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G. Parisi: THE MAGNETIC PROPERTIES OF THE S-K
MODEL FOR SPIN GLASSES: THEORY VERSUS MONTE
CARLO SIMULATIONS.

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G. Parisi: THE MAGNETIC PROPERTIES OF THE S-K MODEL FOR SPIN GLASSES: THEORY VERSUS MONTECARLO SIMULATIONS.

ABSTRACT.

We study the magnetic properties of the Sherrington-Kirkpatrick model for spin glasses doing Montecarlo simulations for 200 spins. Excellent agreement is found with the theoretical predictions of the new version of the replica theory.

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Recently it has been suggested that the appropriate order parameter for spin glasses is a function $q(x)$ defined on the interval 0-1 (Parisi 1979 a, b, c). If this function is a constant we recover the predictions of the standard replica theory. If $q(x)$ is not a constant, the replica symmetry is broken (de Almeida and Thouless 1978, Pytte and Rudnick 1979). This method has been used to compute the properties of the S-K model.

The S-K model (Sherrington and Kirkpatrick 1975) is an infinite range model where N Ising spin σ_i interact via a random Gaussian exchange interaction J_{ik} with:

$$\langle J_{ik}^2 \rangle = \frac{1}{N} \quad i \neq k . \quad (1)$$

The model is not realistic, however it is believed to be soluble, when $N \rightarrow \infty$, in the appropriate mean field theory, so that it is a good testing ground for different approaches.

The predictions for the internal energy $U(T)$ and the entropy $S(T)$ at zero magnetic field H , are in perfect agreement with the Montecarlo simulations of Sherrington and Kirkpatrick (1978).

A sharp disagreement is present for the zero field magnetic susceptibility, $\chi(T)$. The theoretical prediction is (Parisi 1979 c):

$$\chi(T) = 1 \quad \text{for } T < T_c \quad (T_c = 1) \quad (2)$$

while the computer simulations give

$$\chi(T) = aT + O(T^2) . \quad (3)$$

where the value of a is compatible with the suggestion of Thouless, Anderson and Palmer 1977 :

$$a = 2 (\ln 2)^{1/2} \sim 1.665 . \quad (4)$$

The susceptibility $\chi(T)$ has been computed in the Montecarlo simulation using the linear response theory. In this approximation :

$$\chi(T) = (1 - q_{ph})/T \quad (5)$$

where the physical order parameter q_{ph} is defined as (Edward and Anderson 1975) :

$$q_{ph} = \langle \langle \sigma_i \rangle^2 \rangle . \quad (6)$$

The inner bracket indicates the thermodynamic expectation value, the outer bracket indicates the mean over the random couplings. The theoretical predictions of the new replica theory are

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

$$\chi(T) = (1 - \int q(x) dx)/T \neq (1 - q_{ph})/T .$$

Eqs. (5-7) implies that the linear response approximation breaks down at $H = 0$. Indeed massless modes and long range correlations are present at $H = 0$ (Bray and Moore 1978, Parisi 1979 b) and the non validity of eq. (5) is quite likely connected to the overturning of large clusters of spins for small H . According to this analysis the discrepancy between eq. (2) and (3) are due to an unallowed use of the linear response approximation; this possibility is strongly supported by the good agreement of the predictions of the new replica theory for q_{ph} with the Montecarlo simulations.

In order to test the correctness of eq. (3), we have done Montecarlo simulations of the properties of the S-K model at non zero magnetic field. We have computed the magnetization $m(H)$ the internal energy $U(H)$ and $q_{ph}(H)$ as function of the field H at various temperatures. In Figs. 1, 2, 3 we show the results of the Montecarlo simulations and the predictions of the replica theory at $T = 0.3$.

The agreement is quite good. The dashed lines in Figs. 1, 2 are the predictions obtained from eq. (3), which are in neat disagreement with the computer simulations. Similar results hold also at different temperatures.

We have studied 50 systems with $N = 40$, 50 systems with $N = 100$ and 25 with $N = 200$. The standard Montecarlo technique has been used. In order to avoid the danger of locking the system in a metastable state, we have started putting the system at a temperature higher than T_c ($T_c = 1$). After we have gradually frozen it to the final temperature, we have finally let the system evolve for 400 Montecarlo steps for spin and we have averaged the results of the last 200 steps. Longer runs with also different cooling procedures have been done as tests. No systematic changement has been observed. The error bars on our results are purely statistical and are due to variation from system to system. We have checked that the zero field results agrees with those of previous Montecarlo simulations (Kirkpatrick and Sherrington 1978).

The agreement of the predictions of the new version of the replica

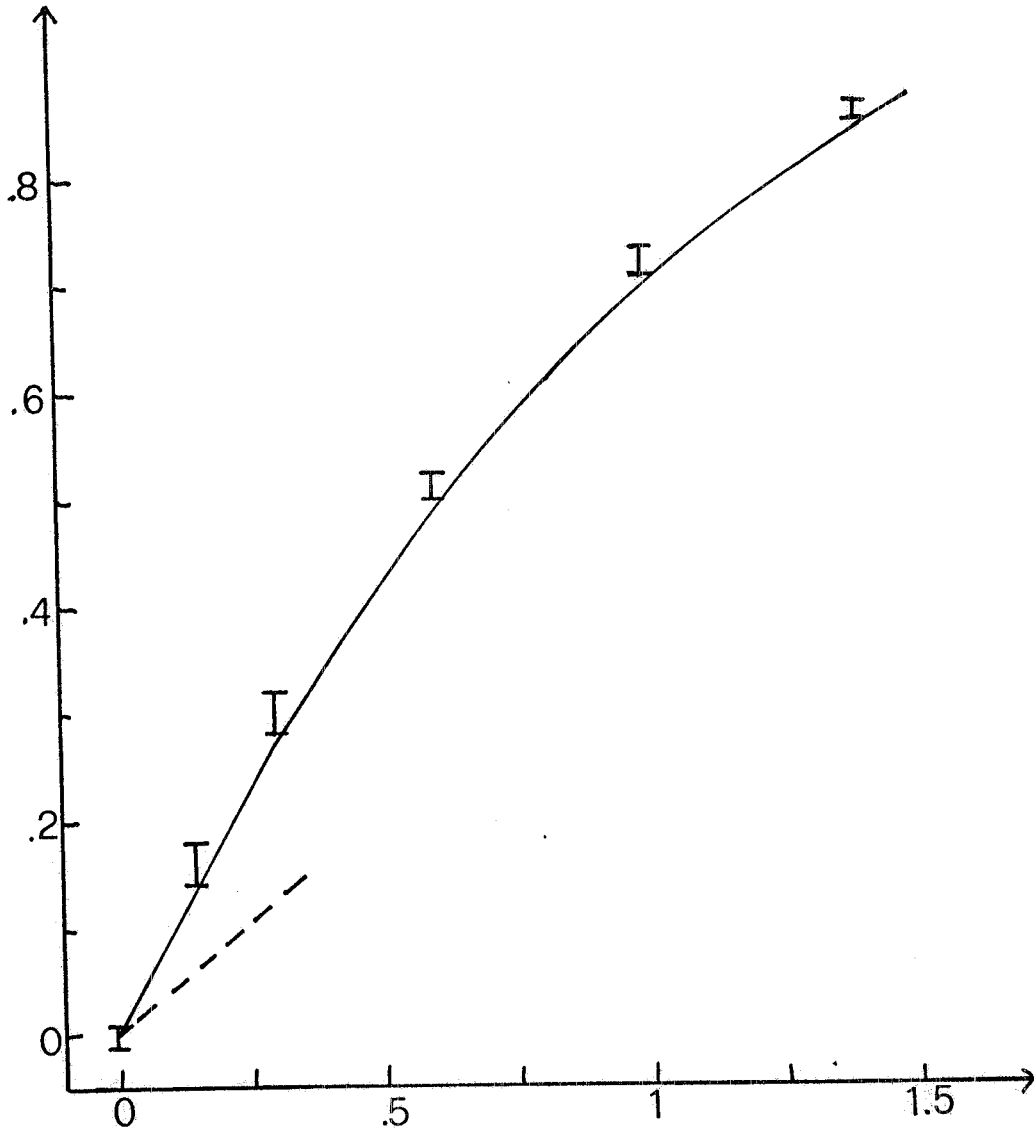


FIG. 1 - The full line is the prediction of the new version of the replica theory (Parisi 1979 b) for the magnetization $m(H)$ as function of H at $T = 0.3$. The outputs of the Montecarlo simulations are shown for $H = 0, 0.15, 0.3, 0.6, 1, 1.41$. 25 systems of 200 spins have been averaged and the error bars denote the statistical error (1 standard deviation). The dashed line is the prediction eq. (3) for small fields.

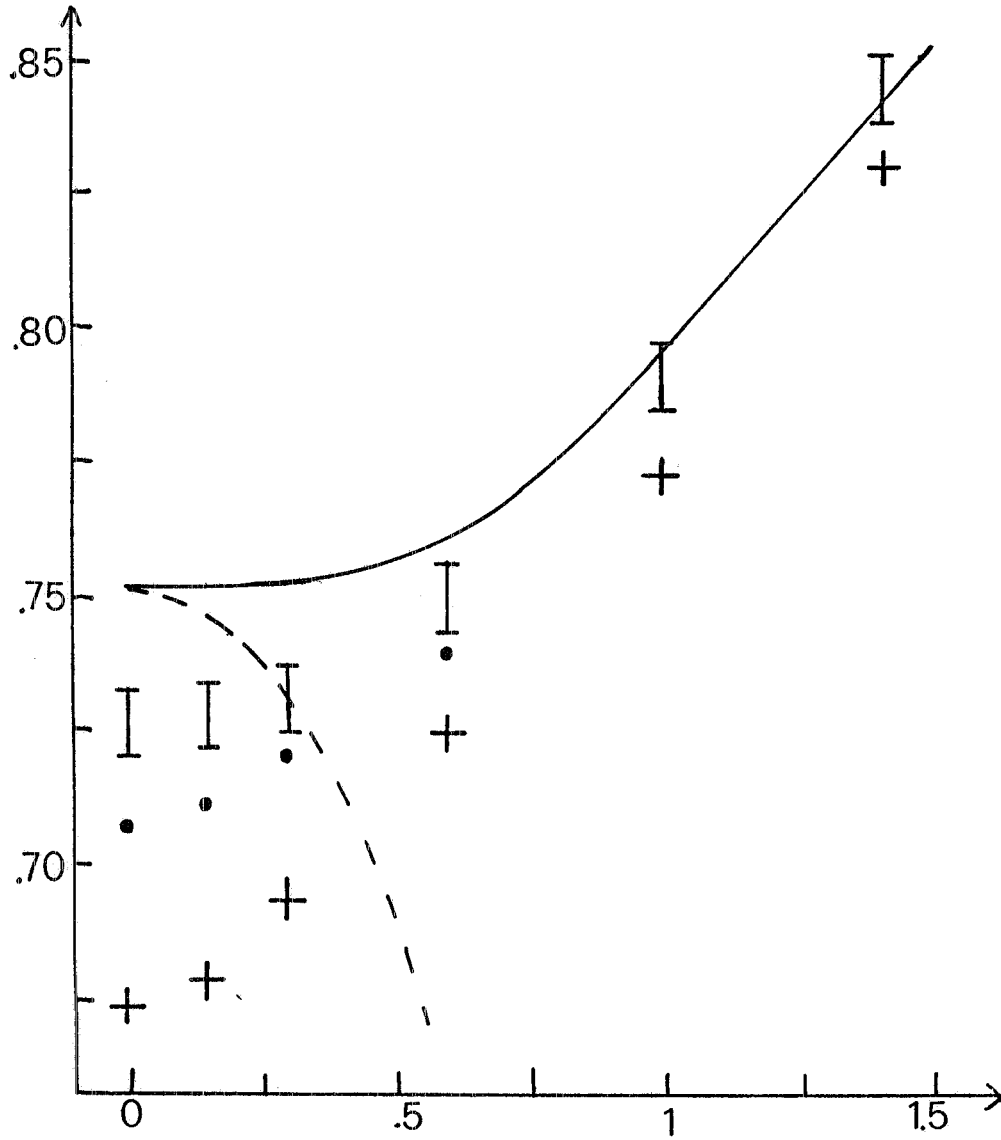


FIG. 2 - We plot $U(H) - \frac{1}{2} H \cdot m(H)$ as function of the magnetic field at $T = 0.3$. The full line is the prediction of the new version of the replica theory, while the dashed line is the prediction coming from eq. (3), using Maxwell type relations. The bars denote the average of 25 systems of 200 spins with their statistical errors. The points and the crosses are the average of 50 systems of 100 spins and 50 systems of 40 spins respectively.

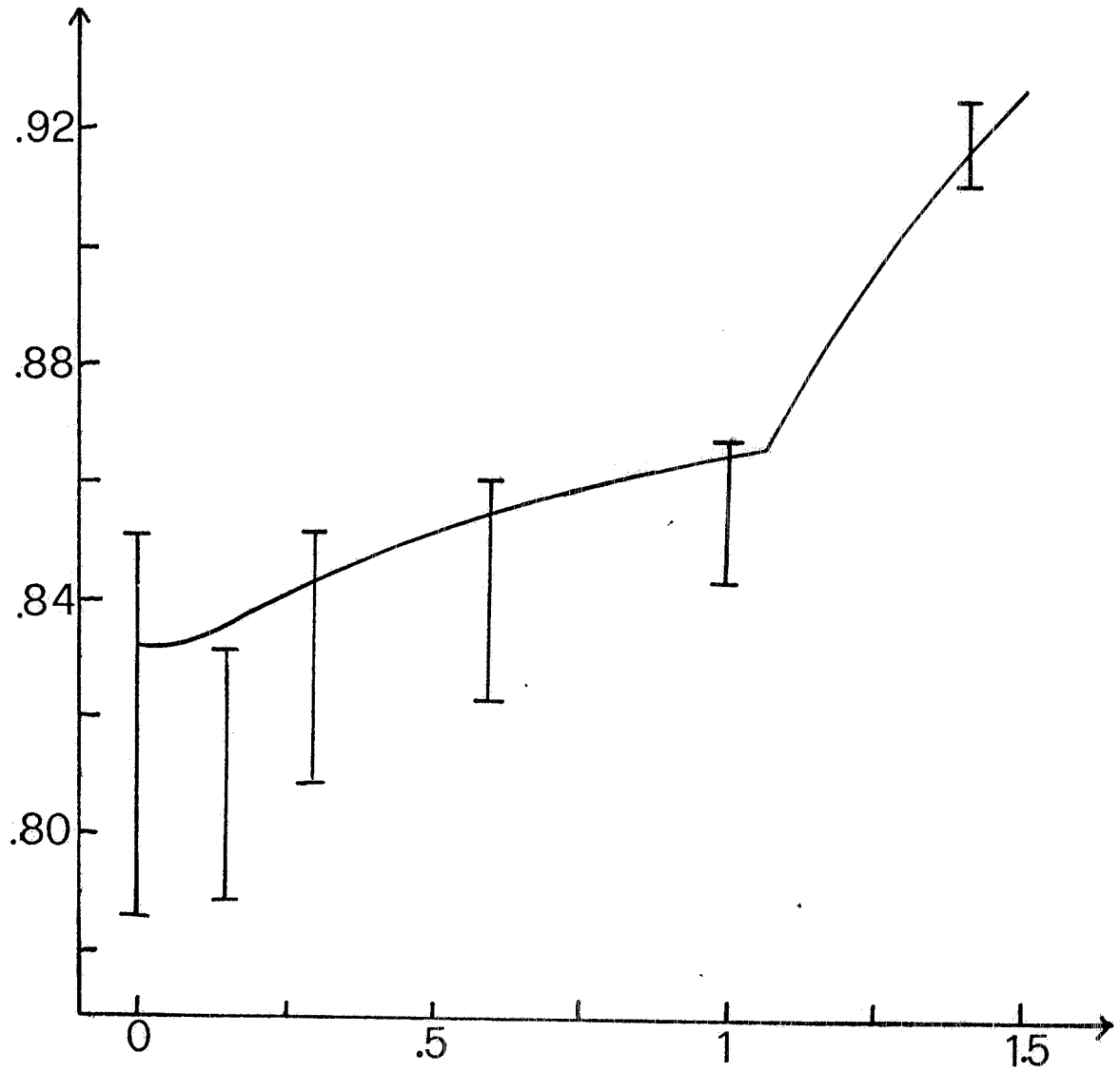


FIG. 3 - We plot q_{ph} as function of H at $T = 0.3$. The bars are the average of 25 systems of 200 spins ; the full line is the prediction of the new version of the replica theory. The discontinuity in the slope of $q_{ph}(H)$ at $H = H_c \approx 1$ is the signal for the transition from unbroken to broken replica symmetry.

theory with the Montecarlo simulations supports the correctness of eq. (2), however it would be interesting to have better simulations for $q_{ph}(H)$ in order to test the predicted changement of slope at $H = H_c(T)$ ($H_c(0.3) \simeq 1$).

We believe that there is convincing evidence that the properties of the S-K model are computed correctly by the new version of the replica theory, and that the "soluble" model for spin glasses is soluble indeed.

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