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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 amorphous 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 (normalised to 1) and $F[J]$ is the J-dependent free energy. In spin glasses:

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

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

Equations (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

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

Obviously one has:

$$\beta F_{\mathrm{R}} = -\lim_{n\to 0}\left(Z_n - \frac{1}{n}\right). \tag{4}$$

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

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

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

Equation (5) is the partition function 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:

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

and a physical order parameter:

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

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 $(1/N)\,\Sigma_i\, Q_i^{\alpha\beta} \equiv Q_{\alpha\beta} = 0$, 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 scheme $\bar{q} = q$.

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 consists 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

$$\beta F_{\mathrm{R}}(T) = \max F_T(q)$$

$$F_T(q) = -\frac{\beta^2}{4}(1+q)^2 + \ln 2$$

$$-(2\pi)^{-1/2}\int \mathrm{d}z\left\{\exp\left(-\frac{z^2}{2}\right)\ln[\cosh(\beta q^{1/2}z)]\right\} \qquad \beta = 1/T. \tag{8}$$

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

From the knowledge of $F_{\mathrm{R}}(T)$ other thermodynamical quantities, like the specific heat ($U(T)$) and the entropy ($S(T)$), can be calculated. However the results disagree with the computer simulations (Sherrington and Kirkpatrick 1978) for $N = 500$, extrapolated up to $N = \infty$ (e.g. the computer simulations give $U(0) = -0{\cdot}76\pm 0{\cdot}01$ while this analytic method gives $U(0) = -\sqrt{2/\pi} \simeq -0{\cdot}80$). The situation worsens if we consider the entropy: by definition $S(T)$ is non-negative and equation (8) implies a negative value of S at low temperatures ($S(0) \simeq -0{\cdot}17$ while $S(\infty) = \ln 2 \simeq 0{\cdot}69$).

The origin 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, Pytte and Rudnik 1979) that the correct expression is

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

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

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 $Q_{\alpha,\beta}$. Equation (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

$$\begin{aligned} &F_T(Q) = F(Q^0) + \Delta_{\alpha\beta} M_{\alpha\beta;\gamma\delta}\Delta_{\gamma\delta} + \mathrm{O}(\Delta^3) \\ &\Delta = Q_{\alpha\beta} - Q^0_{\alpha\beta} \qquad Q^0_{\alpha\beta} = q^0 \end{aligned} \tag{10}$$

where q^0 maximises equation (8).

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

We face the rather difficult problem of parametrising an $n \times n$ matrix in the limit $n = 0$. To work directly in 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 $n \times n$ matrix $Q^{(n)}_{\alpha\beta}$ which depends on a set of parameters $\{q_i, m_i\}$ (e.g. the q_i are the elements of the matrix and the m_i describe the form of the matrix). With a suitable choice of the parametrisation $F_T(Q^{(n)})$ 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 parametrisations.

It is evident that the number of different parametrisations is unbounded 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:

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

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

$$-\lim_{n\to 0}\frac{1}{n}\textstyle\sum_{\alpha,\beta} Q^2_{\alpha,\beta} \geqslant 0. \tag{11c}$$

Requirement (11*a*) comes from the condition that F_R must be finite; the eigenvectors with negative eigenvalue of the matrix M satisfy requirement (11*b*): it is natural to look for a maximum of $F_T(Q)$ in the space spanned by these vectors; at high temperatures we want the maximum of $F_T(Q)$ located at $Q_{\alpha,\beta}=0$ and this happens only if condition (11*c*) is satisfied. We recall that the saddle point method can be applied only if the matrix M has non-negative eigenvalues: this condition implies that the function $F(Q)$ must be maximised, when it is restricted to the subspace where the condition (11*c*) is identically satisfied.

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

In § 2 we describe the parametrisations we propose and we show that a function $q(x)$ defined on the interval 0–1 is naturally associated to each parametrisation 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 schemes $q(x)$ 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 § 3 we apply this approach to the study of the *S–K* model near T_c. In § 4 we show how a very simple-minded approximation ($q(x)$ takes only two values) is sufficient to obtain a substantial improvement with respect to the situation with unbroken replica symmetry for the *S–K* model at all the temperatures (e.g. we obtain $U(0)\simeq -0{\cdot}765$ and $S(0)\simeq -0{\cdot}01$).

2. The parametrisation

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

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

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 an integer $(i\geqslant 1)$. (We let $m_0=1$, $m_{K+1}=n$.)

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

$$Q_{\alpha,\beta}=\left|\begin{array}{cccccccc} 0 & q_0 & q_1 & q_1 & & & & \\ q_0 & 0 & q_1 & q_1 & & q_2 & & \\ q_1 & q_1 & 0 & q_0 & & & & \\ q_1 & q_1 & q_0 & 0 & & & & \\ & & & & 0 & q_0 & q_1 & q_1 \\ & q_2 & & & q_0 & 0 & q_1 & q_1 \\ & & & & q_1 & q_1 & 0 & q_0 \\ & & & & q_1 & q_1 & q_0 & 0 \end{array}\right|. \tag{13}$$

We do not have any serious argument to justify the ansatz equation (12) (apart from the requirement (11)). Its main virtue is its simplicity. It is not evident *a priori* if the solution of the variational problem, equation (9), has the form dictated by equation

(12). The only possible justification of the ansatz equation (12) is its ability to reproduce the results of the computer simulations, as we shall see in § 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-integer n, no conditions on the m_i, are present, i.e. they can be arbitrary real numbers (Parisi 1979a). However, we want conditions (11) to be satisfied.

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

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

Equation (14) follows from the relation:

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

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

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

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

By definition we have:

$$-\lim_{n\to 0} \frac{1}{n} \sum_{\alpha,\beta} Q^2_{\alpha,\beta} = \int_0^1 \mathrm{d}x (q^{(K)}(x))^2. \tag{17}$$

$q^{(K)}(x)$ 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 equation (9) is reached in the limit $K \to \infty$.

At this stage it is unclear if the sequence of functions $q^{(K)}(x)$ 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 Rudnik 1979):

$$F_T(Q) = \lim_{n\to 0} (-\tau \operatorname{Tr} Q^2 + \tfrac{1}{3} \operatorname{Tr} Q^3 + y \sum_{\alpha,\beta} Q^4_{\alpha,\beta} + \mathrm{O}(Q^4))/n \tag{18}$$

where Tr is the standard trace in the n-dimensional vector space. Among the various terms of fourth order we have written the only one which is responsible for the breaking of the replica symmetry.

Indeed, if $y \geqslant 0$ 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 detail the case $y = -\frac{1}{4}$ and look for a maximum of $F(Q)$ with $Q_{\alpha,\beta} = \mathrm{O}(\tau)$.

After some algebra one finds that

$$F_T(Q) = \int_0^1 \mathrm{d}x \left(+\tau q^2(x) + \tfrac{1}{4} q^4(x) - \tfrac{1}{3} x q^3(x) - q^2(x) \int_x^1 q(y)\, \mathrm{d}y \right) \tag{19}$$

where the parametrisation (12) has been used and the function $q(x)$ is defined by equation (6) (for simplicity we have written $q^{(K)}(x)$ as $q(x)$).

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

$$F_T(q_i, m_i) = \sum_{0}^{N}{}_i\, (m_i - m_{i+1})[+\tau q_i^2 + \tfrac{1}{4}q_i^4 - \tfrac{1}{3}(2m_i - m_{i+1})q_i^3 + q_i \sum_{i+1}^{N}{}_j\, (m_j - m_{j+1})q_j^2]. \quad (20)$$

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

$$\begin{aligned} q_0 &= \tau + C^{(K)}\tau^2 + \mathrm{O}(\tau^3) \\ q_i &= B_i^{(K)}\tau + \mathrm{O}(\tau^2) \\ m_i &= L_i^{(K)}\tau + \mathrm{O}(\tau^2). \end{aligned} \quad (21)$$

After some painful algebra one obtains:

$$C^{(K)} = \frac{3}{2} - \frac{1}{(2K+1)^2} \qquad B_i^K = \frac{2(K-i)+1}{2K+1}$$
$$L_i^{(K)} = \frac{6i}{2K+1}. \quad (22)$$

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

$$\begin{aligned} q(x) &= \frac{x}{3} + \mathrm{O}(\tau^2) \qquad &\text{if } x < 3\tau \\ q(x) &= \tau + \mathrm{O}(\tau^2) \qquad &\text{if } x > 3\tau. \end{aligned} \quad (23)$$

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

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

If we consider the internal energy $U(\tau) = \mathrm{d}F/\mathrm{d}\tau$, we find that

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

where:

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

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

For completeness we also write the result:

$$-\sum_{2}^{n}{}_\beta\, Q_{\alpha\beta} \equiv \tilde{q} \equiv \int_0^1 q(x)\,\mathrm{d}x = \tau + q_2^{(K)}\tau^2 + \mathrm{O}(\tau^3)$$
$$q_2^{(K)} = \frac{1}{2(2K+1)^2}. \quad (26)$$

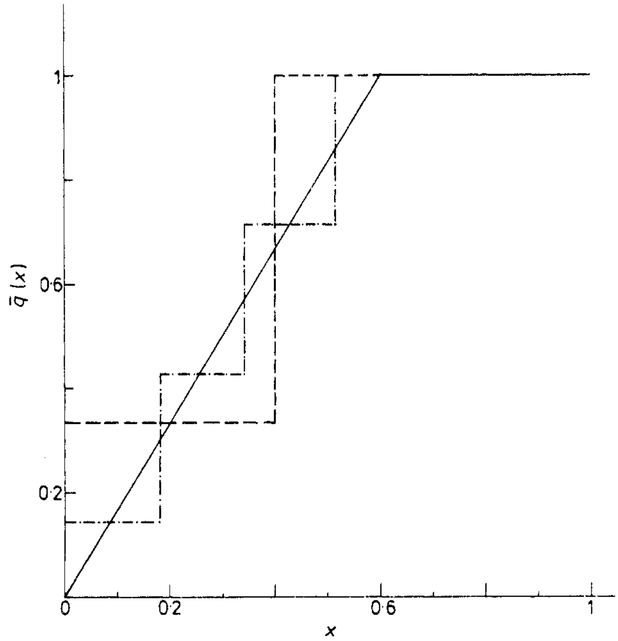

Figure 1. The broken curve, chain curve and full curve are, respectively, the function $q^{(K)}(x)$ for $K = 1$, 4 and ∞ in units of τ.

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

$$\begin{aligned} \bar{q} &= q(1) = \tau + \tfrac{3}{2}\tau^2 + \mathrm{O}(\tau^3) \\ \bar{q} &= \tilde{q} = \tau + \mathrm{O}(\tau^3). \end{aligned} \tag{27}$$

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

4. All 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 temperatures.

One finds (Parisi 1979a):

$$\begin{aligned} \beta F(p, tm) = &-\frac{\beta^2}{4}[1 + mp^2 + (1-m)(p+t)^2 - 2(p+t)] \\ &+ \ln 2 - (2\pi)^{-1/2} \int \mathrm{d}z \bigg\{ \exp\left(-\frac{z^2}{2}\right) m^{-1} \\ &\times \ln\bigg[(2\pi)^{-1/2} \int \mathrm{d}y \, \exp\left(-\frac{y^2}{2}\right) \cosh^m(\beta p^{1/2} z + \beta t^{1/2} y) \bigg] \bigg\} \end{aligned} \tag{28}$$

where $q_1 = p$ and $q_0 = p + t$.

If $m=0$ or $t=0$ we recover the result without breaking of the replica symmetry ($K=0$) (equation (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 maximise equation (28) as a function of p, t and m. This has been done on a computer using a standard minimisation 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 figures 2, 3 and 4 we show, respectively, the internal energy, the specific heat and the entropy as functions of τ, both for $K=0$ and $K=1$. As expected, the difference between the two approximations is relevant only for $T<0{\cdot}5$. For comparison we plot also the low-temperature $C(T)$ and $S(T)$ obtained using a different approach (Thouless *et al* 1977).

The entropy is negative for $T<1$ and $S(0)$ is negative although quite small ($S(0)\simeq-0{\cdot}01$); we expect that $S(0)=0$ only for infinite K. A substantial improvement has been obtained with respect to $K=0$. The computation of the entropy for $K=2$ would be rather long, but straightforward.

The values shown in figures 1, 2, 3 and 4 are in excellent agreement with the computer simulations (e.g. $U(0)=-0{\cdot}765$, while the computer simulations suggest $U(0)=-0{\cdot}76\pm0{\cdot}01$) (Sherrington and Kirkpatrick 1978).

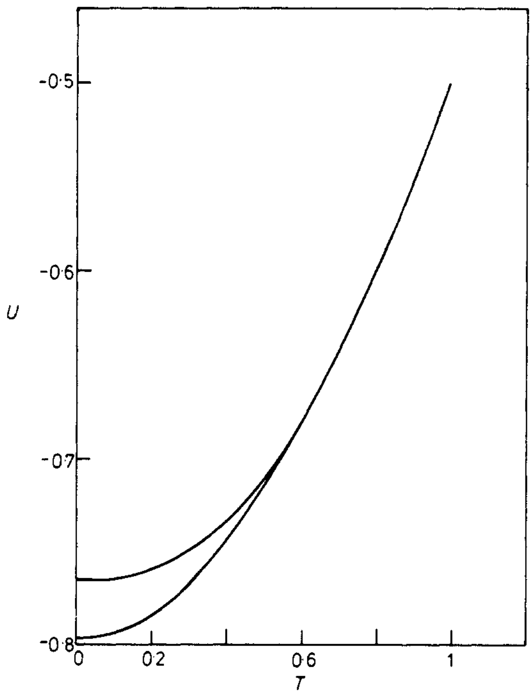

Figure 2. The lower and upper curves are, respectively, the internal energy $U(T)$ for $K=0$ and $K=1$.

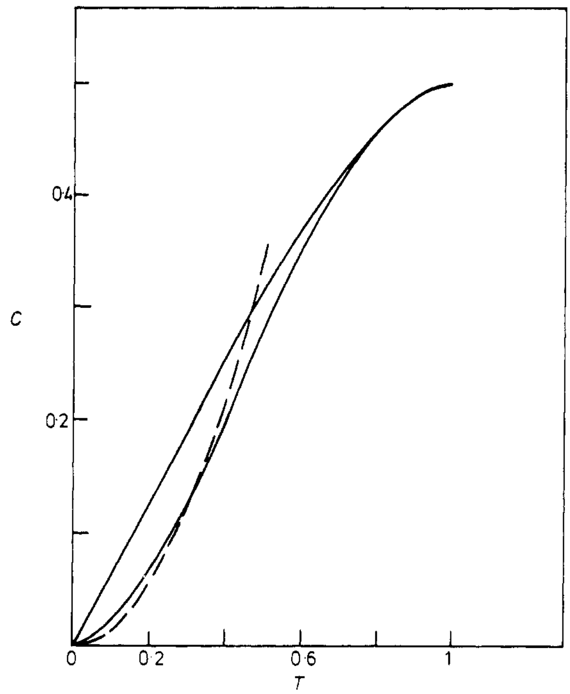

Figure 3. The lower and the upper curves are, respectively, the specific heat $C(T)$ for $K = 1$ and $K = 0$. The broken curve is the prediction $C(T) = 2 \ln 2T^2 + O(T^3)$ (Thouless *et al* 1977).

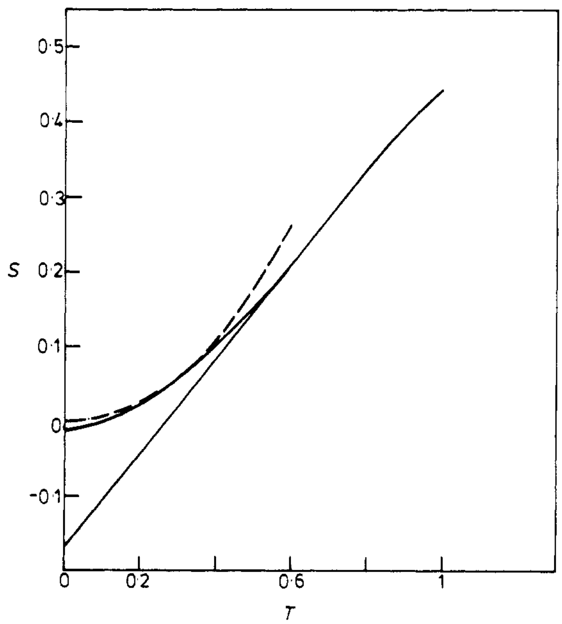

Figure 4. The lower and the upper curves are, respectively, the entropy $S(T)$ for $K = 0$ and $K = 1$. The broken curve is the prediction $S(T) = \ln 2T^2 + O(T^3)$ (Thouless *et al* 1977).

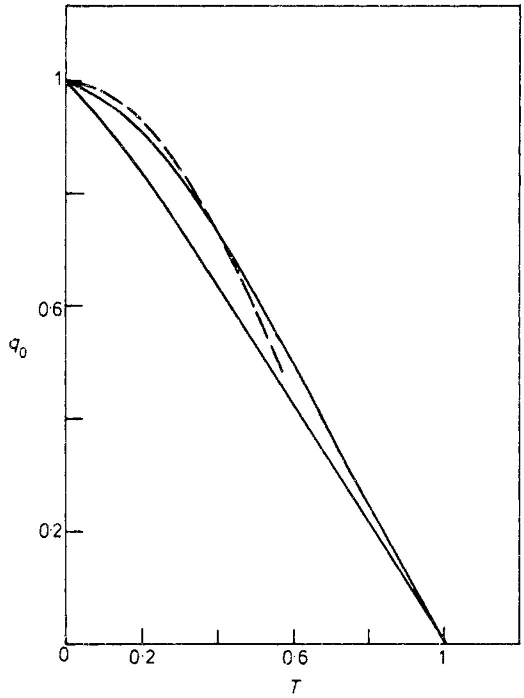

Figure 5. The lower and the upper curves are, respectively, the parameter q_0 as a function of T for $K=0$ and $K=1$. Just for comparison the broken curve is the prediction for the function $\bar{q}(T)$ (Thouless *et al* 1977): $\bar{q}(T)=1-2(\ln 2)^{1/2}T^2+O(T^3)$.

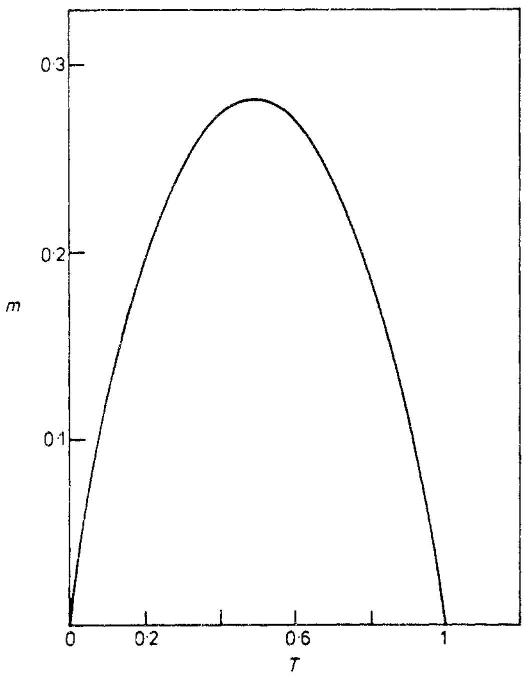

Figure 6. The parameter m_1 for $K=1$ as a function of T.

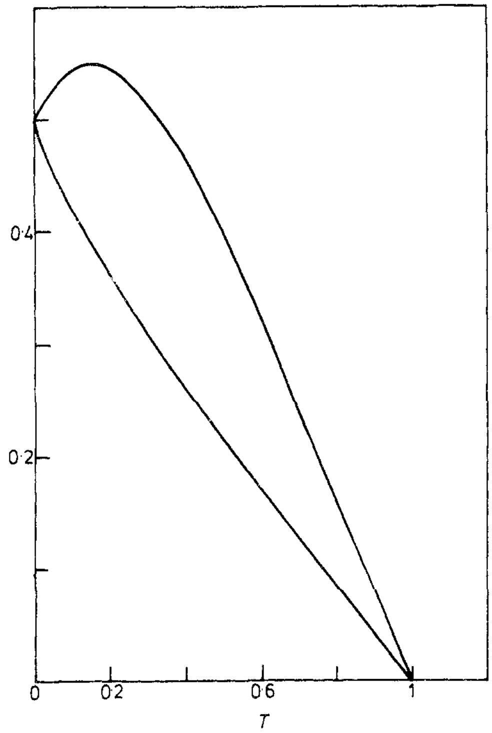

Figure 7. The lower and the upper curves are, respectively, the parameters t and p for $K = 1$ as functions of T.

For completeness we show in figure 5 the parameter q_0 both for $K = 0$ and 1. The broken 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_0 for $K = 0$.

In figures 6 and 7 we show 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.

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