

Classification  
Physics Abstracts  
75.24M — 75.50L

## Numerical study of the Ising spin glass in a magnetic field

Marco Picco<sup>(1)</sup> and Felix Ritort<sup>(2)</sup>

<sup>(1)</sup> LPTHE(\*), Université Pierre et Marie Curie, and Université Denis Diderot, Bte 126, 4 Place Jussieu, 75252 Paris Cedex 05, France

<sup>(2)</sup> Dipartimento di Fisica and INFN, Università di Roma *Tor Vergata*, Viale della Ricerca Scientifica, 00173 Roma, Italy

(Received 4 May 1994, accepted in final form 28 July 1994)

**Abstract.** — We study the order parameter distribution  $P(q)$  in the 4d Ising spin glass with  $\pm J$  couplings in a magnetic field. We also compare these results with simulations for the infinite ranged model (i.e. SK model.) Then we analyse our numerical results in the framework of the droplet picture as well as in the mean field approach.

This work is devoted to the study of spin glasses in presence of a magnetic field. During the last ten years, a large number of works has been devoted to the study of spin glasses [1]. One of the problems which still remains unsolved is to understand the effect of a magnetic field on the spin glass phase. The mean-field theory predicts that the spin glass phase will survive to the application of a magnetic field below the de Almeida-Thouless critical line (AT line) [2]. In the most general case, the main effect should be the destruction of a large number of equilibrium states with a reshuffling of the free energies for the remaining ones. To our knowledge, even at the mean field level, a numerical test of the theoretical predictions of the replica symmetry breaking solution with magnetic field has never been done. Such a test would be interesting because it would give support to the Parisi ansatz as a correct solution to mean-field theory [3].

For the short-range models case, there is still much controversy. In fact, there is no precise theoretical prediction. A usual  $\epsilon$  expansion near dimension 6 will run in trouble because it is not known how to find a non trivial fixed point [4]. Phenomenological models like those initially developed by McMillan [5], Bray and Moore [6] and by Fisher and Huse [7] predict that the spin glass phase disappears for a finite magnetic field. But this result is a consequence depending on some assumption on the real nature of the low temperature spin glass phase. The most recent studies of the AT line were done in Monte Carlo simulations. In these works,

---

(\*) Laboratoire associé No. 280 au CNRS.

the main points of interest were the curves of constant non-linear susceptibility in the  $h$ - $T$  plane [10] or its divergence when approaching the AT line using finite-size scaling methods [11]. Nevertheless the first approach is very indirect and the second one could be plagued by strong corrections to the simple scaling.

In this work we have tried to understand the spin glass with magnetic field by studying the  $P(q)$  order parameter function obtained by means of the Monte Carlo method using the heat bath algorithm. We will first present a brief discussion on the general theoretical predictions of this problem and numerical results for the mean-field theory. Then we will present the numerical results obtained for the  $4d \pm J$  Ising spin glass. It is well established that this model has a finite  $T_c$  and it has been intensively studied [12].

The  $d$ -dimensional Ising spin glass model of interest, with  $\pm J$  couplings, is defined by the following Hamiltonian

$$H = - \sum_{(i,j)} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i \quad (1)$$

The couplings  $J_{ij}$  are quenched variables with equal distribution values  $\pm 1$ . The interaction is restricted to nearest neighbors and  $h$  is the magnetic field. The Ising spins  $\sigma_i$  take two possible values  $\pm 1$  and live in a  $d$ -dimensional hypercubic lattice with periodic boundary conditions. In the limit  $d \rightarrow \infty$ , one expects to converge to mean-field theory, i.e. the SK model [14]. In the SK model, all spins interact among them and the couplings  $J_{ij}$  are normalized by a factor  $1/\sqrt{N}$  where  $N$  is the number of spins.

It is very useful to consider discrete couplings  $J_{ij}$  in the Hamiltonian because this speeds up the updating of the spins in the Monte Carlo numerical simulation. We also hope that their discreteness should not be relevant for the physics at least for not too low temperatures. Now it is convenient to make some comments on this assertion. It is very hard to obtain reliable analytical results in short-ranged spin-glasses. Anyway, some results have been obtained at zero temperature. Bovier and Frohlich [8] have explicitly shown that the exponents associated to the zero temperature fixed point are sensitive to the type of distribution of the coupling variables. In particular, a binary discrete distribution (like the one used in this work) or a Gaussian continuous distribution are expected to give different zero-temperature exponents. In this case both fixed points belong to different universality classes. In case of a finite temperature fixed point the situation is still not fully understood. Within droplet models there are general arguments which suggest that the universality is restored in case of a finite temperature fixed point [9]. Numerical simulations in the four dimensional case at the critical temperature for a Gaussian [15] or binary distribution [11] give the same exponents within error bars (for an opposite assertion on this question see [16]). High precision simulations in this case should clarify the situation. It is not necessary to point out that the problem of the universality becomes much more subtle if we include the effect of a magnetic field. We expect that the existence of a finite temperature transition in a magnetic field should not depend on the distribution of the  $J$ 's. Studies with a magnetic field in the case of the four-dimensional Ising spin glass with a Gaussian distribution would be welcome.

We consider two identical copies of the system equation (1), i.e with the same realization of the bond disorder  $J_{ij}$  [17]. Let us call them  $\{\sigma_i\}$  and  $\{\tau_i\}$ . The overlap  $Q$  among the two copies is defined by

$$Q = \frac{1}{N} \sum_i \sigma_i \tau_i \quad (2)$$

from which we can construct the order parameter function  $P(q)$

$$P(q) = \overline{\langle \delta(q - Q) \rangle} \quad (3)$$

where  $\langle \dots \rangle$  and  $\overline{(\dots)}$  mean the usual statistical Gibbs average over configurations and the average over the quenched disorder respectively.

In mean-field theory, below the critical temperature and at zero magnetic field, there exist an infinity of equilibrium states, all of them having a different statistical weight. Furthermore, all these states have zero magnetization and no state is particularly selected if we apply a magnetic field. In fact, an infinity of equilibrium states still remain and the spin glass phase survives in a magnetic field. At zero magnetic field the order parameter distribution  $P(q)$  is symmetric under the exchange  $q \rightarrow -q$ . The magnetic field breaks this symmetry and the  $P(q)$  is expected to be non-zero only if  $q > 0$ . This means that half of the states have been suppressed by the magnetic field.

Close to  $T_c$ , the free energy of the SK model with magnetic field can be approximate by

$$f = \tau \sum_{a < b} Q_{ab}^2 - \frac{1}{6} \text{Tr} Q^3 - \frac{1}{12} \sum_{a < b} Q_{(ab)}^4 - h^2 \sum_{a < b} Q_{ab} \quad (4)$$

where  $\{Q_{ab}; 1 \leq a, b \leq n\}$  is the order parameter and  $n$  the number of replicas. The equilibrium solution of the free energy in the limit of infinite order of replica symmetry breaking gives a function  $q(x)$  defined in the interval  $(0, 1)$  [3]. This function  $q(x)$  is the analytical continuation of the matrix  $Q_{ab}$  in the limit  $n \rightarrow 0$ . Close to  $T_c$  one gets a  $q(x)$  with two plateaus in the regions  $0 \leq x \leq x_{\min}$  and  $x_{\max} \leq x \leq 1$  ( $x_{\min} \leq x_{\max}$ ) with respective values  $q_{\min}$  and  $q_{\max}$  ( $q_{\min} < q_{\max}$ ). Between  $x_{\min}$  and  $x_{\max}$ ,  $q(x)$  increases with  $x$ .  $q_{\max}$  is nearly independent on the field but  $q_{\min}$  increases with a power of  $h$  smaller than 1 ( $q_{\min} \sim h^{2/3}$ ). Using the static chaos approach to spin glasses [21] it has been suggested that the effect of the magnetic field is the progressive suppression of all equilibrium states  $\alpha$  such that their overlap  $q_{\alpha\beta} < q_{\min} \forall \beta$ . This corresponds to cutting some branches of the ultrametric tree. Using the relation  $P(q) = \frac{dx(q)}{dq}$  [18] one finds that  $P(q)$  is given by a continuous part  $P_0(q)$  which is non zero inside the interval  $(q_{\min}, q_{\max})$  and two singularities at the extremes of this interval

$$P(q) = P_0(q) + a\delta(q - q_{\min}) + b\delta(q - q_{\max}) \quad (5)$$

We have simulated the SK model at  $T = 0.5$  and  $h = 0.3$  (the corresponding field at the AT line at that temperature is  $h \simeq 0.57$ ). We simulated three different sizes  $N = 320, 1048$  and  $3200$ . For these sizes we were able to reach equilibrium for near all samples after 100000 Monte Carlo steps for the largest size. Then statistics was collected over several hundred thousands of Monte Carlo steps. The main source of fluctuations comes from the finite number of samples because the  $P(q)$  is strongly non self-averaging. Self-averageness is restored when the AT line is reached by increasing the field. The number of samples is 500, 30 and 20 respectively. Even though the numbers of samples are small, they are large enough to show the qualitative behavior of the  $P(q)$ . The results are shown in figure 1. The  $P(q)$  begins to display two singularities for sizes of several thousands spins. For smaller sizes, we only found one peak plus a long tail which extends down to the region of negative overlaps. According to the Parisi solution to mean-field theory,  $q_{\min}$  should match the correct value at infinite order of replica symmetry breaking in the infinite-size limit. We can then compute the position of both singularities, at least at first order of replica symmetry breaking and this gives  $q_{\min} = 0.45$ ,  $q_{\max} = 0.63$ . This is in agreement with our numerical results. Other good estimates for  $q_{\min}$  and  $q_{\max}$  are also obtained using the PaT (Parisi-Toulouse) hypothesis [19] (which is a very good approximation at least close to  $T_c$ ). This approximation predicts that  $q_{\min}(h, T) = q(h, T_{AT}(h))$  and  $q_{\max}(h, T) = q(h_{AT}(T), T)$  where  $T_{AT}(h)$  and  $h_{AT}(T)$  are the equations for the AT line. Computing these values, one gets  $q_{\max} \simeq 0.64$  and  $q_{\min} \simeq 0.437$ . This is also in agreement with our simulations.

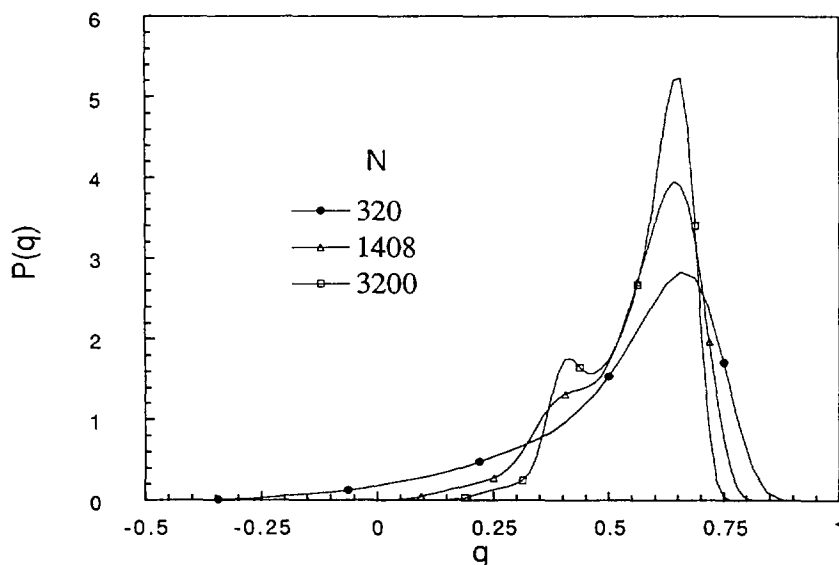


Fig. 1. —  $P(q)$  for the SK model at  $T = 0.5$ ,  $h = 0.3$ . The error bars are of order 20% for  $N = 3200$  and 15% for  $N = 1408$  and less than 5% for  $N = 320$ . The symbols are a guide to the eye.

Now we return to the 4d case. There exists two possible scenarios that we want to compare. First, from the droplet models [7] it is expected that all excitations of droplet of sizes larger than a certain length  $\xi$  will be suppressed by the field. The dependence of this correlation length in function of the magnetic field is given by

$$\xi \sim (q_{EA} h^2)^{\frac{1}{2\theta-d}} \quad (6)$$

with  $q_{EA}$  the Edwards-Anderson order parameter and  $\theta$  the thermal exponent which gives the characteristic energy scale  $L^\theta$  of droplet excitations of typical size  $L$ . This exponent  $\theta$  should be approximately  $(d-3)/2$  (as emerges from numerical studies of chaos in spin glasses [20, 21]). For sizes much larger than  $\xi$  it is expected that the  $P(q)$  will be strongly peaked around a unique value of  $q$ . The expression here reported for the zero temperature exponent  $\theta$  is expected to be valid only in case of continuous symmetric distribution of couplings. In two dimensions one obtains  $\theta = -0.48$  [22] in well agreement with the previous expression and  $\theta = -1$  in one dimension which is the correct solution (see [9]). In three dimensions several results [9] suggest that  $\theta$  is very low but compatible with zero even though a precise determination is lacking in the Gaussian case. In case of binary couplings the exponent  $\theta$  has been shown to be different in agreement with the observation that they belong to a different universality class. In the three-dimensional  $\pm J$  Ising spin glass with nearest neighbors Berg, Hansmann and Celik [23] obtain  $\theta \sim 0.74$ . For a three-dimensional  $\pm J$  Ising spin glass model which incorporates second nearest-neighbor interactions Marinari, Parisi and Ritort [24] obtain, under the assumption that there is not finite  $T$  transition,  $\theta \sim 0.6$  which is in agreement with the previous reported value. There are no simulations (with the same precision as those performed in [23]) in case of a three-dimensional Gaussian Ising spin glass. In this case we expect that more precise computations should give a value well compatible with  $\theta = 0$ .

We have simulated  $L = 3, 5, 6, 8$  in a 4d lattice with periodic boundary conditions with  $\pm J$  couplings. Simulations were performed at  $T = 1.2 (\sim 0.6 T_c)$  and  $h = 0.4$ . The number of

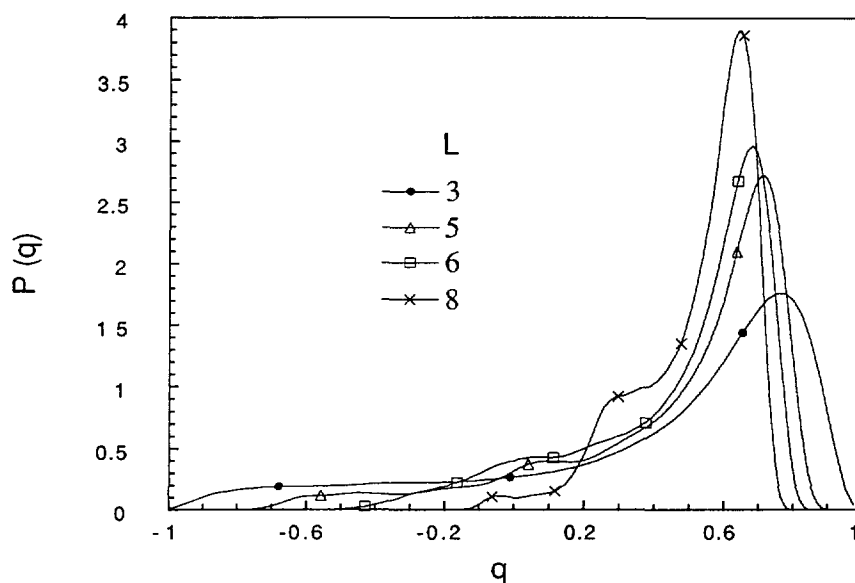


Fig. 2. —  $P(q)$  for the 4d Ising spin glass. Error bars are smaller than 15% in all cases. The symbols are a guide to the eye.

sample are 320, 128, 100, 50 respectively. From finite-size scaling studies [11], we expect to be within the spin glass phase if there is an AT line. It is not very difficult to reach the equilibrium in case of  $L = 3, 5$ . 100000 Monte Carlo steps were enough after a slow cooling procedure. Now we will try to convince the reader that we effectively thermalized for  $L = 6, 8$ . To this end we performed a simulated annealing of half a million of Monte Carlo steps from the high to the low temperature phase at constant magnetic field. After that, statistics was collected over the next half a million Msteps. During this collecting, we computed the four moments of the  $P(q)$  distribution which show no apparent drift in time. To increase the statistics we simulated in parallel eight identical copies of the system computing the four overlaps among four different pairs at each Monte Carlo step. Figure 2 shows the numerical results for the  $P(q)$ . We can immediately notice that there is no singularity at  $q = q_{\min}$  if we compare to the previous figure for the SK model.

Looking at this results it is difficult to draw a definite conclusion on what is the correct scenario in 4d Ising spin glasses. Two facts are interesting to point out. The first one is the existence of a long tail for sizes up to  $L = 6$  which extends down to negative overlaps. So,  $P(q = 0)$  is finite which means that reversal of compact domains of characteristic size  $L$  are still present with a finite probability. Within the droplet model, we can estimate how domain excitations of typical size  $L$  are suppressed by the magnetic field. The effect of the magnetic field depends on the regime in which the system is, either  $L \gg \xi$  or  $L \ll \xi$ ,  $\xi$  being given by equation (6). We can estimate the value of  $\xi$  by using numerical simulations of static chaos [21]. A typical value of order 5 is obtained. If  $L \gg \xi$  we expect that the droplets excitations of size  $L$  are suppressed with a factor  $\simeq \exp(-\beta\chi(L)^d h^2)$  respectively to the case  $h = 0$  ( $\chi$  being the linear susceptibility.) So, in this regime, the tails would be suppressed. Unfortunately, we are in the regime where  $\xi \sim L$ . As a lower bound, when  $L \ll \xi$ , tails are suppressed with a factor  $\simeq \exp(-(L)^{d/2} h^2)$ . In our range of sizes, this factor is of order  $10^{-1}$  which is smaller than what we can see on our plots ( $P(q = 0)$  being 0.3 at zero magnetic field, we would expect

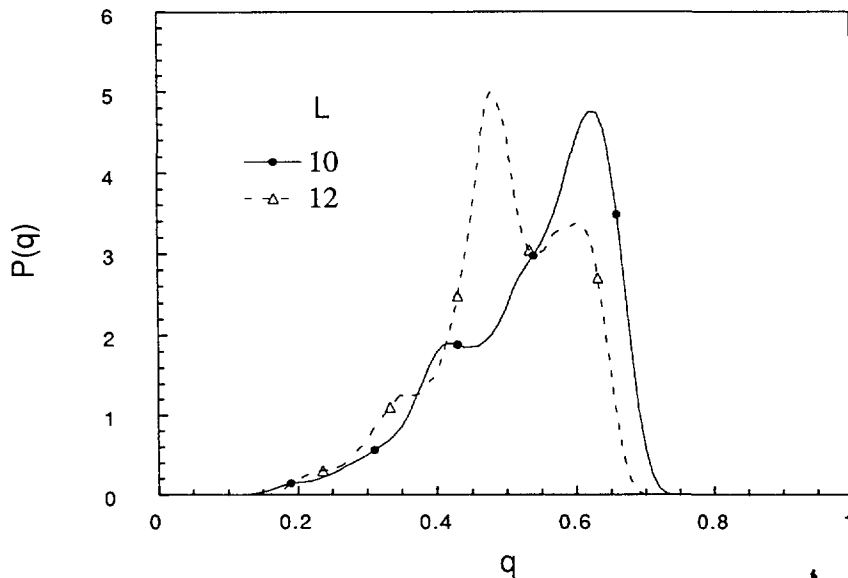


Fig. 3. — Non thermalized  $P(q)$  for the 4d Ising spin glass.

$P(q=0) \sim 0.03$  [12]) The second fact regards the absence of a second peak of  $P(q)$  at  $q_{\min}$ . Presumably, such a peak could appear for larger sizes. In the case of SK model, the  $q_{\min}$  peaks already arise for size of order 1000 spins, as oppose to the 4d case. One possible reason for such a difference reside in the fact that, for the 4d case, we can be very close to the AT line. A second reason is that we can surely expect stronger finite size effects than in the mean-field case. For instance, the singularity in  $P(q)$  for  $q = q_{\max}$  is less pronounced as can be seen in numerical simulation [12].

In order to reach more definite conclusion, we need to study larger sizes lattices. In practice, such a task is very difficult because for larger sizes lattices we are not able to thermalize. In fact, we have performed numerical simulations for  $L = 10$  and  $L = 12$ . Despite that these are non equilibrium results, interesting hints can be obtained. In figure 3 we show the  $P(q)$  distribution. Starting from uncorrelated configurations, the overlap among two copies grows with time. In several cases it remains stacked in a value of  $q$  close to 0.4 giving two singularities for the  $P(q)$  distribution. This indicates that we are in the good region in the  $h$ - $T$  plane in order to test if there exists a spin glass phase.

Still, in order to have a more definite conclusion, we need to take advantage of new numerical simulation techniques like the simulated tempering [25]. This method has revealed much effective for the 2d [26] and 3d [27] Ising spin glasses. A work using such techniques is under progress.

Summarizing, we have studied the 4d Ising spin glass with magnetic field. For comparison, we have also simulated the SK model. This is also a test of the Parisi solution to mean-field theory and our numerical results are in agreement with it. In the 4d case we present results for lattice size up to  $L = 8$ . Then we tried to interpret them in the mean-field picture and the droplet one. It seems that the effect of the magnetic field is weaker than what droplet picture predicts. Non thermalized results for larger sizes suggest that fully equilibrated simulations should be able to select in a definite way between these two pictures. We hope that using numerical techniques like simulated tempering should be able to decide the question in the near future.

## Acknowledgments.

We thank D. Huse and G. Parisi for very interesting suggestions. F. R. has been supported by the EC fellowship B/SC1\*/915198 and the INFN. M. P. has been partially supported by the EU Science grant SC1\*0394 and EU Capital Humain et Mobilité grant - Euronetwork ERB 4050PL92 0982/0035.

## References

- [1] Mézard M., Parisi G. and Virasoro M.A., "Spin Glass Theory and Beyond" (World Scientific, 1987);  
Binder K. and Young A.P., *Rev. Mod. Phys.* **58** (1986) 801;  
Fischer K.H. and Hertz J.A., "Spin Glasses" (Cambridge University Press, 1991).
- [2] de Almeida J.R. and Thouless D.J., *J. Phys. A* **11** (1978) 983.
- [3] Parisi G., *J. Phys. A* **13** (1980) 1101; *J. Phys. A* **13** (1980) 1887.
- [4] Bray A.J. and Roberts S.A., *J. Phys. C* **13** (1980) 5405.
- [5] McMillan W.L., *J. Phys. C* **17** (1984) 3179.
- [6] Bray A.J. and Moore M.A., *J. Phys. C* **18** (1985) L699.
- [7] Fisher D.S. and Huse D.A., *Phys. Rev. Lett.* **56** (1986) 1601; *Phys. Rev. B* **38** (1988) 386.
- [8] Bovier A. and Frohlich A., *J. Stat. Phys.* **44** (1986) 347.
- [9] Bray A.J. and Moore M.A. in *Heidelberg Colloquium in Spin Glasses*, Springer Lecture Notes in Physics, Vol. 275 (1986).
- [10] Grannan E.R. and Hetzel R.E., *Phys. Rev. Lett.* **67** (1992) 907.
- [11] Badoni D., Ciria J.C., Parisi G., Pech J., Ritort F. and Ruiz J.J., *Europhys. Lett.* **21** (1993) 495;  
Ciria J.C., Parisi G., Ritort F. and Ruiz J.J., *J. Phys. I France* **3** (1993) 2207.
- [12] Reger J.D., Bhatt R.N. and Young A.P., *Phys. Rev. Lett.* **16** (1990) 1859;  
Parisi G. and Ritort F., *J. Phys. A* **17** (1993) 3179;  
Ciria J.C., Parisi G. and Ritort F., *J. Phys. A* **17** (1993) 3179.
- [13] Marinari E., Parisi G. and Ritort F., preprint cond-mat 9310041.
- [14] Sherrington D. and Kirkpatrick S., *Phys. Rev. B* **17** (1978) 4384.
- [15] Bhatt R.N. and Young A.P., *Phys. Rev. B* **37** (1988) 5606.
- [16] Bernardi L. and Campbell I.A., received preprint.
- [17] Young A.P., *Phys. Rev. Lett.* **51** (1983) 1206.
- [18] De Dominicis C. and Young A.P., *J. Phys. A* **16** (1983) 2063.
- [19] Parisi G. and Toulouse G., *J. Phys. Lett. France* **41** (1980) L361.
- [20] Kondor I., *J. Phys. A* **22** (1989) L163.
- [21] Ritort F., to appear in *Phys. Rev. B*.
- [22] Kawashima N., Hatano N. and Suzuki M., *J. Phys. A* **25** (1992) 4985.
- [23] Celik T., Hansmann U. and Berg B., preprint cond-mat 9303025.
- [24] Marinari E., Parisi G. and Ritort F., *J. Phys. A* **27** (1994) 2687.
- [25] Berg B.A. and Celik T., *Phys. Rev. Lett.* **69** (1992) 2292;  
Berg B.A. and Neuhaus T., *Phys. Lett. B* **67** (1992) 249;  
Marinari E. and Parisi G., *Europhys. Lett.* **19** (1992) 451.
- [26] Kerler W. and Rehberg P., preprint cond-mat 9402049.
- [27] Marinari E., Parisi G. and Ritort F., in preparation.