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LETTER TO THE EDITOR

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 recently been 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 1980b, c). 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

$$U(0) = -0{\cdot}7633 \pm 10^{-4}.$$

The computer simulations give $U(0) = -0{\cdot}76 \pm 0{\cdot}01$.

As in the conventional approach, we use the replica trick to integrate over the random spin couplings (Sherrington and Kirkpatrick 1975); in the saddle-point approximation (which is supposed to become exact in the thermodynamic limit) one finds that the free energy density F_R, as a function of the magnetic field h, is

$$F_R = TF_T(Q^0), \qquad \partial F_T/\partial Q_{ab}\,|_{Q=Q^0} = 0, \qquad \beta = 1/T,$$

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

where Tr stands for the sum over all the 2^n possible values of the Ising spin variables S_a, and $Q_{a,b}$ is an $n\times n$ matrix, identically zero on the diagonal ($Q_{a,a}=0$). In the limit $n\to 0$, Q becomes a 0×0 matrix, which is not a well defined object; the standard solution to this problem consists of writing the matrix Q as a function of some

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parameters q_i for generic integer n: at fixed q_i the free energy is analytically continued in n up to the point $n=0$ (Blandin 1978, Bray and Moore 1978, Palmer and Van Hemmer 1979).

Equation (2) does not fix the matrix Q^0 uniquely; for positive integer n the saddle-point method gives the correct result only if the function $F_T(Q)$ has a minimum at the point Q^0. This condition implies that the Hessian matrix

$$H_{(a,b);(c,d)} = \partial^2 F_T/\partial Q_{a,b}\partial Q_{c,d} \tag{2}$$

has positive eigenvalues: if we consider variations which leave the matrix $Q_{a,b}$ symmetric and zero on the diagonal, the matrix H will act on a space of dimensions $n(n-1)/2$, whose axes are labelled by a pair of indices (a, b), with $a \neq b$. If $n<1$, the dimensions of the space on which H acts (the number of independent components of Q) becomes negative. Now, it has been remarked that in this unusual situation, in order to apply the saddle-point method correctly, the eigenvalues of H must be non-negative (de Almeida and Thouless 1978, Pytte and Rudnik 1979, Bray and Moore 1978); unfortunately the positivity of H (i.e. the positivity of its eigenvalues) does not imply that F_T is a minimum as a function of the q_i. For example, if we restrict ourselves to studying the problem in the subspace of matrices having the form $Q_{a,b}=q$, the condition of positivity of the eigenvalues of H restricted in this subspace implies that F_T must be a maximum and not a minimum as a function of q; this happens because

$$(1/n)\,\mathrm{Tr}\,Q^2 = (n-1)q^2 \tag{3}$$

becomes negative definite for $n<1$.

In the general case we cannot say if F_T should be maximised or minimised as a function of the parameters q_i; however, if we restrict ourselves to studying the problem in a subspace in which $\mathrm{Tr}(Q^2)/n$ is negative definite, we must maximise and not minimise F_T as a function of q_i.

The condition that the matrix H does not have negative eigenvalues in a subspace does not imply that H has no negative eigenvalue. Indeed it has been found (de Almeida and Thouless 1978, Pytte and Rudnik 1979) that there are negative eigenvalues of H, if we choose the replica symmetric solution ($Q^0_{a,b}=q$). It is necessary to look for other solutions of equation (2) where the matrix Q^0 has a non-trivial dependence on the indices. The space of 0×0 matrices is a very large space (infinite dimensional) and we do not know how to write the generic matrix of this space; at the present moment the only viable approach consists of doing a simple ansatz for the matrix Q^0 and studying the problem in a smaller space; at the end of the computation one should compute the eigenvalues of the Hessian in order to check if the eigenvalues of H are positive.

It has been suggested that the following parametrisation should be considered (Parisi 1980a):

$$Q_{a,b}=q_i \qquad \text{If: } I\left(\frac{a}{m_i}\right) \neq I\left(\frac{b}{m_i}\right) \text{ and } I\left(\frac{a}{m_{i+1}}\right) = I\left(\frac{b}{m_{i+1}}\right), \qquad i=0, K, \tag{4}$$

where the m_i are integer numbers such that m_{i+1}/m_i is an integer ($i=1, K$) with $m_0=1$ and $m_{K+1}=n$; $I(x)$ is an integer valued function: its value is the smallest integer greater than or equal to x. The matrix Q depends on $K+1$ real parameters (q_i) and K integer parameters (m_i); if we call M_K the space of matrices having the form dictated by equation (4), it is easy to see that $M_{K+1} \supset M_K$. It has been suggested that if n is not integer, there is no reason to restrict ourselves to the case where the m_i are integers and we can treat the variable m_i as a real number: the free energy will be computed as the analytic continuation from the integer m_i.

Let us restrict ourselves to the space M_K^+ where the m_i satisfy the following condition:

$$m_i > m_{i+1}. \tag{5}$$

To work in M_K^+ presents two advantages: $(1/n)\,\mathrm{Tr}\,Q^2$ is negative definite,

$$\lim_{n\to 0}\frac{1}{n}\,\mathrm{Tr}\,Q^2 = -\sum_0^K{}_i\,(m_i - m_{i+1})q_i^2, \tag{6}$$

and it is possible to associate with the matrix Q a function $q(x)$ on the interval 0–1 defined by

$$q(x) = q_i, \qquad m_{i+1} \leqslant x \leqslant m_i. \tag{7}$$

For finite K the function $q(x)$ is piecewise constant and for $K \to \infty$ we can obtain a smooth function. Equation (6) implies that F_T must be maximised as a function of the q_i. If $K = 0$, $q(x)$ is a constant function; we recover the traditional approach with unbroken replica symmetry.

It is easy to show that the internal energy and the susceptibility are given by

$$U = -\beta/2\int_0^1 (1 - q^2(x))\,\mathrm{d}x, \qquad \chi = \beta\int_0^1 (1 - q(x))\,\mathrm{d}x. \tag{8}$$

The identification of the Edwards–Anderson order parameter $q_{\mathrm{EA}} = \langle\langle\sigma\rangle^2\rangle$ is not easy in this framework; this difficulty is also present in the approach of Blandin (1978) and Blandin *et al* (1979), which corresponds in our language to the case $K = 1$, integer m_1. They have suggested that

$$q_{\mathrm{EA}} = \lim_{\epsilon\to 0} Q_{a,b}(\epsilon), \tag{9}$$

where $Q_{a,b}$ has been computed after we have added to the argument of the exponential in equation (1) a term proportional to $\epsilon S_a S_b$. This term is an infinitesimal breaking of the replica symmetry; it removes the ambiguity that would be present in equation (9) for $\epsilon = 0$. If we apply this suggestion to our case, we find

$$q_{\mathrm{EA}} = \max_x q(x). \tag{10}$$

The derivation of equation (10) is far from being rigorous, and it should be justified by a more careful analysis; equations (8) and (10) together show that the breaking of the replica symmetry is connected with the failure of the relation $\chi = \beta(1 - q_{\mathrm{EA}})$ (Fisher 1975).

Analytic results can be obtained near the critical temperature ($T_c = 1$) (Parisi 1980a); the maximum of F_T is located at $K = \infty$, and for finite K the errors in the free energy and in the magnetic susceptibility decrease respectively like $(2K+1)^{-4}$ and $(2K+1)^{-2}$. The bulk of the corrections for going from $K = 0$ to $K = \infty$ are obtained also for K as small as 1. Numerical results for $K = 1$ (Parisi 1979, 1980b) are indeed in good agreement with the computer simulation. In this Letter we report on the numerical results for $K = 2$ and we present a formalism which allows us to obtain the results also for higher values of K.

Using the Gaussian integral representation to disentangle the sum over different spins, $F_T(Q)$ can be written as a K-fold integral: in the case $K=2$ we find

$$
\begin{aligned}
F_T(Q) = &-\tfrac{1}{4}\beta^2\left(1+\int_0^1 q^2(x)\,\mathrm{d}x - 2q(1)\right) \\
&-\int_{-\infty}^{+\infty} \mathrm{d}z_0\, G_{q_0}(z_0) \ln\left[\int_{-\infty}^{+\infty} \mathrm{d}z_1\, G_{q_1-q_0}(z_1-z_0)\right. \\
&\left.\times\left(\int_{-\infty}^{+\infty} \mathrm{d}z_2\, G_{q_2-q_1}(z_2-z_1)\cosh^{m_2}(\beta z_2+\beta h)\right)^{m_2/m_1}\right]^{1/m_1}, \qquad (11)\\
&G_q(z) = (2\pi q)^{-1/2}\exp(-z^2/2q).
\end{aligned}
$$

Using the fact that $G_q(z)$ is the Green function of the heat equation, equation (11) can be formally written as

$$
\begin{aligned}
F_T(Q) = &-\tfrac{1}{4}\beta^2(1+S_0^1 q^2(x)\,\mathrm{d}x - 2q(1)) \\
&- C_{q_0}\ln\{C_{q_1-q_0}[C_{q_2-q_1}\exp(m_2 f_S(z+h))]^{m_2/m_1}\}^{1/m_1}|_{z=0}, \qquad (12)\\
&f_S^{(h)} = \ln[2\cosh(\beta h)], \qquad C_q = \exp(\tfrac{1}{2}q\,\mathrm{d}^2/\mathrm{d}z^2).
\end{aligned}
$$

The numerical evaluation of equation (11) is rather simple; by maximising the free energy as a function of the parameters q_i and m_i, one finds the results shown in table 1.

Table 1. 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

As expected, the convergence with increasing K is fairly fast. The absolute value of the negative entropy decreases with increasing K and it is quite likely that $S(0)=0$ for $K=\infty$. The problem of negative zero-temperature entropy, which plagues the conventional approach to spin glasses, seems to be absent here; this result strongly suggests that in the limit $K\to\infty$ one obtains the correct solution of the S–K model.

When $T\to 0$, the q_i have a finite limit, while the x_i are proportional to T. As an example we show in figure 1 the function $q(x)$ in the approximations $K=1$, 2 for $T=0{\cdot}3$.

The values we obtain for the magnetic susceptibility do not agree with the results of the Monte Carlo simulations of Sherrington and Kirkpatrick (1978); however, in their computations they have implicitly assumed the validity of the Fisher relation $\chi=\beta(1-q_{\mathrm{EA}})$, which is not valid in this approach; on the other hand, the value we obtain for q_{EA}, using equation (10), is in good agreement with their Monte Carlo simulations.

According to Thouless *et al* (1977), in the low-temperature region we have

$$
S(T) \simeq \beta T^2, \qquad q_{\mathrm{EA}} \simeq 1-\alpha T^2, \qquad \beta = \tfrac{1}{4}\alpha^2 = \ln 2. \qquad (13)
$$

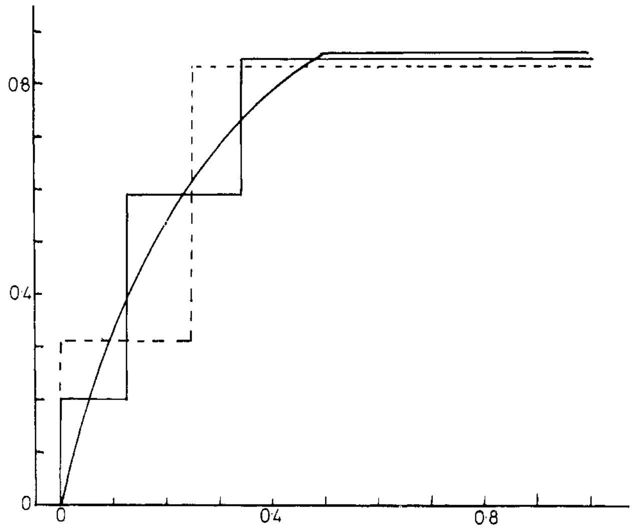

Figure 1. The dashed line and the full line are the functions $q(x)$ in the approximations $K=1$ and $K=2$, respectively. The full curve is an educated guess for the true function $q(x)$.

In order to see if equation (13) holds in our approach, we have plotted in figures 2 and 3 the functions

$$s(T)=S(T)/T^2, \qquad r(T)=(1-q_{\mathrm{EA}}(T))/[T^2(2-T)]. \tag{14}$$

The approximation of keeping $q(x)$ piecewise constant worsens with decreasing T, and the division by T^2 enhances the errors in our approximation (the difference between q_{EA} in the two cases $K=1$ and $K=2$ is always less than 0·015), so we cannot expect that for finite K the functions s and r have a finite limit for $T\to 0$. In the

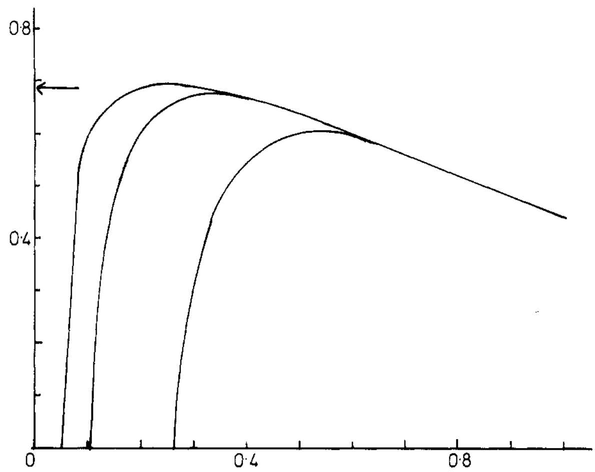

Figure 2. The three curves are from below the functions $s(T)$ in the approximations $K=0$, 1 and 2, respectively. The arrow is the zero-temperature prediction of Thouless *et al* (1977).

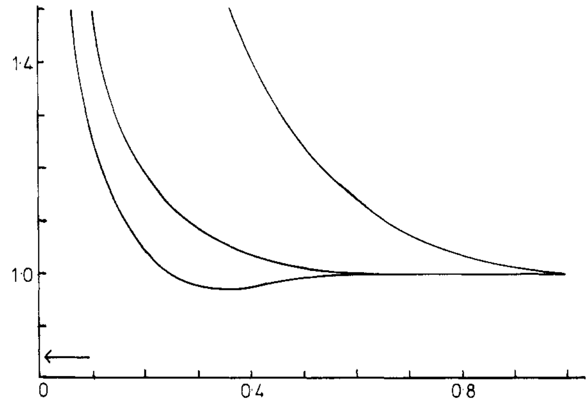

Figure 3. The three curves are from above the functions $r(T)$ in the approximations $K = 0, 1$ and 2, respectively. The arrow is the zero-temperature prediction of Thouless *et al* (1977).

intermediate T region our results are in qualitative agreement with equation (10), although we are unable to extract the values of α and β, using such a low value of K.

From explicit computations done near the critical temperature, we know that in the limit $K \to \infty$, $q(x)$ becomes a smooth function (Parisi 1980a, b); it is straightforward to write the generalisation of equations (11) and (12) to an arbitrary K: in the limit $K \to \infty$ one finds that

$$F_R = \max_{q(x)} TF_T[q], \tag{15}$$

$$F_T[q] = -\frac{1}{4}\beta^2\left(1 + \int_0^1 q^2(x)\,\mathrm{d}x + 2q(1)\right) + \tilde{F}_T[q],$$

$$\tilde{F}_T[q] = -f(0, h),$$

where the function $f(x, h)$ satisfies the following nonlinear differential equation:

$$\frac{\partial f}{\partial x} = -\frac{1}{2}\frac{\mathrm{d}q}{\mathrm{d}x}\left[\frac{\partial^2 f}{\partial h^2} + x\left(\frac{\partial f}{\partial h}\right)^2\right] \tag{16}$$

with the boundary condition

$$f(1, h) = \ln[2\cosh(\beta h)]. \tag{17}$$

Equation (15) is correct as it stands only if $q(0) = 0$, otherwise we would have

$$\tilde{F}_T[q] = -\int_{-\infty}^{+\infty} \mathrm{d}z\, G_{q(0)}(z) f(0, z + h). \tag{18}$$

Equation (18) can also be derived by approximating a function with $q(0) \neq 0$ by a sequence of functions with $q(0) = 0$, i.e. by using the continuity of the functional $\tilde{F}_T[q]$ with respect to its argument, the function $q(x)$.

The shape of the functions $q(x)$ in figure 1, exact results near the critical temperature and preliminary results for high values of K strongly suggest that $q(0) = 0$, if the magnetic field h is equal to zero; (an analysis of equation (15) shows that this is possible only if $\chi = 1$).

If the function $q(x)$ is monotonically increasing, we can define the function $x(q)$; in this case equations (15)–(17) simplify to

$$\tilde{F}_T(q) = -f(q, h)|_{q=0}, \qquad f(q, h)|_{q=q_{\mathrm{EA}}} = \ln[2\cosh(\beta h)],$$
$$\frac{\partial f}{\partial q} = -\frac{1}{2}\left[\frac{\partial^2 f}{\partial h^2} + x(q)\left(\frac{\partial f}{\partial h}\right)^2\right]. \tag{19}$$

The conventional treatment of the model, i.e. no breaking of the replica symmetry, corresponds to $x(q) = 0$. It would be very interesting to understand if and how equation (19) can be derived, starting from the TAP equations of Thouless *et al* (1977).

The method presented in this Letter enables us to compute thermodynamic properties of the S–K model with arbitrary precision (it would be quite interesting to do analytic computations near $T = 0$). The main unsolved problem consists in the computation of the eigenvalues of the Hessian near our solution, in order to verify that non-negative eigenvalues are present. For finite K we expect the presence of negative eigenvalues; their absolute value should decrease with K, and become zero only for infinite K, leaving to us a massless mode (i.e. a zero eigenvalue), the so-called replicon (Bray and Moore 1978). Knowledge of the Hessian is also needed to compute the corrections to the saddle-point approximation: it would be the key step toward the application of this formalism to more realistic models of spin glasses.

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