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G. Parisi: A SEQUENCE OF APPROXIMATED SOLUTIONS TO THE S-K MODEL FOR SPIN GLASSES.

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ABSTRACT

In the framework of the new version of the replica theory, we compute a sequence of approximated solutions to the Sherrington-Kirkpatrick model of spin glasses.

It has been recently shown that in the replica approach to spin glasses (Edwards and Anderson 1975), if the replica symmetry is broken (de Almeida and Thouless 1978, Pytte and Rudnik 1979), as happens in the spin glass phase at low magnetic field, the local order parameter is a function $q(x)$ defined on the interval 0-1 (Parisi, 1979 c, d). If the replica symmetry is unbroken, the function $q(x)$ is a constant.

The S-K model for spin glasses (Sherrington and Kirkpatrick 1975) is supposed to be soluble in the mean field approximation (the range of the interaction is infinite) and it is a good testing ground for this approach.

We derive here a convergent sequence of approximations to the free energy of the S-K model; excellent agreement is obtained with the computer simulations of Sherrington and Kirkpatrick 1978. The zero temperature entropy is consistent with zero, while the zero temperature internal energy is estimated to be:

$$U(0) = -0.7633 \pm 10^{-4} \quad . \tag{1}$$

The computer simulations give $U(0) = -0.76 \pm 10^{-2}$.

As in the conventional approach, one uses the replica trick to integrate over the random spin couplings; in the saddle point approximation (which becomes exact in the thermodynamical limit) one finds that the free energy density F_R given by

$$F_R = T \max F_T\left[Q\right] \quad ; \qquad \beta = 1/T \quad , \tag{2}$$

$$F_T(Q) = -\frac{\beta^2}{4} + \lim_{n \to 0} \left\{ \frac{1}{4} \sum_{a,b} \beta^2 Q^2_{a,b} - \ln\left[\mathrm{Tr}\exp\left(\sum_{a,b} \beta^2 Q_{a,b} S_a S_b\right)\right]\right\}$$

where Tr stands for the sum over all the 2^n possible values of the n Ising spin variables S_a and the maximum is taken over all the possible $n \times n$ matrices Q, h being the external magnetic field. After that the limit $n \to 0$ is taken, Q is a 0×0 matrix, which is defined as analytic continuation from integer n. The replica symmetry is broken, i.e. the matrix Q, which maximize $F_T(Q)$, has a non trivial dependence on the indeces. There is a very large number of ways in which this dependence may be realized (Blandin 1978, Bray and Moore 1978, Blandin, Gabay and Garel 1979), the spàce of 0×0 matrices being in reality an infinite dimensional space. It was realized by Parisi 1979 c, that this space contains a subspace S, which is isomorfic to the space of continuous functions on the interval 0-1. A matrix Q belonging to S can be represented by a function $q(x)$. It has been suggested that the maximum of $F_T(Q)$ belongs to S, and in this note we will restrict in S the search of the maximum.

The evaluation of (2) for a generical function $q(x)$ is not evident, however by extending the results of Parisi 1979 a, c, d one finds that:

$$F_T(q) = -\frac{1}{4}\beta^2\left[1 + \int_0^1 q^2(x)\,dx - 2\,q(1)\right] - f(0,h) \ , \tag{3}$$

where the function f(x, h) satisfies the following non-linear differential equation:

$$\frac{\partial f}{\partial x} = -\frac{1}{2}\frac{dq}{dx}\left[\frac{\partial^2 f}{\partial h^2} + x\left(\frac{\partial f}{\partial h}\right)^2\right] \qquad (4)$$

with the boundary conditon:

$$f(1, h) = \ln\left[2\, \mathrm{ch}(\beta h)\right] . \qquad (5)$$

Eqs. (3-5) are correct as they stands only if $q(0) = 0$, if $q(0) \neq 0$ the correct expression can be obtained by continuity arguments. It is easy to show that the internal energy and the susceptibility are given by:

$$U = -\frac{\beta}{2}\int_0^1 \left[1 - q^2(x)\right] dx , \qquad \chi = \beta \int_0^1 \left[1 - q(x)\right] dx . \qquad (6)$$

The identification of the physical order parameter ($q_{ph} = \langle\langle\sigma\rangle^2\rangle$) is not easy in this framework; it has been suggested that:

$$q_{ph} = q(1) . \qquad (7)$$

Analytic results can be obtained near the critical temperature ($T_c = 1$) outside from the critical region approximated numerical techniques must be used: however without doing any numerical calculation, one can argue (Parisi 1979 d) that for small magnetic field:

$$q(0) \approx h^{2/3} \; ; \qquad \chi = 1 - 0\,(h^{4/3}) \; ; \qquad T < 1 . \qquad (8)$$

The singular behaviour of χ is a signal for the existence of long range correlations in the spin glass phase, the independence from T of the zero field susceptibility for $T < 1$ is a remarkable prediction of this approach, which unfortunately is in variance with the existing computer simulations.

To simplify the calculations, we have avoided the task to solve directly the eqs. (4-5), we have approximated the function $q(x)$ with a piecewise constant function (Parisi 1979 b, c):

$$q(x) = q_i \qquad \text{if} \quad x_i < x < x_{i+1} \qquad i = 0, \dots, k \tag{9}$$

$$0 \equiv x_o \leq x_1 \leq \dots\dots \leq x_k \leq x_{k+1} \equiv 1 .$$

In the limit $k \to \infty$ one obtains exact results. The advantage of this approximation is that $f(0, h)$ can be written in a closed form, e. g. for $k = 3$, we have:

$$f(0, h) = T_{q_o} \ln \left\{ T_{\bar{q}_1} \left\{ T_{\bar{q}_2} \left\{ T_{\bar{q}_3} \cdot \exp\left[x_3 f(1, h) \right] \right\}^{x_2/x_3} \right\}^{x_2/x_1} \right\}^{1/x_1} \tag{10}$$

$$T_q = \exp\left[\frac{1}{2} q \left(\frac{\partial}{\partial h} \right)^2 \right] \qquad \bar{q}_i = q_i - q_{i-1} .$$

Using the well known Green function of the heat equation, $f(0, h)$ can be written as a $(K+1)$-folded integral. If $K = 0$ we recover the results of unbroken replica symmetry. The case $K = 1$ has been discussed in details in Parisi 1979 a, c; in this note we will concentrate our attention on the case $K = 2$.

From the exact solution of the problem near the critical temperature, we know that, if $F(q)$ is maximized with respect to both q_i and x_i, the error for F decrease like $(2K+1)^{-4}$, while the errors for $q(1)$ and χ decrease slowly, i. e. as $(2K+1)^{-2}$: in variational methods the energy is known with much greater precison than the wave function.

In Table I we show the calculated zero temperatures parameters. As expected the convergence with K is rather fast. The negative entropy increases with K and it is quite likely that $S(0) = 0$ for $K = \infty$. The problem of negative zero temperature entropy, which pla gues the conventional approach to spin glasses, is absent here ; this result strongly suggests that the maximum of F(Q) really belongs to S.

TABLE I

We show the zero temperature entropy, the internal energy and susceptibility for K = 0, 1, 2.

K	S(0)	U(0)	$\chi(0)$
0	- 0.16	- 0.798	0.80
1	- 0.01	- 0.7652	0.95
2	- 0.004	- 0.7636	0.98

When $T \to 0$, the q_i have a finite limit while the x_i are proportional to T. In Fig. 1 we show the function q(x) in the approximations K = 1, 2 for T = 0.3.

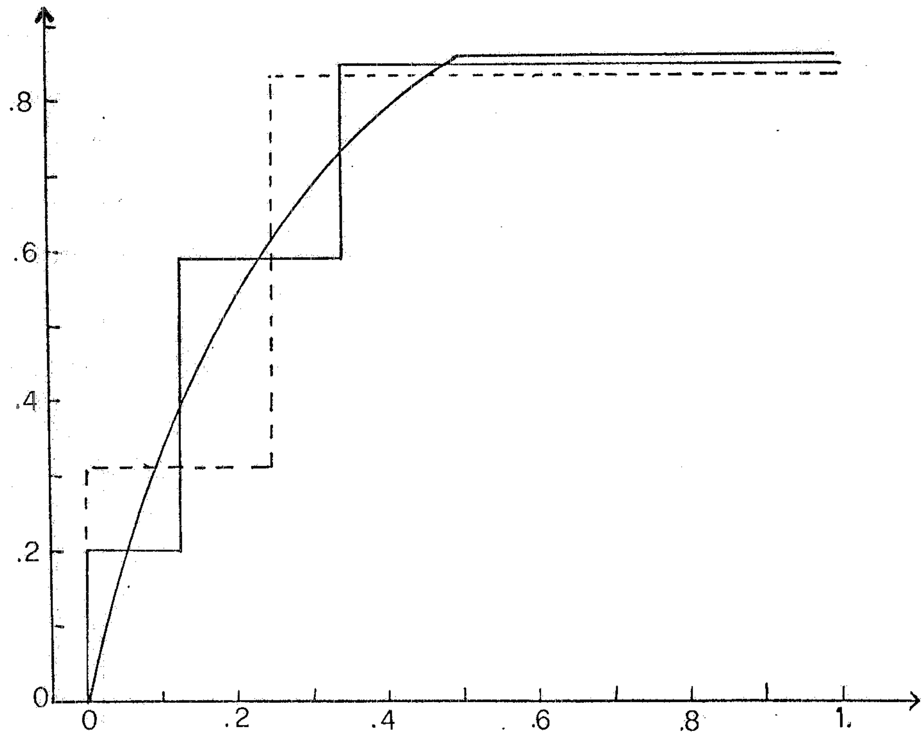

FIG. 1 - The dashed line and the full line are the functions q(x) in the approximations K = 1 and K = 2, respectively. The full curve is an educated guess for the true function q(x).

According to Thouless, Anderson and Palmer 1977, in the low temperature region we have:

$$S(T) \simeq \beta T^2 , \qquad q_{ph}(T) = 1 - \alpha T^2 , \qquad \beta = \frac{\alpha^2}{4} = \ln 2 . \tag{11}$$

In order to test the correctnes of eq. (10), we have plotted in Figs. 2 and 3 the functions:

$$s(T) = S(T)/T^2 , \qquad r(T) = \left[1 - q_{ph}(T)\right] / \left[T^2 (2 - T)\right] . \tag{12}$$

The approximation of keeping q(x) piecewise constant worsens by decreasing T, and the division by T^2 enhance the errors in our approximation (the difference between q(1) for K = 1 and K = 2 is always less 0.015), so that we cannot expect that for finite K the functions S and r have a finite limit for $T \to 0$. In the intermediate T region our results are in qualitative agreement with eq. (10), although we are unable to extract the values of α and β.

The method presented here enables us to compute thermodynamic properties of the S-K model with arbitrary precision (it would be quite interesting to understand if and how analytic calculation can be done near T = 0). It is rather annoying that the magnetic susceptibility does not agree with the computer simulations of Sherrington-Kirkpatrick; the origine of this discrepancy is unclear, although it is quite possible that, if the approach to the equilibrium is rather slow, computer simulations may give a wrong result for the susceptibility. This issue may be vlaryfied by calculating, via computer simulations, the magnetization as function of the magnetic field.

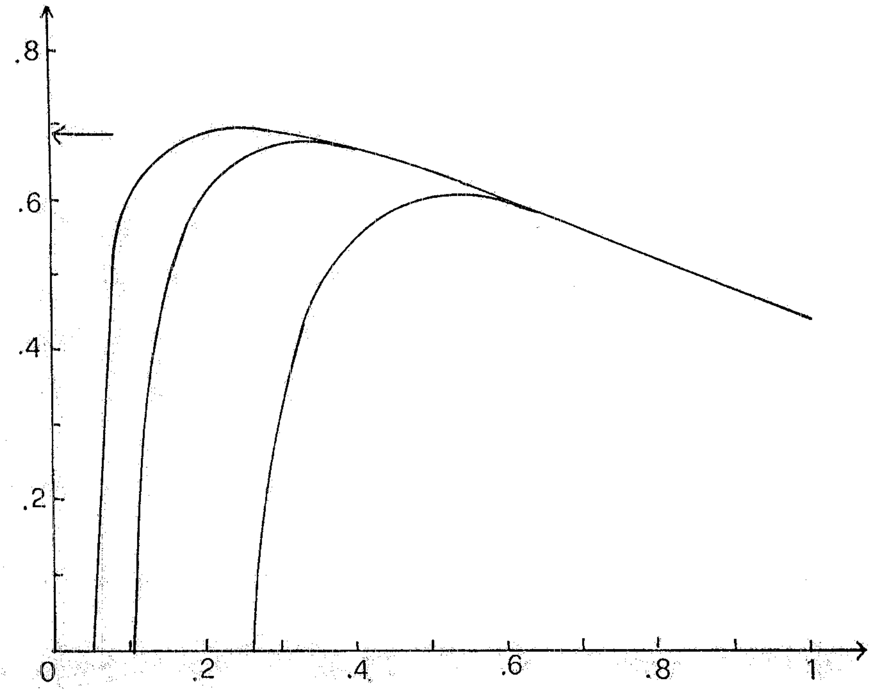

FIG. 2 - The three curves are from below the functions s(T) in the approximations K = 0, 1 and 2, respectively. The arrow is zero temperature prediction of Thouless et al. 1977.

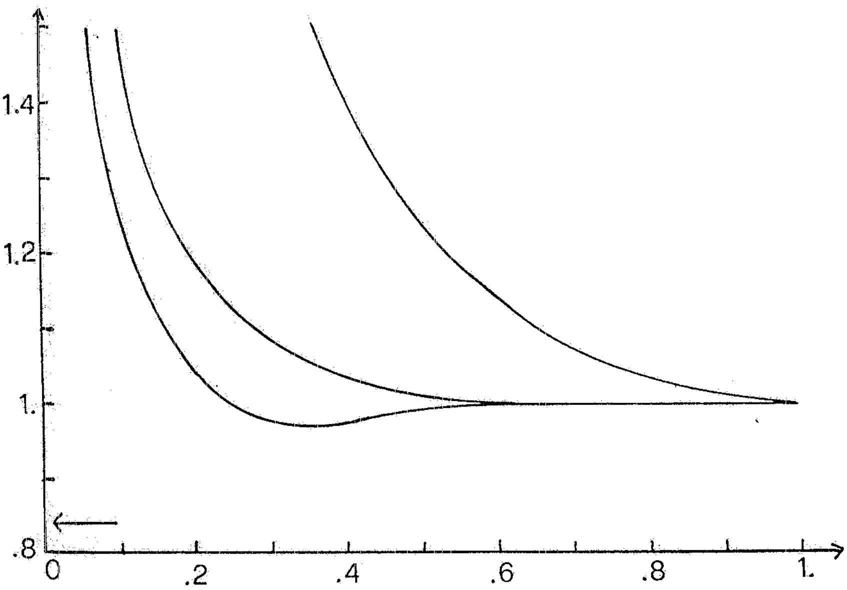

FIG. 3 - The three curves are from above the functions r(T) in the approximations K = 0, 1 and 2, respectively. The arrow is the zero temperature prediction of Thouless et al. 1977.

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