

To be submitted to
Jnl. of Physics A

ISTITUTO NAZIONALE DI FISICA NUCLEARE
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LNF-79/46(P)
24 Luglio 1979

G. Parisi: MAGNETIC PROPERTIES OF SPIN GLASSES IN A
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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 1979 a, b, c) 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 (Edward and Anderson 1975); if $q(x)$ is x dependent, the replica symmetry is broken.

These 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 value of the 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 $q(x) = \text{const} \neq 0$.

In Section 2 we recall the formalism of Parisi 1979 c, which has been cast in a more compact form. In Section 3 exact results are obtained for the S-K model near the critical temperature. Approximated results are obtained at all the temperatures in Section 4. In Section 5 we compare our results with the computer simulations (Sherrington and Kirkpatrick 1978), we discuss also the problem of computing the "physical" order parameter q_{ph} defined by

$$q_{ph} = \langle \langle m \rangle^2 \rangle, \quad (1)$$

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 $n \rightarrow 0$. These matrices are defined as analytic continuation in n from integer n up to $n \rightarrow 0$. 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 under the form :

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

where q_i are $k+1$ real parameters ($i=0, k$), m_i are $k+2$ integer parameter ($i=0, k+1$), 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 or equal to x (e. g. $I(0.5) = 1$).

This parametrization of the matrix $Q_{\alpha\beta}$ is a generalization of the one introduced by Blandin 1978 and by Blandin, Gabay and Garel 1979. The motivations for this particular choice of parametrization are discussed in Parisi 1979 c.

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 ($\tilde{q} = 0$); indeed the matrices defined in eq. (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

$$1 \geq m_1 \geq m_2 \geq \dots \geq m_k \geq m_{k+1} \cong 0. \quad (3)$$

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:

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

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

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

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

We have

$$\begin{aligned}
 A + B = C &\leftrightarrow \begin{cases} \tilde{c} = \tilde{a} + \tilde{b} \\ c(x) = a(x) + b(x) \end{cases} \\
 A \cdot B = C &\leftrightarrow \begin{cases} \tilde{c} = \tilde{a}\tilde{b} - \langle ab \rangle \\ c(x) = (\tilde{b} - \langle b \rangle) a(x) + (\tilde{a} - \langle a \rangle) b(x) + \\ \quad + \int_0^x [a(x) - a(y)] \cdot [b(x) - b(y)] dy \end{cases} \quad (6)
 \end{aligned}$$

where :

$$\begin{aligned}
 \langle a \rangle &= \int_0^1 a(x) dx, & \langle b \rangle &= \int_0^1 b(x) dx, \\
 \langle ab \rangle &= \int_0^1 a(x) b(x) dx. \quad (7)
 \end{aligned}$$

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

$$\begin{aligned}
 \lim_{n \rightarrow 0} \frac{1}{n} \text{Tr}(A) &= \tilde{a} \\
 \lim_{n \rightarrow 0} \frac{1}{n} \sum_{\alpha, \beta} (A_{\alpha, \beta})^{\ell} &= \tilde{a}^{\ell} - \langle a^{\ell} \rangle. \quad (8)
 \end{aligned}$$

By continuity eqs. (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-KIRKPATRIK MODEL NEAR T_c .

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

$$\begin{aligned}
 F(T) = \max_{\{Q\}} F[\bar{Q}] \quad , \quad \beta F[\bar{Q}] &= \lim_{n \rightarrow 0} \frac{1}{n} \left\{ -\frac{n}{4} \beta^2 + \right. \\
 &\left. + \frac{1}{4} \beta^2 \text{Tr}(Q^2) - \ln \left[\sum_{S_{\alpha} = \pm 1} \exp(-\beta^2 S_{\alpha} Q_{\alpha\beta} S_{\beta}) \right] \right\} \quad (9)
 \end{aligned}$$

Where the sum runs over the 2^n configuration of the n spin variables S_α , and the maximum is taken over all the zero dimensional matrices, zero on the diagonal. We suppose that the matrix Q , which maximize $F(Q)$ has the form described in eq. (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 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 note and it is postponed to further investigations.

It is not simple to write down $F[Q]$ as 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

$$F(Q) = - \lim_{n \rightarrow 0} \frac{1}{n} \frac{1}{2} \left[\tau \text{Tr}(Q^2) - \frac{1}{3} \text{Tr}(Q^3) + \right. \\ \left. + \frac{y}{4} \sum_{\alpha, \beta} Q_{\alpha\beta}^4, + \dots + h^2 \sum_{\alpha, \beta} Q_{\alpha\beta} \right] + F(Q) \Big|_{Q=0} \quad (10)$$

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:

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

Using the Ansatz eq. (2) for the matrix Q , one finds

$$2 q(x) \left[\tau - \bar{q} \right] + y q^3 = \int_0^x \left[q(x) - q(y) \right]^2 - h^2 \\ \bar{q} = \int_0^1 q(x) dx. \quad (12)$$

Differentiating with respect to x twice one obtains

$$q'(x) [3y q(x) - x] = 0 . \quad (13)$$

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

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

If $y > 0$ there is also an other solution:

$$\begin{aligned} q(x) &= \frac{x}{3y} , & x \leq x_1 \\ q(x) &= q(1) = \frac{x_1}{3y} , & x \geq x_1 \end{aligned} \quad (15)$$

$$\bar{q} = \tau .$$

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

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

One finds

$$q(1) = \tau + \frac{3}{2} y q^2(1) , \quad x_1 = 3y \tau + \frac{1}{2} x_1^2 . \quad (17)$$

Notice that

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

The second solution has an 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

$$q(0) = 0 . \quad (19)$$

A preliminary analysis shows that eq. (19) is an exact statement which remains valid at all the orders in τ .

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

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

The symmetric solution is always possible

$$q(x) = q_s , \quad 2q_s \left[\tau - q_s \right] + \frac{2}{3} q_s^3 = h^2 . \quad (21)$$

The non trivial solution of eq. (12) is

$$\begin{aligned} q(x) &= q(0) & 0 \leq x \leq x_0 \\ q(x) &= 2x & x_0 \leq x \leq x_1 \\ q(x) &= q(1) & x_1 \leq x \leq 1 , \end{aligned} \quad (22)$$

where

$$\begin{aligned} q(0) &= \left(\frac{3}{4} h^2 \right)^{1/3} , \quad x_0 = \frac{1}{2} q(0) , \quad x_1 = \frac{1}{2} q(1) , \\ \bar{q} &= \tau + q^2(0) = \tau + \left(\frac{3}{4} \right)^{2/3} h^{4/3} . \end{aligned} \quad (23)$$

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

$$q^c(0) = \tau + \frac{3}{2} (q^c(0))^2 , \quad h^c = \left[\frac{4}{3} (q^c_0)^3 \right]^{1/2} . \quad (24)$$

Eq. (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 characterized by the breaking of the replica symmetry.

In the low field region we find that the magnetic susceptibility is $\chi(h)$ is given by

$$\chi(h) = 1 - \left(\frac{3}{4}\right)^{2/3} h^{4/3}. \quad (25)$$

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

$$\frac{d^2\chi}{dh^2} \sim h^{-2/3}. \quad (26)$$

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. Eq. (26) is a prediction peculiar to this approach and it would be very interesting to check it directly on 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 $F_{\text{ef}}[\bar{q}]$ if we write

$$q(x) = \bar{q} + p(x), \quad \int_0^1 p(x) dx = 0, \quad F_{\text{ef}}[\bar{q}] = \text{Max}_{p(x)} F[q] \quad (27)$$

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

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

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

We have obtained some of the results of Thouless, Anderson and Palmer 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 $U(0) \sim -0.753$ and $S(0) \sim 0.06$, which is an improvement with respect to the standard treatment.

4. - AT ALL THE TEMPERATURES.

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

$$\begin{aligned} q(x) &= q_0, & x < m \\ q(x) &= q_1, & x > m. \end{aligned} \quad (29)$$

Excellent results are obtained at zero magnetic field especially in the region $T \geq 0.2$ (Parisi 1979 a). In this case the functional $F[\underline{Q}]$ can be simply written as :

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

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

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

$$(q_1 - q_0) m (1 - m) \neq 0. \quad (31)$$

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

Eq. (20) implies that

$$\chi(h) = \beta \left[1 - q_0 m - q_1 (1 - m) \right]. \quad (32)$$

In Fig. 1, we show χ 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 susceptibility while the low curve is χ_S , the susceptibility in the conventional replica symmetric

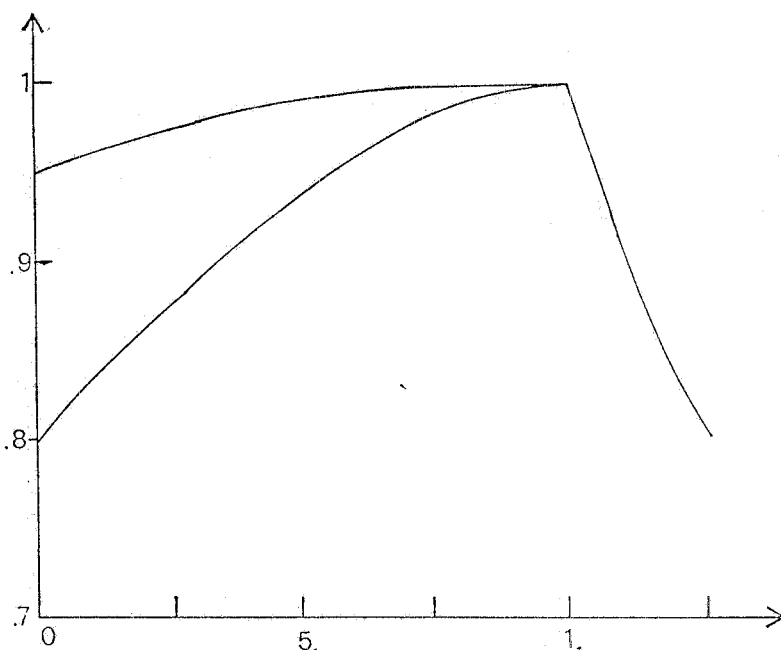


FIG. 1 - The higher curve is the zero field susceptibility (χ) plotted against the temperature. The lower curve is the prediction of the replica symmetric approach (χ_S).

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 Figs. 2-4 various quantities as

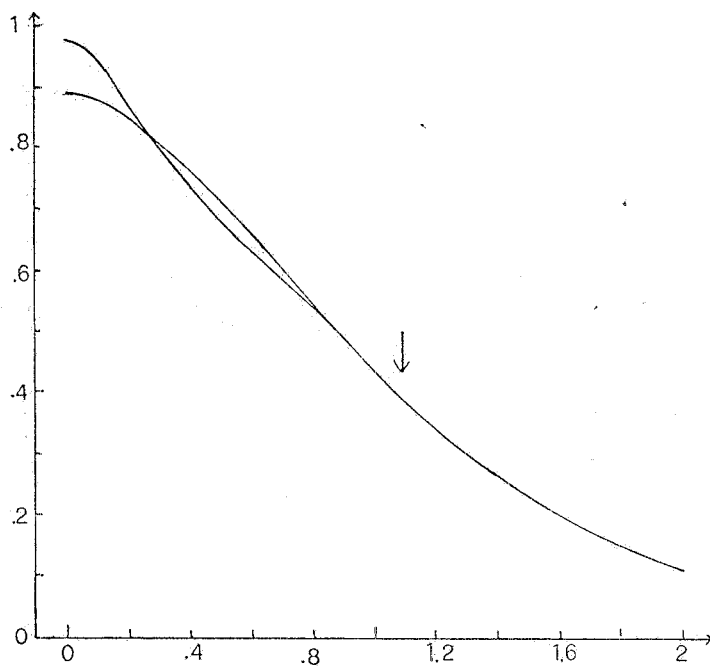


FIG. 2 - We plot the magnetic susceptibility $\chi(h)$ against h for $T = 0.3$. The curve, which is higher at $h = 0$, is the result of our calculation, the other curve is $\chi_S(h)$. The two curves coincide for $h > h_c \approx 1$, which is indicated by an arrow.

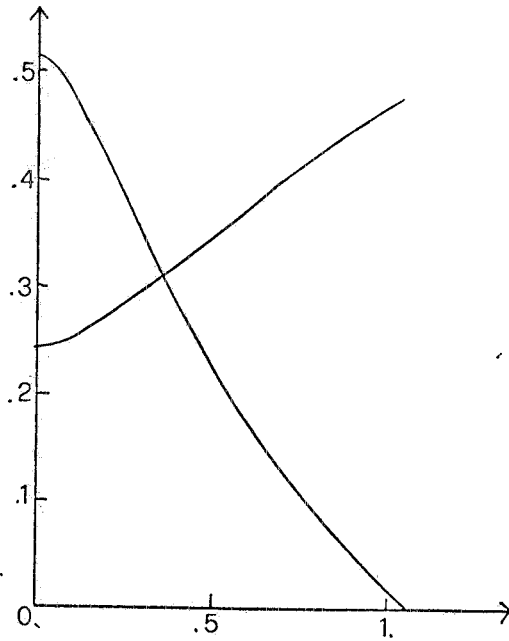


FIG. 3 - The decreasing and the increasing curve are respectively $q_1 - q_0$ and m as functions of h . At $h = h_c$, $q_1 - q_0 = 0$ and $m \neq 0$.

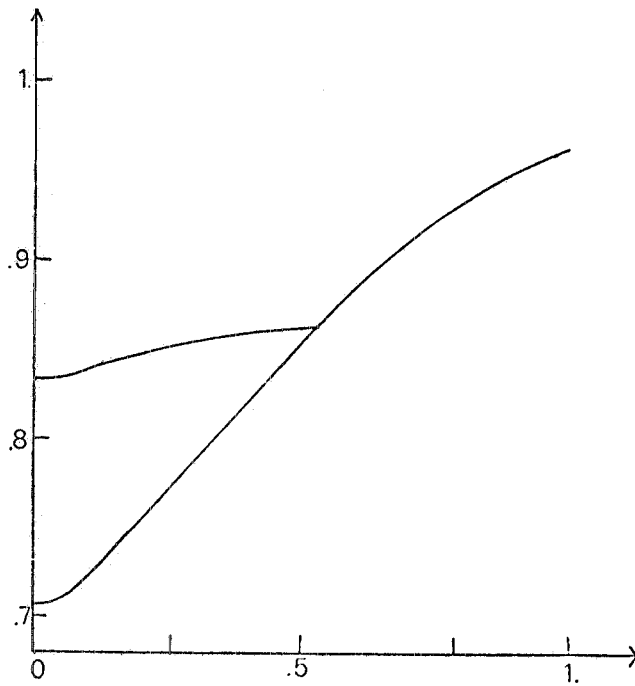


FIG. 4 - The lower and higher curves are respectively \bar{q} and $q(1)$ as function of h . They coincide for $h \geq h_c$.

functions of h at $T = 0.3$. At this temperature $h_c \approx 1$. No unsuspected 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 dq_1/dh is discontinuous.

5. - DISCUSSION.

The expert reader has probably realized 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 clusters is a slow phenomenon and it may be invisible in a not enough long Montecarlo 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 exacting the susceptibility from Montecarlo 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 is unclear how to compute the physical order parameter q_{ph} (defined in eq. (1)). A simple minded argument gives

$$q_{ph} = \max_x q(x); \quad (33)$$

Eq. (33) does agrees with the computer simulations, If eq. (33) is correct, when the replica symmetry is broken:

$$q_{\text{ph}} \neq \bar{q} , \quad \chi \neq \beta [1 - q_{\text{ph}}] . \quad (34)$$

It is suggestive to consider the validity of eq. (34) as a signal for the breaking of the replica symmetry, unfortunately the arguments leading to eq. (33) are not very strong. The soundness of eq. (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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