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# Magnetic properties of spin glasses in a new mean field theory

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**Abstract.** We study the magnetic properties of spin glasses in a recently proposed mean field theory; in this approach the replica symmetry is broken and the order parameter is a function ($q(x)$) on the interval 0–1. Exact results at the critical temperature and approximated results at all the temperatures are derived. The comparison with the computer simulations is briefly presented.

## 1. Introduction

In previous papers (Parisi 1979a, b, 1980) we have proposed a new mean field theory for spin glasses in the framework of the replica theory: the local order parameter is a function ($q(x)$) defined on the interval 0–1. If $q(x)$ is constant, the replica symmetry (i.e. the permutations among different replicas) is exact and we recover the standard mean field theory (Edwards and Anderson 1975); if $q(x)$ is $x$-dependent, the replica symmetry is broken.

This scheme has been successfully applied to the study of the properties of the S–K model (Sherrington and Kirkpatrick 1975) at zero magnetic field. This model is quite interesting: it is believed that the correct mean field theory should give exact results, so it is a good testing ground for different approaches. In this note we use the same techniques to study the magnetic properties of the S–K model also at $h \neq 0$. In perfect agreement with the results of de Almeida and Thouless (1978), we find that for high values of $h$, the replica symmetry is exact and at a temperature-dependent critical value ($h_c$) of the magnetic field $h$ a transition is present from the regime where $q(x)$ is $x$-dependent, to the regime where $q(x) = \text{constant} \neq 0$.

In § 2 we recall the formalism of Parisi (1980), which has been cast in a more compact form. In § 3 exact results are obtained for the S–K model near the critical temperature. Approximate results are obtained at all temperatures in § 4. In § 5 we compare our results with the computer simulations (Sherrington and Kirkpatrick 1978), and we also discuss the problem of computing the 'physical' order parameter $q_{\text{ph}}$ defined by

$$q_{\text{ph}} = \langle\langle m \rangle^2\rangle \tag{1}$$

where the inner bracket indicates the thermodynamic expectation value over the spin variables, while the outer bracket indicates the mean over the random spin couplings.

  

## 2. Algebraic preliminaries

The order parameter in the replica theory approach to spin glasses is an $n \times n$ matrix $(Q_{\alpha\beta})$ in the limit $n = 0$. These matrices are defined as analytic continuation in $n$ from integer $n$ up to $n = 0$. It is not a simple job to write down the generical matrix of this infinite-dimensional space. We will consider only a very restricted class of matrices, those which can be written in the form:

$$
\begin{aligned}
&Q_{\alpha\alpha} = \tilde{q} \\
&Q_{\alpha\beta} = q_i \qquad \text{if } I(\alpha/m_i) \neq I(\beta/m_i),\ I(\alpha/m_{i+1}) = I(\beta/m_{i+1})
\end{aligned}
\tag{2}
$$

where $q_i$ are $(k+1)$ real parameters $(i = 0, k)$, $m_i$ are $(k+2)$ integer parameters $(i = 0, k+1)$, and the ratios $m_{i+1}/m_i$ are also integer numbers; by definition we have $m_0 = 1$ and $m_{k+1} = n$. The integer-valued function $I(x)$ is equal to the smallest integer greater than or equal to $x$ (e.g. $I(0{\cdot}5) = 1$).

This parametrisation of the matrix $Q_{\alpha\beta}$ is a generalisation of the one introduced by Blandin (1978) and Blandin *et al* (1979). The motivations for this particular choice of parametrisation are discussed in Parisi (1980).

In the spin glasses the order parameter $Q_{\alpha\beta}$ is zero on the diagonal, so that $\tilde{q} = 0$. We prefer to consider the slightly more general case $(\tilde{q} \neq 0)$; indeed the matrices defined in equation (2) form an algebra closed under addition and multiplication; in the rest of this section we will study the properties of this algebra.

It is crucial to remark that if $n$ is not a positive integer, there is no reason to have integer $m_i$; in the most interesting case, they satisfy (for $n = 0$) the inequalities

$$
1 \geqslant m_1 \geqslant m_2 \geqslant \ldots \geqslant m_k \geqslant m_{k+1} \equiv 0. \tag{3}
$$

If the inequalities (3) are satisfied we can represent the matrix $Q_{\alpha\beta}$ with a pair $[\tilde{q}, q(x)]$, $q(x)$ being a piecewise constant function on the interval 0–1, defined by:

$$
q(x) = q_i \qquad \text{for } m_i > x > m_{i+1} (i = 1, k). \tag{4}
$$

In this representation the addition and the multiplication take a rather simple form. Let us define:

$$
\begin{aligned}
&A_{\alpha,\beta} \leftrightarrow [\tilde{a}, a(x)] \\
&B_{\alpha,\beta} \leftrightarrow [\tilde{b}, b(x)] \\
&C_{\alpha,\beta} \leftrightarrow [\tilde{c}, c(x)]
\end{aligned}
\tag{5}
$$

where we denote by the double arrow the canonical representation (4). We have

$$
\begin{aligned}
&A + B = C \leftrightarrow \begin{cases} \tilde{c} = \tilde{a} + \tilde{b} \\ c(x) = a(x) + b(x) \end{cases} \\
&AB = C \leftrightarrow \begin{cases} \tilde{c} = \tilde{a}\tilde{b} - \langle ab \rangle \\ c(x) = (\tilde{b} - \langle b \rangle) a(x) + (\tilde{a} - \langle a \rangle) b(x) + \displaystyle\int_0^x [a(x) - a(y)][b(x) - b(y)]\, \mathrm{d}y \end{cases}
\end{aligned}
\tag{6}
$$

where

$$\langle a\rangle=\int_0^1 a(x)\,\mathrm{d}x \qquad \langle b\rangle=\int_0^1 b(x)\,\mathrm{d}x$$
$$\langle ab\rangle=\int_0^1 a(x)b(x)\,\mathrm{d}x. \tag{7}$$

The addition rule is trivial while some algebra is needed to verify the multiplication rule. One also finds that

$$\lim_{n\to 0}\frac{1}{n}\operatorname{Tr}(A)=\tilde{a}$$
$$\lim_{n\to 0}\frac{1}{n}\sum_{\alpha,\beta}(A_{\alpha,\beta})^l=\tilde{a}^l-\langle a^l\rangle. \tag{8}$$

By continuity equations (5)–(8) can be extended to the case where $q(x)$ is an arbitrary (not piecewise constant) continuous function, this last case being the most interesting for spin glasses.

## 3. The Sherrington–Kirkpatrick model near $T_c$

In the S–K model the free energy ($F(T)$) is supposed to be given by:

$$F(T)=\max_{\{Q\}}F[Q]$$
$$\beta F[Q]=\lim_{n\to 0}\frac{1}{n}\left\{-\frac{n}{4}\beta^2+\tfrac{1}{4}\beta^2\operatorname{Tr}(Q^2)-\ln\left[\sum_{S_\alpha=\pm 1}\exp(-\beta^2 S_\alpha Q_{\alpha\beta}S_\beta)\right]\right\} \tag{9}$$

where the sum runs over the $2^n$ configurations of the $n$ spin variables $S_\alpha$, and the maximum is taken over all the zero-dimensional matrices, zero on the diagonal. We suppose that the matrix $Q$, which maximises $F(Q)$, has the form described in equation (2); this hypothesis can be verified by checking that the maximum of $F[Q]$ restricted on the matrices of the form (2) is a real maximum and not a saddle point. This can be done by computing the eigenvalue of the second derivative of $F$ (de Almeida and Thouless 1978, Pytte and Rudnik 1979), but this task goes beyond the aim of this paper and it is postponed to further investigations.

It is not simple to write $F[Q]$ as a functional of $q(x)$; in this section we restrict ourselves to the case where $Q$ is small, i.e. $T$ is near to the critical temperature ($T_c=1$).

In this situation $F(Q)$ may be approximated by

$$F(Q)=-\lim_{n\to 0}\frac{1}{n}\frac{1}{2}\left(\tau\operatorname{Tr}(Q^2)-\tfrac{1}{3}\operatorname{Tr}(Q^3)+\frac{y}{4}\sum_{\alpha,\beta}Q^4+\ldots+h^2\sum_{\alpha,\beta}Q_{\alpha\beta}\right)+F(Q)\Big|_{Q=0} \tag{10}$$

where we have retained the only term of order $Q^4$ which is responsible for the breaking of the replica symmetry (Bray and Moore 1978, Pytte and Rudnik 1979); we have also neglected higher-order terms in the magnetic field.

The equations for a stationary point of $F$ are:

$$0=\frac{\partial F}{\partial Q_{\alpha\beta}}=-2\tau Q_{\alpha\beta}-y(Q_{\alpha\beta})^3+(Q^2)_{\alpha\beta}-h^2=0. \tag{11}$$

Using the ansatz equation (2) for the matrix $Q$, one finds

$$2q(x)[\tau-\bar{q}]+yq^3=\int_0^x [q(x)-q(y)]^2-h^2$$
$$\bar{q}=\int_0^1 q(x)\,\mathrm{d}x. \tag{12}$$

Differentiating with respect to $x$ twice one obtains

$$q'(x)(3yq(x)-x)=0. \tag{13}$$

Let us consider firstly $h=0$. For simplicity we restrict ourselves to the case $q(x)\geqslant 0$. Obviously, if $y<0$, the only solution is the replica symmetric one, where

$$q(x)=q_s \qquad q_s=\tau+\frac{y}{2}q_s^2. \tag{14}$$

If $y>0$ there is also another solution:

$$q(x)=\frac{x}{3y} \qquad x\leqslant x_1$$
$$q(x)=q(1)=\frac{x_1}{3y} \qquad x\geqslant x_1 \tag{15}$$
$$\bar{q}=\tau.$$

The value of $q(1)$ can be found by computing $q$ as a function of $q(1)$ and imposing the last condition:

$$\bar{q}=(1-\tfrac{1}{2}x_1)q(1)=\tau. \tag{16}$$

One finds

$$q(1)=\tau+\tfrac{3}{2}yq^2(1) \qquad x_1=3y\tau+\tfrac{1}{2}x_1^2. \tag{17}$$

Notice that

$$\bar{q}<q_s<q(1). \tag{18}$$

The second solution has a higher value of the free energy. For Ising spin $y$ is positive ($y=\frac{2}{3}$); the correct solution is (15) and replica symmetry is broken.

The inclusion of higher orders in $Q$ is long but straightforward and a systematic expansion near $T_c$ is possible.

It may be interesting to note that at this order

$$q(0)=0. \tag{19}$$

A preliminary analysis shows that equation (19) is an exact statement which remains valid at all orders in $\tau$.

Let us consider now the case $h^2\geqslant 0$ and let us put $y=\frac{2}{3}$. The magnetic susceptibility is given for small $h$ by

$$\chi=\beta(1-\bar{q}). \tag{20}$$

The symmetric solution is always possible:

$$q(x)=q_s \qquad 2q_s(\tau-q_s)+\tfrac{2}{3}q_s^3=h^2. \tag{21}$$

The non-trivial solution of equation (12) is

$$\begin{aligned} q(x) &= q(0) \qquad & 0 \leqslant x \leqslant x_0 \\ q(x) &= 2x \qquad & x_0 \leqslant x \leqslant x_1 \\ q(x) &= q(1) \qquad & x_1 \leqslant x \leqslant 1 \end{aligned} \tag{22}$$

where

$$\begin{aligned} & q(0) = (\tfrac{3}{4}h^2)^{1/3} \qquad x_0 = \tfrac{1}{2}q(0) \qquad x_1 = \tfrac{1}{2}q(1) \\ & \bar{q} = \tau + q^2(0) = \tau + (\tfrac{3}{4})^{2/3}h^{4/3} \end{aligned} \tag{23}$$

where $q(1)$ is fixed by the last condition on $\bar{q}$.

The solution (23) make sense only if $x_1 > x_0$. We find that $x_1 = x_0$ when $h = h_c$ where

$$q^c(0) = \tau + \tfrac{3}{2}(q^c(0))^2 \qquad h^c = [\tfrac{4}{3}(q_0^c)^3]^{1/2}. \tag{24}$$

Equation (23) implies that $h^c$ is of order $\tau^{3/2}$ in agreement with previous computations (de Almeida and Thouless 1978).

For $h > h_c$ only the symmetric solution is possible; for $h < h_c$ the asymmetric solution is favoured. At $h = h_c$ we have a second-order transition characterised by the breaking of the replica symmetry.

In the low-field region we find that the magnetic susceptibility is given by

$$\chi(h) = 1 - (\tfrac{3}{4})^{2/3}h^{4/3}. \tag{25}$$

The second derivative of the susceptibility is divergent for $h \to 0$:

$$d^2\chi/dh^2 \sim h^{-2/3}. \tag{26}$$

The singular behaviour of the susceptibility for small fields is connected to the fact that $q(0) = 0$ for $h = 0$, and seems to be stable against the addition of higher-order terms in the free energy. Equation (26) is a prediction peculiar to this approach and it would be very interesting to check it directly in the computer simulations. $d^2\chi/dh^2$ is also the $\bar{q}$ susceptibility, which behaves like $(\bar{q} - \tau)^{-1/2}$. More precisely we can define an effective free energy $F_{ef}[\bar{q}]$ if we write

$$q(x) = \bar{q} + p(x) \qquad \int_0^1 p(x) = 0 \qquad F_{ef}[\bar{q}] = \max_{p(x)} F[q] \tag{27}$$

where the maximum is taken over all the functions $p$ at fixed $\bar{q}$. We find

$$F_{ef}(\bar{q}) \simeq (\bar{q} - \bar{q}_0)^{5/2} \tag{28}$$

where $\bar{q}_0$ is the value at zero magnetic field.

We have obtained some of the results of Thouless *et al* (1977), in particular the existence of a forbidden region for $\bar{q} < q_0$ and the infinite value of the $\bar{q}$ susceptibility.

The method presented in this section can be used only near to the critical temperature; at lower values of $T$ a different approach is needed. This is the subject of the next section. We note, however, that if we write $F(T) = F_s(T) + \frac{2}{45}(T_c - T)^5 + O(T_c - T)^6$, and we neglect higher orders in $T - T_c$, we find $U(0) \sim -0{\cdot}753$ and $S(0) \sim 0{\cdot}06$, which is an improvement with respect to the standard treatment.

## 4. At all temperatures

A rather simple-minded approximation which works rather well at all temperatures consists in approximating the function $q(x)$ with a function taking only two values:

$$q(x) = q_0 \qquad x < m$$
$$q(x) = q_1 \qquad x > m. \tag{29}$$

Excellent results are obtained at zero magnetic field especially in the region $T \geqslant 0{\cdot}2$ (Parisi 1979a). In this case the functional $F[Q]$ can be simply written as:

$$\begin{aligned}\beta F(q_0, q_1, m) = &-\frac{\beta^2}{4}[1 + mq_0^2 + (1-m)q_1^2 - 2q_1] \\ &+ \ln 2 - (2\pi)^{-1/2} \int dz \left\{ \exp(-z^2/2) m^{-1} \ln \left[ (2\pi)^{-1/2} \right.\right. \\ &\left.\left. \times \int dy \exp(-y^2/2)(ch\tilde{H})^m \right] \right\}\end{aligned} \tag{30}$$

$$\tilde{H} = \beta(q_0^{1/2} z + t^{1/2} y + h) \qquad t = q_1 - q_0.$$

The maximum of (29) can easily be found numerically. The replica symmetry is broken if

$$(q_1 - q_0) m (1-m) \neq 0. \tag{31}$$

For all fields $h < h_c(T)$ and $T < T_c = 1$ equation (31) holds at the maximum. For $T > T_c$, $q_1 = q_0 = 0$.

Equation (20) implies that for small $h$

$$\chi(h) = \beta[1 - q_0 m - q_1(1-m)]. \tag{32}$$

In figure 1, we show $\chi$ against the temperature for $h = 0$. For $T > 1$, the antiferromagnetic result $\chi = 1/T$ holds. For $T$ less than $T_c$ the upper curve is the calculated

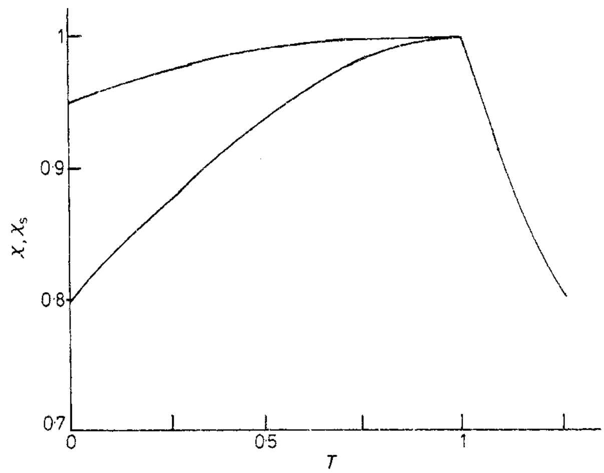


**Figure 1.** The higher curve is the zero-field susceptibility ($\chi$) plotted against temperature. The lower curve is the prediction of the replica symmetric approach ($\chi_s$).

susceptibility while the lower curve is $\chi_s$, the susceptibility in the conventional replica symmetric treatment of the model ($\chi_s = \beta(1-q_s)$).

As a typical example of the behaviour of the system in an external magnetic field $h$, we show in figures 2–4 various quantities as functions of $h$ at $T = 0{\cdot}3$. At this temperature $h_c \simeq 1$. No unexpected phenomenon is present; in this approximation the singular behaviour of $\chi(h)$ at $h = 0$ is absent.

We notice that both $\bar{q}$ and $q(1) = q_1$ are increasing functions of $h$; $\bar{q}$ behaves quite smoothly at the transition point, while $\mathrm{d}q_1/\mathrm{d}h$ is discontinuous.

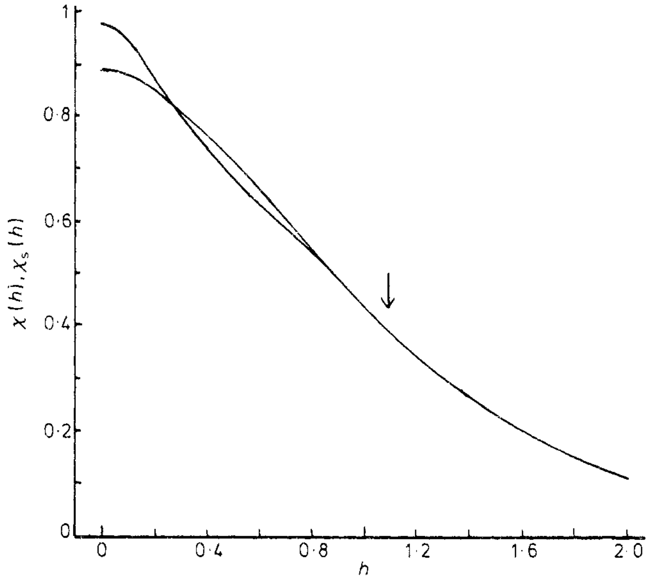


**Figure 2.** We plot the magnetic susceptibility $\chi(h)$ against $h$ for $T = 0{\cdot}3$. The curve, which is higher at $h = 0$, is the result of our calculation; the other curve is $\chi_s(h)$. The two curves coincide for $h \geqslant h_c \simeq 1$, which is indicated by an arrow.

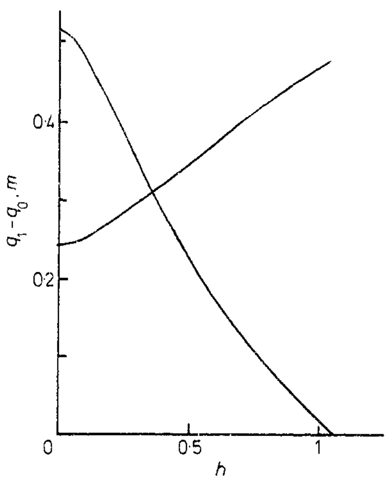


**Figure 3.** The decreasing and the increasing curve are, respectively, $q_1 - q_0$ and $m$ as functions of $h$. At $h = h_c$, $q_1 - q_0 = 0$ and $m \neq 0$.

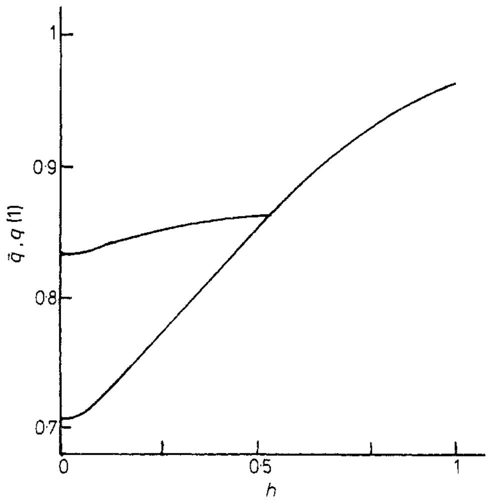


**Figure 4.** The lower and upper curves are, respectively, $\bar{q}$ and $q(1)$ as functions of $h$. They coincide for $h \geqslant h_c$.

## 5. Discussion

The expert reader has probably realised that our results for the susceptibility do not agree with the computer simulations of Sherrington and Kirkpatrick (1978). These authors find that at $h = 0$, $\chi < \chi_s$ ($\chi = 0$ at $T = 0$), i.e. the opposite of our results.

The origin of this discrepancy is not clear: we notice that the inequality $F > F_s$ (Chalupa 1978) implies that $\chi > \chi_s$, at least in the mean. $\chi \neq 0$ at $T = 0$ is not in variance with a quadratic specific heat only if very large size clusters are relevant: the onset of equilibrium in a large-scale cluster is a slow phenomenon and it may be invisible in a not long enough Monte Carlo approach (Fernandez and Medina 1979).

It is not known if hysteresis or remanence is present in the S–K model; if that happens one should be very careful in extracting the susceptibility from Monte Carlo data. Unfortunately no accurate simulations exist at non-zero magnetic field; the zero-field susceptibility has been extracted from the spin–spin correlations. A direct computation of the susceptibility would be welcomed.

In this approach it is unclear how to compute the physical order parameter $q_{\mathrm{ph}}$ (defined in equation (1)). A simple-minded argument gives

$$q_{\mathrm{ph}} = \max_x q(x). \tag{33}$$

Equation (33) does agree with the computer simulations. If equation (33) is correct, when the replica symmetry is broken:

$$q_{\mathrm{ph}} \neq \bar{q} \qquad \chi \neq \beta(1 - q_{\mathrm{ph}}). \tag{34}$$

It is suggested that one should consider the validity of equation (34) as a signal for the breaking of the replica symmetry. Unfortunately the arguments leading to equation (33) are not very strong. The soundness of equation (33) may be investigated by studying the time-dependent correlations (De Dominicis 1979). However, we insist that good-quality computer simulations at non-zero $h$ would be very useful to clarify the situation.

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