To be submitted to
Journal of Physics A

ISTITUTO NAZIONALE DI FISICA NUCLEARE
Laboratori Nazionali di Frascati

LNF-79/38(P)
25 Giugno 1979

G. Parisi: THE ORDER PARAMETER FOR SPIN GLASSES: A FUNCTION ON THE INTERVAL 0-1.

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ABSTRACT.

We study the breaking of the replica symmetry in spin glasses. We find that the order parameter is a function on the interval 0 - 1. This approach is used to study the Sherrington-Kirkpatrick model. Exact results are obtained near the critical temperature. Approximated results at all the temperatures are in excellent agreement with the computer simulations, at zero external magnetic field.

1. - INTRODUCTION.

Magnetic transitions in ferromagnetic or antiferromagnetic materials are well understood theoretically ; one of the most interesting open problems is the nature of the transitions in spin glasses (i. e. systems which are neither ferromagnetic nor antiferromagnetic, because the sign of the exchange interaction changes randomly from bond to bond). Spin glasses are the simplest amorfous materials we can study: we face the problem of finding the order parameter which is appropriate to describe the onset of ordering in a disordered medium.

The general framework in which we study this problem, is the replica theory (Edwards and Anderson, 1975). The main idea is rather simple : the free energy (F_R) of a random system can be written as :

$$F_R = \int d[J]\,\mu[J]\,F[J] \, , \tag{1}$$

where J stands for the random variables, $\mu[J]$ is their probability measure (normalized to 1) and $F[J]$ is the J dependent free energy. In spin glasses :

$$\beta F[J] = -\ln \int \prod_{i=1}^{N} \varrho(\sigma_i)\, d\sigma_i \, \exp -\beta H[J,\sigma] \doteq -\ln Z[J] \, ,$$
$$H[J,\sigma] = \sum_{i,k=1}^{N} J_{ik}\,\sigma_i\sigma_k \, , \tag{2}$$

where σ_i are the spin variables, $\varrho(\sigma)$ is their distribution (in the Ising model $\varrho(\sigma) = \delta(\sigma^2 - 1)$) and N is the number of spins.

Eq. (1) and (2) are not easy to study under this form, because F_R is not written as the integral of the exponential of an Hamiltonian, as normally happens. In order to present the problem under a more familiar form, it is useful to introduce the function

$$Z_n = \frac{1}{n} \int d[J]\,\mu[J]\,Z^n[J] \, . \tag{3}$$

Obviously one has :

$$\beta F_R = - \lim_{n \to 0} (Z_n - \frac{1}{n}) \quad . \tag{4}$$

Now, for integer n, Z_n can be written as :

$$Z_n = \int d[J]\, \mu[J] \int \prod_{\alpha=1}^{n} \prod_{i=1}^{N} \varrho(\sigma_i^\alpha)\, d\sigma_i^\alpha \exp\left[-\beta \sum_{\alpha=1}^{n} H[J, \sigma^\alpha]\right] \tag{5}$$

where σ_i^α are $n \times N$ spin variables.

Eq. (5) is the partition functionn of n identical replicas of the same system, interacting with the same J dependent hamiltonian.

The strategy consists in finding the partition function Z_n for generic integer n and finally performing the analytic continuation up to the point $n = 0$. In this way one is led to introduce, as an order parameter, the $n \times n$ matrix

$$Q_i^{\alpha,\beta} = \langle \sigma_i^\alpha \sigma_i^\beta \rangle \qquad \alpha \neq \beta \tag{6}$$

a physical order parameter is

$$\bar{q} = \frac{1}{N} \sum_{i=1}^{N} \langle \langle \sigma_i \rangle^2 \rangle \quad , \tag{7}$$

where the internal bracket indicates the thermodynamic expectation value at fixed J, while the external bracket indicates the mean value over J.

In the high temperature phase $\frac{1}{N} \Sigma_i Q_i^{\alpha\beta} \equiv Q_{\alpha\beta} = 0$, while in the spin glass phase $Q_{\alpha,\beta} \neq 0$. In the standard treatment it is assumed that $Q_{\alpha,\beta} = q$ independently from α and β. This possibility is the only one symmetric under permutations of the replicas. In this scheeme $\bar{q} = q$.

In order to test the correctness of this approach, it is useful to investigate a model (the S-K model) (Sherrington and Kirkpatrick, 1975) in which the mean field approximation should be exact ; this model con sists of N Ising spins interacting one with all the others with a random gaussian interaction ($\langle J_{ik}^2 \rangle = 1/N$). Assuming that $Q_{\alpha\beta} = q$, the model can be solved, using the saddle point method when $N \to \infty$. One finds that

$$\beta F_R(T) = \max F_T(q) ,$$

$$F_T(q) = -\frac{\beta^2}{4}(1+q)^2 + \ln 2 - (2\pi)^{-1/2} \int dz \left\{ \exp - \frac{z^2}{2} \cdot \ln \left[ch(\beta q^{1/2} z) \right] \right\} , \qquad \beta = 1/T . \tag{8}$$

A transition is present at $T = 1$ and $q \neq 0$ when $T < 1$.

From the knowlidge of $F_R(T)$ other thermodynamical quantities ,like the specific heat (U(T)) and the entropy (S(T)), can be calculated,however the results desagree with the computer simulations (Sherrington and Kirkpatrick, 1978) for $N = 500$, extrapolated up to $N = \infty$ (e. g. the computer simulations give $U(0) = -0.76 \pm 0.01$ while this analytic method gives $U(0) = -\sqrt{2/\pi} \simeq -0.80$). The situation worsens if we consider the entropy: by definition S(T) is non negative and eq. (8) implies a negative value of S at low temperatures ($S(0) \simeq -0.17$ while $S(\infty) = \ln 2 \simeq 0.69$).

The origine of this failure remained unexplained for some time: it is possible to blame the exchange of limits $n \to 0$ with $N \to \infty$ (Van Hemmer and Palmer, 1979) but no constructive approach can be found to avoid this difficulty.

It has been finally remarked (de Almeida and Thouless, 1978 ; and Pytte and Rudnik, 1979) that the correct expression is

$$F_R = T \max F_T(Q) ,$$

$$F_T(Q) = -\frac{\beta^2}{4} + \ln 2 + \lim_{n \to 0} \left\{ \frac{1}{4} \Sigma_{\alpha,\beta}\, \beta^2 Q^2_{\alpha,\beta} - \ln \left[\mathrm{Tr} \exp (\Sigma_{\alpha,\beta}\, \beta^2 Q_{\alpha,\beta}\, S_\alpha S_\beta) \right] \right\} , \tag{9}$$

where Tr stands for the sum over all the 2^n possible values of the n Ising spin variables S_α and the maximum is taken over all possible matrices $Q_{\alpha,\beta}$. Eq. (8) is correct only if F(Q) has its maximum at a symmetric point ; in reality the symmetric point is only a saddle point. This can be seen by computing the eigenvalues of the matrix $M_{\alpha\beta;\gamma\delta}$ defined by :

$$F_T(Q) = F(Q^o) + \Delta_{\alpha\beta} M_{\alpha\beta;\gamma\delta} \Delta_{\gamma\delta} + O(\Delta^3) \,,$$
$$\Delta = Q_{\alpha\beta} - Q^o_{\alpha\beta} \,, \qquad Q^o_{\alpha\beta} = q^o \,, \tag{10}$$

where q^o minimizes eq. (8).

A straightforward computation shows that the matrix M has negative eigenvalues for $T < 1$. The replica symmetry invariant point does not maximize F(Q) and replica symmetry must be broken : we have to look for solutions of eq. (9) which are not symmetric in α and β.

We face the rather difficult problem of parametrize an n x n matrix in the limit $n = 0$. To work directly in the zero dimensional space is rather difficult ; to circumvent this problem we will define also the matrix $Q_{\alpha\beta}$ by analytic continuation. We define an n x n matrix $Q^{(n)}_{\alpha\beta}$ which depends on a set of parameter $\{ q_i, m_i \}$ (e. g. the q_i are the elements of matrix and the m_i describe the form of the matrix). With a suitable choice of the parametrization $F_T(Q^{(n)})$ can be extended to an analytic function of n (at this end we need that $Q^{(n)}_{\alpha,\beta}$ is defined only for n multiples of a fixed integer) and the maximum of $F_T(Q)$ should be taken over all the possible parametrizations.

It is evident that the number of different parametrization is unbonded and the space of $O \otimes O$ matrices with these definitions is an infinite dimensional space.

The search for a maximum is not simple in such a big space. We have been guided by the following three requirements :

$$\left[\lim_{n\to 0} \frac{1}{n} \Sigma_{\alpha,\beta} Q^2_{\alpha,\beta} \right] < \infty \;; \tag{11a}$$

$$\sum_{1}^{N}{}_{\beta} Q_{\alpha\beta} = \sum_{1}^{N}{}_{\beta} Q_{\gamma\beta} , \qquad \alpha \neq \gamma \tag{11b}$$

$$-\lim_{n \to 0} \frac{1}{n} \Sigma_{\alpha,\beta} Q^2_{\alpha,\beta} > 0 \quad . \tag{11c}$$

Requirement (11a) comes from the condition that F_R must be finite; the eigenvectors with negative eigenvalue of the matrix M satisfies requirement (11b): it is natural to look for a maximum of $F_T(Q)$ in the space spanned by these vectors; at high temperatures we want that the maximum of $F_T(Q)$ is located at $Q_{\alpha,\beta} = 0$ and this happens only if condition (11c) is satisfied.

Although the requirements (11) do not fix the symmetry breaking pattern, they exclude those previously proposed in the past (Blandin, 1978) and (Bray and Moore, 1978). In the first case requirement (11c) is not satisfied, in the second case requirement (11a) is violated. In this paper we investigate the simplest parametrizations of the matrix $Q_{\alpha,\beta}$ satisfying requirements (11).

In Section 2 we describe the parametrizations we propose and we show that a function q(x) defined on the interval 0-1 is naturally associated to each parametrization of the class we consider. In this approach the order parameter belongs to $L^2(0,1)$. If replica symmetry is unbroken q(x) is a constant. In simple approximation scheemes q(x) is a piecewise constant function which takes only a finite number of values. A direct interpretation of q(x) is lacking although it may have the meaning of probability distribution. This point deserves more accurate investigations.

In Section 3 we apply this approach to the study of the S-K model near T_c. In Section 4 we show how a very simple minded approximation (q(x) takes only two values) is sufficient to obtain a substantial improvement respect to the situation with unbroken replica symmetry for the S-K model at all the temperatures (e. g. we obtain $U(0) \simeq -0.765$ and $S(0) \simeq -0.01$).

2. - THE PARAMETRIZATION.

In this paper we will study the following parametrization of the matrix $Q_{\alpha,\beta}$ (G. Parisi, 1979 b) :

$$\begin{aligned} Q_{\alpha,\alpha} &= 0 \ , \\ Q_{\alpha,\beta} &= q_i \qquad \text{if} \quad I(\alpha/m_i) \neq I(\beta/m_i) \\ &\qquad\qquad \text{and} \quad I(\alpha/m_{i+1}) = I(\beta/m_{i+1}) \ , \end{aligned} \tag{12}$$

where q_i $(i = 0, K)$ are real numbers and m_i $(i = 1, K)$ are integer numbers such that m_{i-1}/m_i is integer $(i \geq 1)$ (We pose $m_o = 1$, $m_{K+1} = n$).

The matrix $Q_{\alpha,\beta}$ depends on $K+1$ real parameters (the q_i's) and on K integer parameters (the m_i's). For $n = 8$, $K = 2$, $m_1 = 2$, $m_2 = 4$, we have :

$$Q_{\alpha,\beta} = \left| \begin{array}{cccccccc} 0 & q_o & q_1 & q_1 & & & & \\ q_o & 0 & q_1 & q_1 & & & & \\ q_1 & q_1 & 0 & q_o & & q_2 & & \\ q_1 & q_1 & q_o & 0 & & & & \\ & & & & 0 & q_o & q_1 & q_1 \\ & & & & q_o & 0 & q_1 & q_1 \\ & & q_2 & & q_1 & q_1 & 0 & q_o \\ & & & & q_1 & q_1 & q_o & 0 \end{array} \right| \tag{13}$$

We do not have any serious argument to justify the Ansatz eq. (12) (apart from the requirement (11)). Its main virtue is its semplicity. It is not evident a priori if the solution of the variational problem, eq. (9), has the form dictated by eq. (12). The only possible justification of the Ansatz eq. (12) is its ability to reproduce the results of the computer simulations, as we shall see in Section 4.

We must now continue the matrix $Q_{\alpha\beta}$ up to $n = 0$. In doing so it is not evident if the m_i must remain integers, we suppose that for non in teger n, no conditions on the m_i is present and they can be arbitrary real number (Parisi, 1979 a). However we want that conditions (11) are satisfied.

Conditions (11a) and (11b) are identically satisfied while condition (11c) implies

$$1 \geq m_1 \geq m_2 \ldots\ldots m_K \geq 0 \;. \tag{14}$$

Eq. (14) follows from the relation:

$$\lim_{n \to 0} \frac{1}{n} \Sigma_{\alpha,\beta} Q^2_{\alpha\beta} = \sum_0^K {}_i (m_i - m_{i+1}) q_i^2 \;. \tag{15}$$

The scheeme of Blandin (Blandin, 1978) is $K = 1$, $m_1 = 2$ and obviously does not satisfy condition (11c).

It is natural to define the function $q^{(K)}(x)$ as

$$q^{(K)}(x) = q_i \;, \qquad \text{if} \quad m_i < x < m_{i+1} \;. \tag{16}$$

With definition we have:

$$-\lim_{n \to \infty} \Sigma_{\alpha,\beta} Q^2_{\alpha,\beta} = \int_0^1 dx\, (q^{(K)}(x))^2 \;. \tag{17}$$

$q^{(K)}(x)$ is a piecewise function which takes at most K+1 different values. In the limit $K \to \infty$, we obtain a generical function of $L^2(0,1)$. In the next Section we will argue that the maximum of eq. (9) is reached in the limit $K \to \infty$.

At this stage is unclear if the sequences of function $q^{(K)}(x)$ converges toward a function $q(x)$ when $K \to \infty$. We shall verify that this happens in an explicit example in the next Section.

3. - ANALYTIC RESULTS NEAR T_c.

Near the critical temperature T_c ($T_c = 1$) the matrix $Q_{\alpha\beta}$ is small (proportional to $\tau = T_c - T$) so that it is reasonable to expand it in powers of Q.

One finds (Bray and Moore, 1978 ; Pytte and Rudnick, 1979) :

$$F_T(Q) = \lim_{n \to 0} \left(-\tau \, \mathrm{tr}\, Q^2 + \frac{1}{3} \mathrm{tr}\, Q^3 + y \, \Sigma_{\alpha,\beta} \, Q^4_{\alpha,\beta} + O(Q^4)\right) \qquad (18)$$

where tr is the standard trace in the n dimensional vector space. Among the various term of forth order we have written the only one which is responsible for the breaking of the replica symmetry.

Indeed if $y \gtrsim 0$ the symmetric solution would be a maximum and not a saddle point. In the S-K model y is negative and replica symmetry is broken. We will study in details the case $y = -1/4$ and look for a maximum of F(Q) with $Q_{\alpha,\beta} = O(\tau)$.

After some algebra one finds that

$$F_T(Q) = \int_0^1 dx \left\{ + \tau \, q^2(x) + \frac{1}{4} q^4(x) - \frac{1}{3} x \, q^3(x) - q^2(x) \int_x^1 q(y) \, dy \right\} \qquad (19)$$

where the parametrization (12) has been used and the function q(x) is defined by eq. (6) (For semplicity we have written $q^{(K)}(x)$ as q(x)).

Eq. (19) can also be written using the parameters q_i and m_i as :

$$F_T(q_i . m_i) = \sum_0^N {}_i (m_i - m_{i+1}) \left\{ + \tau \, q_i^2 + \frac{1}{4} q_i^4 - \frac{1}{3}(2m_i - m_{i+1}) q_i^3 + q_i \sum_{i+1}^N {}_j (m_j - m_{j+1}) \, q_j^2 \right\} \qquad (20)$$

At fixed K we look for a local maximum of F(Q), under the conditions $q_i = O(\tau)$. One finds :

$$q_o = \tau + C^{(K)}\tau^2 + O(\tau^3) ,$$

$$q_i = B_i^{(K)}\tau + O(\tau^2) , \qquad (21)$$

$$m_i = L_i^{(K)}\tau + O(\tau^2) .$$

After some painful algebra one obtains :

$$C^{(K)} = \frac{3}{2} - \frac{1}{(2K+1)^2} \quad ; \qquad B_i^K = \frac{2(K-i)+1}{2K+1} \quad ;$$

$$L_i^{(K)} = \frac{6i}{2K+1} . \qquad (22)$$

When $K \to \infty$ the function $q^{(K)}(x)$ converges toward:

$$q(x) = \frac{x}{3} + O(\tau^2) \qquad \text{if} \quad x < 3\tau ,$$

$$q(x) = \tau + O(\tau^2) \qquad \text{if} \quad x > 3\tau . \qquad (23)$$

In Fig. 1 we have shown the function $q^{(K)}(x)$ taking only the terms of $O(\tau)$, for $K = 1$, 4 and ∞.

It would be tempting to interpret $q(x)$ as the mean value of the parameter q (eq. (7)) inside a cluster of size xN, but the rationale for this interpretation is rather misterious.

If we consider the internal energy $U(\tau) = dF/d\tau$, we find that

$$U(\tau) = \int_0^1 q^2(x)\, dx = \tau^2 + \tau^3 + U_4^{(K)}\tau^4 + O(\tau^5) , \qquad (24)$$

where :

$$U_4^{(K)} = \frac{q}{4} - \frac{1}{(2K+1)^4} . \qquad (25)$$

It is remarkable that $U_4^{(K)}$ for $K = 1$ differs from the exact result less than 1% ; we expect rather good results at all temperatures from the approximation $K = 1$; this expectation is confirmed from the results

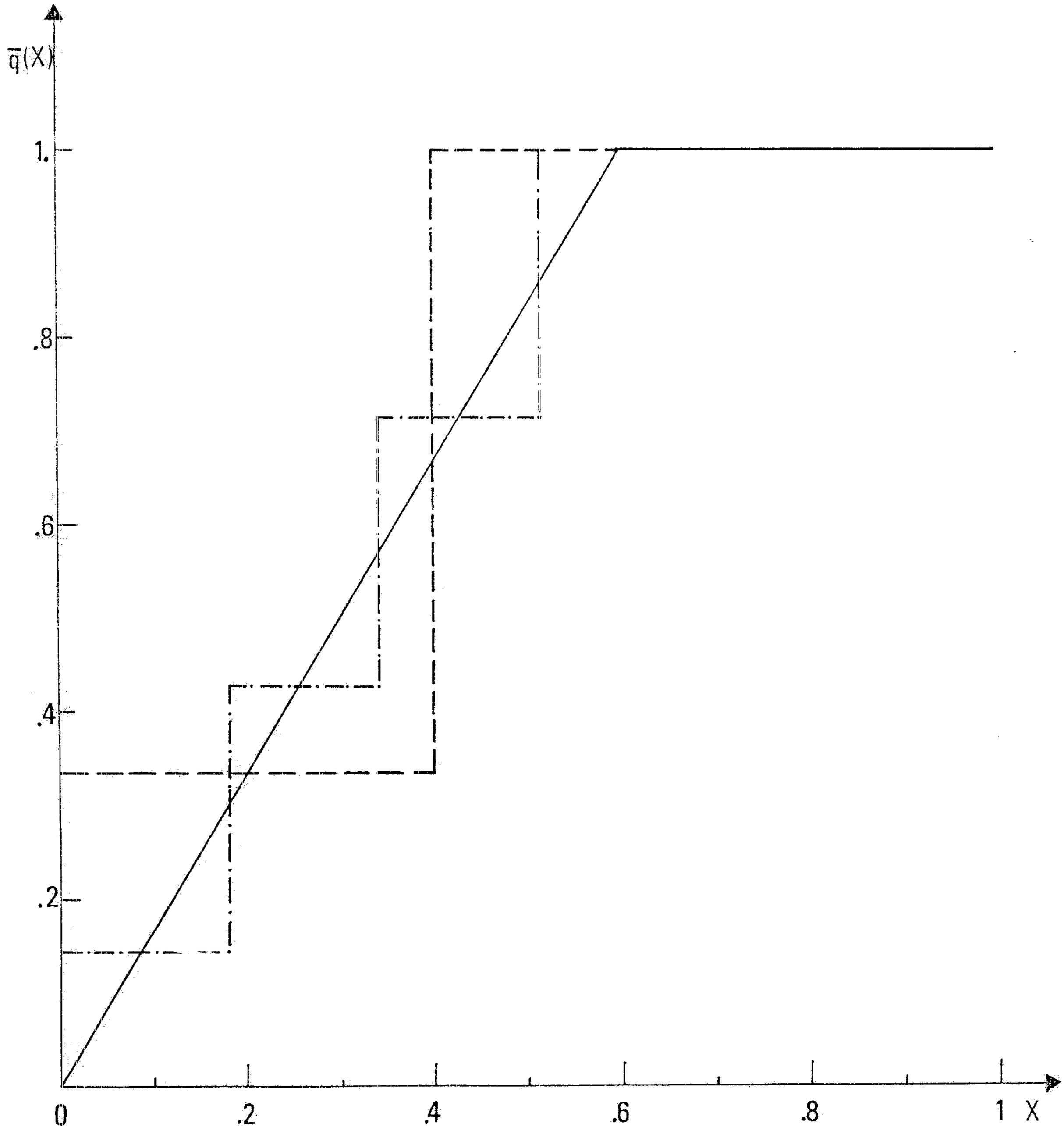

FIG. 1 - The dashed curve, the point-dashed curve and the full curve are respectively the function $q^{(K)}(x)$ for $K = 1$, 4 and ∞.

of the next Section.

For compleatness we also write the result :

$$- \Sigma_{2}^{n}{}_{\beta} Q_{\alpha\beta} \equiv \tilde{q} \equiv \int_0^1 q(x)\,dx = \tau + q_2^{(K)} \tau^2 + O(\tau^3) \ ,$$

$$q_2^{(K)} = \frac{1}{2(2K+1)^2} \ . \tag{26}$$

At this stage is unclear which of the two equations is correct for q (eq. (7)) :

$$\bar{q} = q(1) = \tau + \frac{3}{2}\ \tau^2 + O(\tau^3) \ ,$$

$$\bar{q} = \tilde{q} = \tau + O(\tau^3) \ . \tag{27}$$

This ambiguity can be claryfied by studying the magnetic properties of a spin glass ; this task goes beyond the limits of this paper and it will be dealt in a future publication.

4. - ALL THE TEMPERATURES.

In the previous Section we have seen that the approximation K = 1 gives very good results near $T_c = 1$. We study it now at all the temperatures.

One finds (G. Parisi, 1979 a) :

$$\beta F(p, tm) = - \frac{\beta^2}{4} \left[1 + mp^2 + (1-m)(p+t)^2 - 2(p+t) \right] + \ln 2 -$$

$$- (2\pi)^{-1/2} \int dz \left\{ \exp(- \frac{z^2}{2}) m^{-1} \ln \left[(2\pi)^{-1/2} \ \cdot \right.\right. \tag{28}$$

$$\left.\left. \cdot \int dy \exp(- \frac{y^2}{2}) \, ch^m(\beta p^{1/2} z + \beta t^{1/2} y) \right] \right\} \ ,$$

where $q_1 = p$ and $q_o = p+t$.

If $m = 0$ or $t = 0$ we recover the result without breaking of the replica symmetry ($K = 0$) eq. (8), where $q = p + t$.

The internal energy is given by:

$$U(\tau) = -\beta(1 - q^2)/2 , \qquad q^2 \equiv mp^2 + (1 - m)(p + t)^2 . \tag{29}$$

We must now maximize eq. (28) as function of p, t and m. This has been done on a computer using a standard minimization program.

One finds that for $T > T_c = 1$

$$p = t = 0 .$$

For $T < 1$, p, t and m are all different from zero and the $K = 1$ free energy is always greater than the $K = 0$ free energy. In Figs. 2, 3 and 4 we show respectively the internal energy, the specific heat and the entropy as function of τ, both for $K = 0$ and $K = 1$. As expected the difference between the two approximations is relevant only for $T < 0.5$. For comparison we plot also the low temperature C(T) and S(T) obtained within a different approach (Thouless, Anderson and Palmer, 1977).

The entropy is negative for $T < 1$ and S(0) is negative although quite small ($S(0) \simeq -0.01$); we expect that $S(0) = 0$ only for infinite K. A substantial improvent has been obtained respect to $K = 0$. The computation of the entropy for $K = 2$ would be as rather long, but straightforward.

The values shown in Figs. 1, 2, 3 and 4 are in excellent agreement with the computer simulations (e.g. $U(0) = -0.765$, while the computer simulations suggest $U(0) = -0.76 \pm 0.01$) (Sherrington and Kirkpatrick, 1978).

For compleatness we show in Fig. 5 the parameter q_o both for $K = 0$ and 1. The dashed line is the prediction of TAP for q (Thouless et al., 1977).

The value of $\tilde{q}$ is not shown: it would be a curve slightly lower than q_o for $K = 0$.

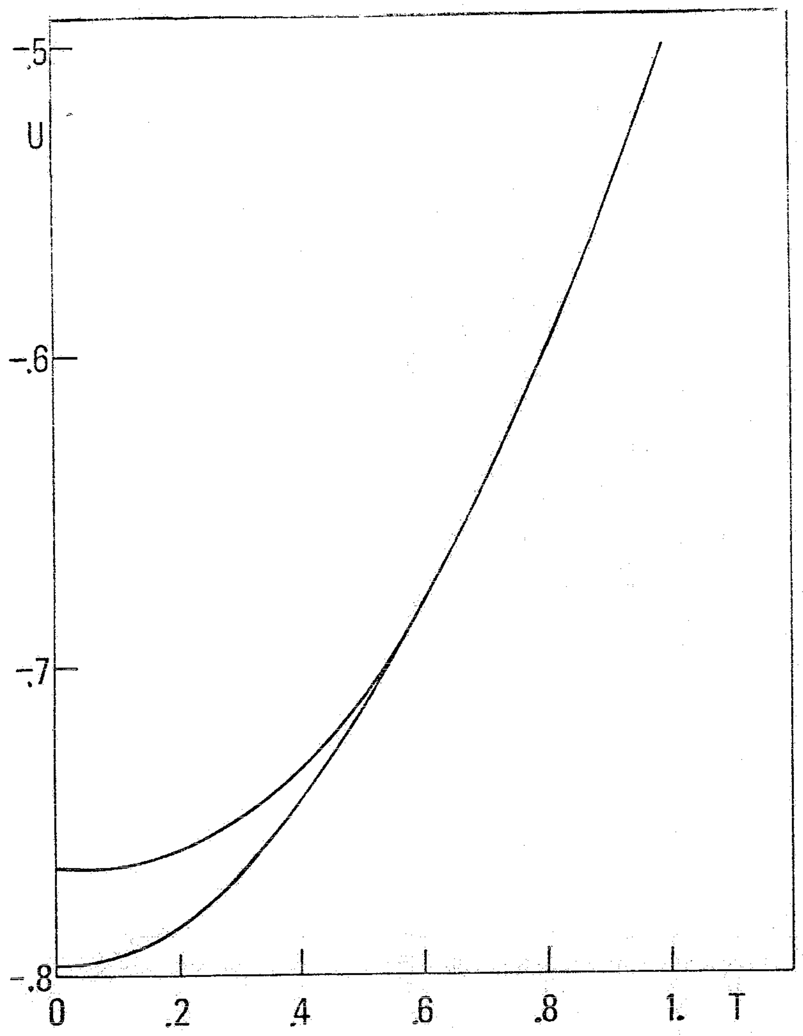

FIG. 2 - The lower and the upper curve are respectively the internal energy U_T) for K = 0 and K = 1.

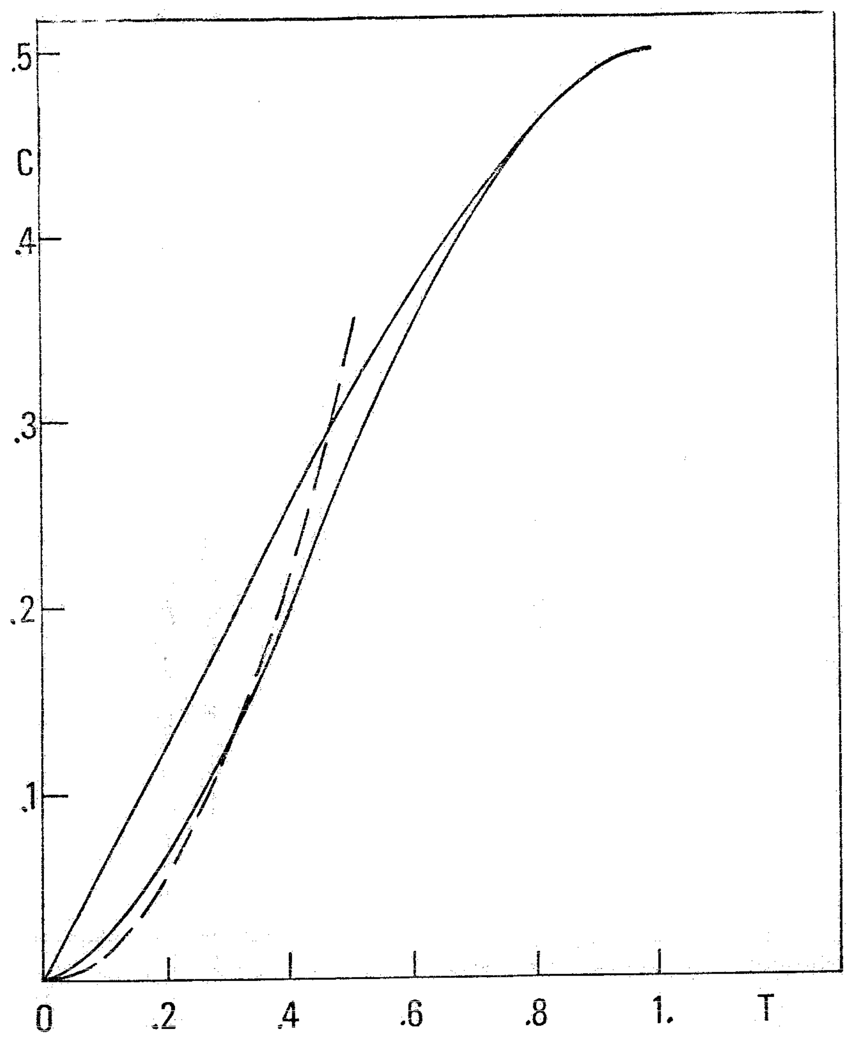

FIG. 3 - The lower and the upper curve are respectively the specific heat C(T) for K = 1 and K = 0. The dashed curve is the prediction $C(T) = 2 \ln 2\, T^2 + O(T^3)$ (Thouless et al., 1977).

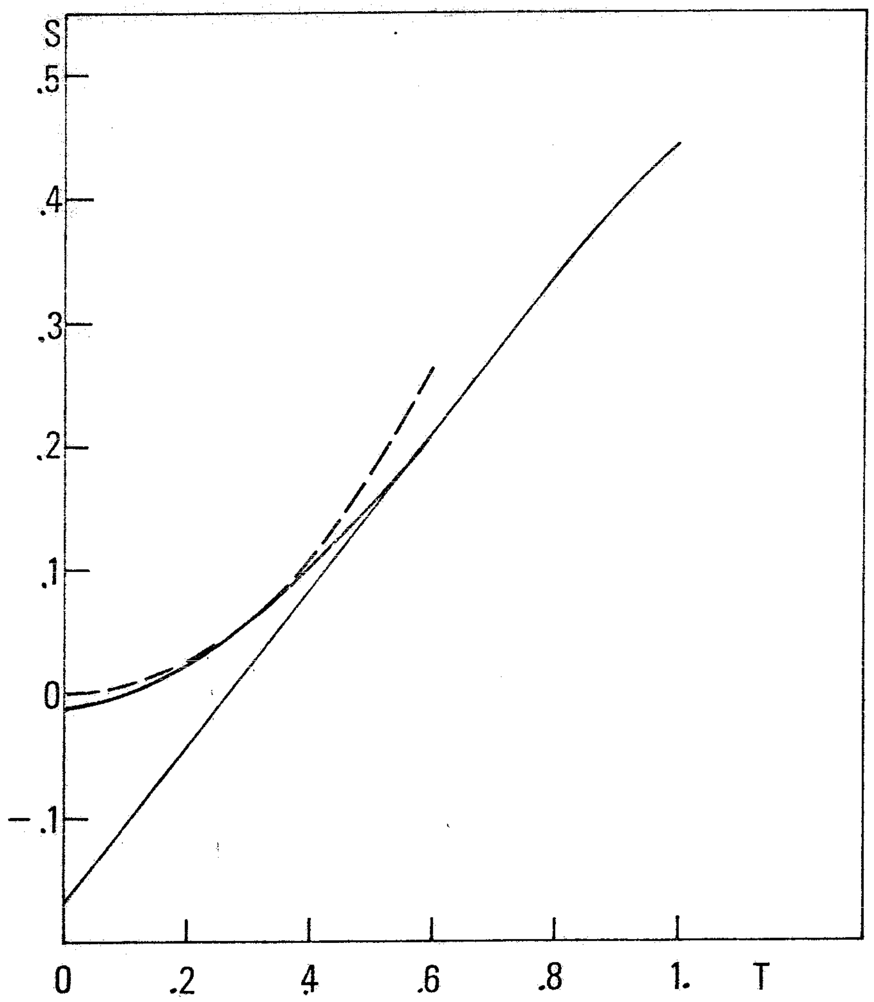

FIG. 4 - The lower and the upper curve are respectively the entropy S(T) for K = 0 and K = 1. The dashed curve is the prediction $S(T) = \ln 2\, T^2 + O(T^3)$ (Thouless et al., 1977).

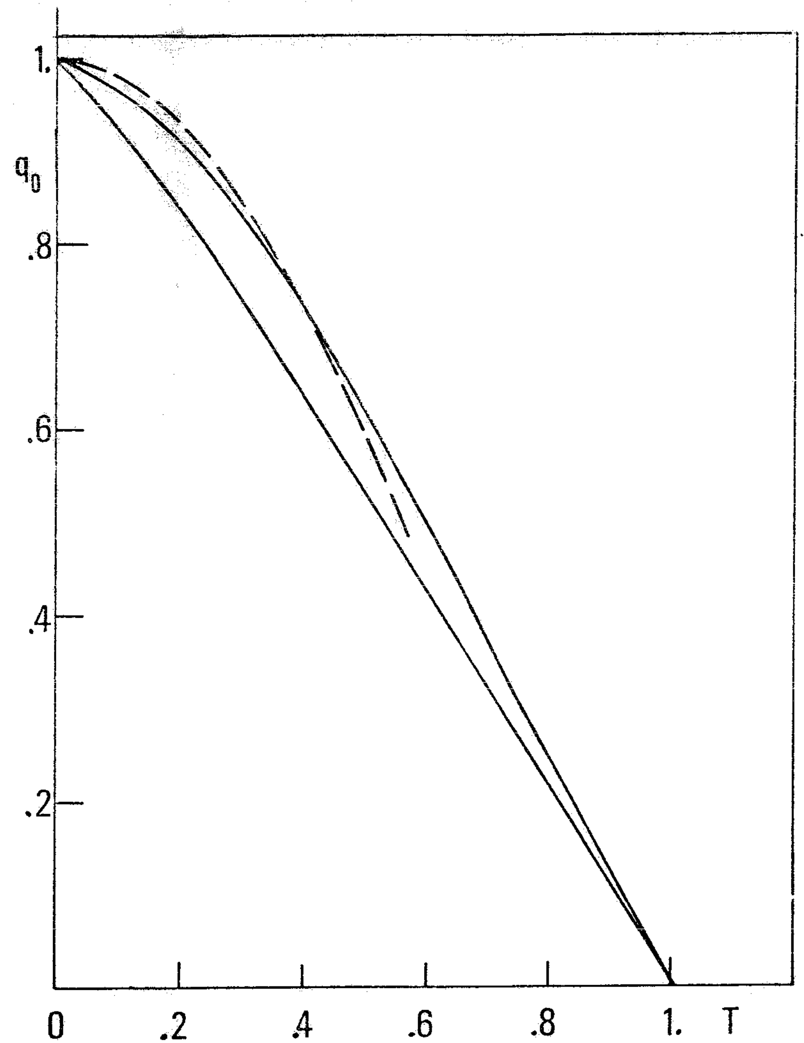

FIG. 5 - The lower and the upper curve are respectively the parameter q_o as function of T for K=0 and K=1. Just for comparison the dashed curve is the prediction for the function $\overline{q}(T)$ (Thouless et al., 1977): $\overline{q}(T) = 1 - 2(\ln 2)^{1/2} T^2 + O(T^3)$.

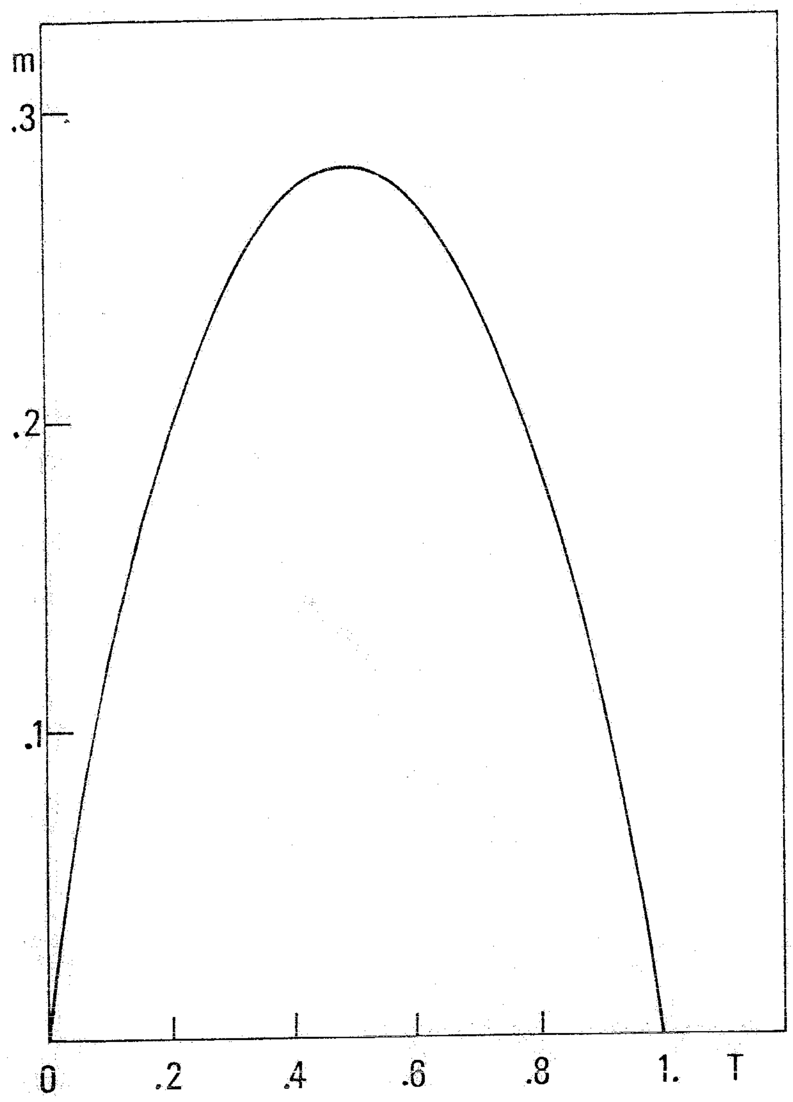

FIG. 6 - The parameter m_1 for $K = 1$ as function of T.

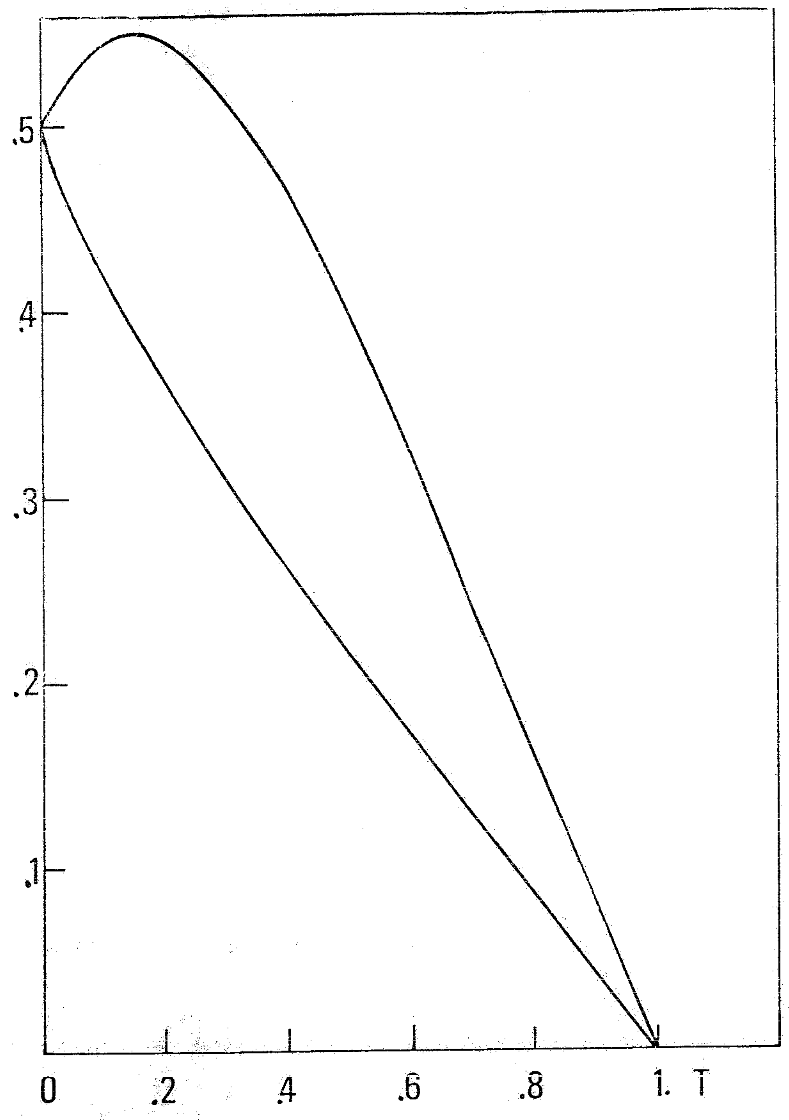

FIG. 7 - The lower and the upper curve are respectively the parameter t and p for $K = 1$ as functions of T.

In Figs. 6 and 7 we shown the T dependence of p, t and m. It is interesting to note that m becomes zero both at T = 0 and T = 1, and that the ratio t/p decreases monotonously with the temperature from t/p = 2 at T = 1 to t/p = 1 at T = 0.

It seems that this approach leads to the exact solution of the S-K model in the limit $K \to \infty$; a crucial test of this conjecture would be obtained by calculating the thermodynamic quantities for higher K and by studying the dependence on the magnetic field of the computer simulations.

The author is grateful to C. de Dominicis, C. Natoli and L. Peliti for useful discussions and suggestions.

REFERENCES.

Blandin J. 1978 J. Physique C6, 1578.
Bray A. J. and Moore M. A. 1978 Phys. Rev. Letters 41, 1069.
de Almeida J. R. L. and Touless D. J. 1978 J. Physique A11, 983.
Edwards S. F. and Anderson P. W. 1975 J. Physique F5, 965
Parisi G. 1979 a submitted to Phys. Letters A.
Parisi G. 1979 b submitted to Phys. Rev. Letters.
Pytte F. and Rudnik J. 1979 Phys. Rev. B19, 3603.
Sherrington D. and Kirkpatrick S. 1975 Phys. Rev. Letters 35, 1972.
Sherrington D. and Kirkpatrick S. 1978 Phys. Rev. 17B, 4385.
Thouless D. J., Anderson P. W. and Palmer R. G. 1977 Phil. Mag. 35, 593.
Van Hemmer J. L. and Palmer R. G. 1979 J. Physique A12, 567.