, B. Selman, and L. Troyansky, *Nature* **400**:133 (1999).

3. S. Kirkpatrick and B. Selman, *Science* **264**:1297 (1994).
4. S. A. Cook, in *Proc. 3rd Annu. ACM Symp. on Theory of Computing 151* (Assoc. Comput. Machinery, New York, 1971).
5. M. Mézard, G. Parisi, and M. A. Virasoro, *Spin glass theory and beyond* (World Scientific, Singapore 1987).
6. G. Biroli, R. Monasson, and M. Weigt, *Eur. Phys. J. B* **14**:551 (2000).
7. B. Aspvall, M. F. Plass, and R. E. Tarjan, *Inf. Process. Lett.* **8**:121 (1979).
8. D. Sherrington and S. Kirkpatrick, *Phys. Rev. Lett.* **26**:1782 (1975); S. Kirkpatrick, D. Sherrington, *Phys. Rev. B* **17**:4384 (1978).
9. T. R. Kirkpatrick and D. Thirumalai, *Phys. Rev. Lett.* **58**:2091 (1987); T. R. Kirkpatrick and D. Thirumalai, *Phys. Rev.* **B36**:5388 (1987); T. R. Kirkpatrick, D. Thirumalai, and P. G. Wolynes, *Phys. Rev.* **A40**:1045 (1989).