Tempering simulations in the four dimensional $\pm J$ Ising spin glass in a magnetic field

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We study the four dimensional (4D) $\pm J$ Ising spin glass in a magnetic field by using the simulated tempering method recently introduced by Marinari and Parisi. We compute numerically the first four moments of the order parameter probability distribution $P(q)$. We find a finite cusp in the spin-glass susceptibility and strong tendency to paramagnetic ordering at low temperatures. Assuming a well defined transition we are able to bound its critical temperature.

Spin glasses are systems which deserve considerable theoretical interest due to the interplay between randomness and frustration [1]. The role of the frustration in the statics and dynamics is essential to understand the nature of the low temperature phase. Despite great progress during the last decade in the understanding of the mean-field theory of spin glasses, a large number of topics are still poorly understood. In particular, it is completely unclear which features of the mean-field theory survive in finite dimensions. This problem has recently received considerable attention [2] and has become the cornerstone to validate the correct description of the spin glass state.

The reason why this topic still remains open relies on the absence of a convincing final theory for the spin glass state. Efforts to construct a field theory of the glass state, based on the Parisi solution to the mean-field theory, have been done mainly by De Dominicis, Kondor and Temesvari [3]. Despite a large number of new results, a clear answer to the finite dimensional issue is still missing.

After the Parisi solution to the mean-field theory, a new phenomenological approach to the spin-glass state based on the Migdal-Kadanoff renormalization group approach was proposed by McMillan [4], Bray and Moore [5] and later on analyzed in detail by Koper and Hilhorst [6] and Fisher and Huse [7]. In this approach, the zero-temperature fixed point completely determines the properties of the low temperature phase. This approach gave a description of the spin-glass state, now called the droplet model, where the thermodynamics is determined by two Gibbs states (related by spin inversion symmetry) plus a spectrum of excitations and corresponds to the inversion of compact domains of finite size (droplets). This picture of the spin-glass state lacks the most peculiar feature of the mean-field theory, i.e. the coexistence of a large number of phases or states in the spin-glass phase.

Recently, exact results have been obtained by Newman and Stein [8] and also by Guerra [9] on which features of the spin glass state, present in the Sherrington-Kirkpatrick (SK) model [10], survive in finite dimensions. Numerical simulations are one of the few confident tools that we can use to investigate this problem and clarify the controversy [11]. With the aid of numerical simulations, two main questions in spin glasses have been addressed. The first one concerns the low temperature behavior of the model in zero magnetic field. The second one concerns the existence of the spin-glass transition in a magnetic field similar to the one found by de Almeida and Thouless in the mean-field case [12] (the so called AT line). A clearcut answer to these questions would be very useful as a guide for constructing a theory of the spin glass state in finite dimensions. While the first problem has received considerable attention, very few results have been obtained for the second one.

The purpose of this work is the study of the existence of spin-glass state in a magnetic field. This work is the natural continuation of previous numerical simulations done in the SK model in a magnetic field, where the existence of a replica symmetry broken phase, as predicted by Parisi [13], was verified through the study of the overlap probability distribution $P(q)$ [14]. In that work we also studied the four dimensional (4D) $\pm J$ Ising spin glass in a magnetic field in the low $T$ phase but did not find evidence for a $P(q)$ of the mean-field type, even though we were not sure that equilibrium was achieved for the
largest sizes. In order to investigate the existence of a transition line in a magnetic field we have performed extensive tempering Monte Carlo simulations in the ±J Ising spin glass in four dimensions.

The model and the numerical algorithm. We have considered the model described by the Hamiltonian,

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

where the spin variables $\sigma_i$ take the values ±1, the $J_{ij}$ are random discrete ±1 quenched variables and $h$ denotes the magnetic field. The spins are located in the sites of a 4D cubic lattice of size $L$ and $N = L^4$ sites with periodic boundary conditions.

In order to reach the maximum efficiency in the Monte Carlo simulations we have used the tempering method introduced by Marinari and Parisi [20]. This is a Monte Carlo method in which the temperature is a dynamical variable and the system can change the temperature while always being in thermal equilibrium. The system performs a random walk in temperature in such a way that low temperature equiprobable configurations separated by high energy barriers can be efficiently sampled. For a description and details about this algorithm, the reader is referred to [21].

In what follows we briefly describe the numerical procedure we have followed. Samples are cooled down, at constant magnetic field $h$, starting from the high temperature phase (above the critical temperature at zero field $T_c \approx 2.0$ [13]) down to $T = 1.0$ and the internal energy $e_\beta = \langle H \rangle$ is estimated as a function of $\beta$ for a selected set of $N_\beta$ different values of $\beta$ ($N_\beta = 50$ for the largest sizes). The separation $\Delta \beta$ between the different values of $\beta$ is taken such that the tails of the probability distributions of the energy for different neighboring temperatures do superimpose. For sake of simplicity the different values of $\beta$ are taken equidistant with $\Delta \beta = 0.03$ for the largest sizes. It is important to note that all multicanonical methods are expected to work if the thermodynamic chaos (to be discussed below) is small. The weakness of chaotic effects in temperature for finite sizes was numerically checked for the SK model [22] as well as for 4D ±J Ising spin glasses [23].

Starting from a random initial condition and an initial temperature $\beta_r$, all the spins are sequentially updated at each Monte Carlo step (MCS) and single spin flips are accepted with a probability given by the heat bath algorithm. After each MCS a change in temperature is proposed $\beta_r \rightarrow \beta_{r+1}$ or $\beta_r \rightarrow \beta_{r-1}$, each with a probability $1/2$. The change in temperature $\Delta \beta$ is accepted with probability $\exp(-\Delta \beta (E(\sigma) - (e_\beta + e_{\beta + \Delta \beta})/2))$. The spins are again updated and the change of temperature is again proposed. In this way one is able to compute the equilibrium values of different observables for all values of $\beta$. In order to increase the statistics we have simulated 8 different replicas in parallel in a multispin coding program.

Before presenting the numerical results, we will comment about chaotic effects in spin glasses and then explain how we choose the value of the magnetic field for our simulations.

Thermodynamic chaos in spin glasses. One of the main properties of spin glasses is the existence of chaotic effects when some external parameter like the temperature or the magnetic field is changed [24]. This feature is present in the mean-field approach as well as in the droplet model at zero magnetic field. In the framework of mean-field theory of spin glasses, the physical meaning of thermodynamic chaos is rather intuitive. It is related to the fact that small energy perturbations can redistribute the (small) free energy differences of the many equilibrium states modifying completely their equilibrium statistical weights. In the framework of droplet models, energy perturbations can strongly modify spin correlations due to the fractal nature of the droplet domain walls. We note that thermodynamic chaos is a real effect of the spin glass phase. According to the droplet model, the effect of a uniform magnetic field is to suppress the spin glass phase, hence chaotic effects in temperature disappear if the system becomes magnetized. The simplest way to measure chaoticity in spin glasses is by defining the chaos correlation length associated to the $q-q$ correlation function at large spatial distances $x$ [10,23].

$$C_{chaos}(x) = \left| q_1 q_{i+x} \right| \sim x^{-\mu} \exp(-x/\xi_c)$$  \hspace{1cm} (2)$$

where $q_i = \sigma_i \tau_i$ and $\sigma_i, \tau_i$ denote the spins of the unper- turbated ($H_0(\sigma)$) and perturbed system ($H_p(\tau)$) respectively and the expectation value $< .. >$ is taken over the equilibrium Boltzmann distribution associated to the full Hamiltonian $H(\sigma, \tau) = H_0(\sigma) + H_p(\tau)$. $\mu$ is a positive exponent. The chaos correlation length $\xi_c$ gives an estimate of the typical size of spatial regions which are similar in the unper turbated and perturbed system. When the intensity of the perturbation goes to zero, the chaos correlation length $\xi_c$ diverges and the divergence is related to the particular type of perturbation.

For magnetic field perturbations, we know that chaotic effects are quite strong [3]. This effect sets a limit for the

*We chose to study 4D instead of 3D because the evidence in favor of a phase transition at zero field is less obvious in this last case [16,19]. Moreover the 4D model is easier to thermalize than in 3D.

†In contrast with chaotic effects in the presence of temperature perturbations which are small [24,23,23].
value of the magnetic field that we can use in simulations. This is the most relevant parameter in the simulations because it determines how close we are to the $h = 0$ spin-glass phase. The value of $h$ cannot be too large otherwise, if a spin glass transition exists, it will be pushed down to very low temperatures. Also it cannot be too small otherwise the results are strongly affected by the $h = 0$ spin-glass phase for the finite sizes we have studied. The crossover between the $h = 0$ behavior and the finite $h$ behavior depends on the chaos correlation length $\xi_c(h)$ defined in eq. (3). The value of the magnetic field $h$ has to be chosen in such a way that $\xi_c(h) < L$ for the explored lattice sizes but not too large as explained previously. We have found that a good compromise is $h = 0.4$ which yields a macroscopic magnetization at low temperatures of order $0.15$. Then, we can estimate from independent Monte Carlo simulations (see [22]) that $\xi_c \simeq 5$ for the lowest temperature $T = 1$. We expect that simulations for sizes above $L = 5$ can yield convincing results on the existence or absence of phase transition at this value of the field.

**Numerical results.** Simulations were performed for the following sizes $L = 3, 5, 7, 9$ with 1000, 325, 120, 130 samples and $N_{\beta} = 20, 40, 50, 50$ respectively ranging from $T_{\text{min}} = 1.0$ up to $T_{\text{max}} = 2.5$ (or $T_{\text{max}} = 3.0$ for the smallest sizes $L = 3, 5$). For the largest size $L = 9$ the number of temperatures was not large enough to achieve equilibrium at low temperatures, hence we will show the data only for temperatures above $T \simeq 1.6$ for that size. In figure 1 we present results for the magnetization $M = \frac{1}{N} \sum_i \sigma_i$ at different temperatures and sizes. Instead of plotting directly the magnetization we plot the ratio $r(T, L) = \frac{MT}{k}$. This quantity (due to a local gauge symmetry of the disorder [14]) should be equal to 1 above $T_c(h = 0) \simeq 2.0$ in the limit of very small $h$. For finite $h$, because of the divergence of the spin-glass susceptibility at zero field, $r$ is smaller than 1 (at $T = 2.5$ it is of order $0.7$) but converges to 1 quite fast at high temperatures where the spin-glass susceptibility vanishes like $\beta^3$. The important result which emerges in figure 1 is that below $T_c(h = 0)$, $r$ is linear with $T$. Consequently the magnetization is nearly constant in the low temperature phase. This feature is also present in the mean-field theory and has been observed in the 3D case [20] as well as in field cooled experiments in spin glasses [21].

![FIG. 1. Parameter $r = \frac{MT}{k}$ as a function of temperature. From top to bottom $L = 3, 5, 7, 9$. Data for $L = 9$ is hardly distinguishable from $L = 7$.](image)

More information about a possible phase transition can be obtained by directly measuring the spin-glass order parameter $Q$ between two different replicas $\{\sigma, \tau\}$ with the same set of $J_{ij}$, $Q = \frac{1}{N} \sum_i \sigma_i \tau_i$ and its associated probability distribution,

$$P_J(q) = \langle \delta(q - Q) \rangle$$

(3)

where $\langle \cdot \rangle$ denotes the thermal Gibbs average. In particular, for each sample we calculated the first four moments of the distribution (3). We have computed the mean value, the variance $X$, the skewness $Y$ and the kurtosis $Z$ of the distribution $P(q) = P_J(q)$ where $\langle \cdot \rangle$ means average over the disorder. The skewness and the kurtosis are a measure of the asymmetry and Gaussianity respectively of the overlap distribution. More precisely, if we define the following averages $[f(q)] = \int dq f(q) P(q)$ we have,

$$X = \langle [q - \langle q \rangle]^2 \rangle$$

(4)

$$Y = \frac{\langle [q - \langle q \rangle]^3 \rangle}{\langle [q - \langle q \rangle]^2 \rangle^2}$$

(5)

$$Z = \frac{1}{2} \frac{\langle [q - \langle q \rangle]^4 \rangle}{\langle [q - \langle q \rangle]^2 \rangle^2}$$

(6)

In figure 2, we plot the mean value $[q]$ as a function of the temperature for different sizes. Data for $L = 9$ above $T \simeq 1.6$ is nearly indistinguishable from data for $L = 7$. As shown in figure 2, we expect that $[q]$ converges to a value close to 1 at zero temperature (but smaller than 1 if
there is ground state degeneracy). The cumulants $X, Y, Z$ give more information about a possible phase transition. They are expected to vanish in the $L \to \infty$ limit in the paramagnetic phase. Within an ordered phase of the mean-field type, where several pure states contribute to the Gibbs average, we expect $X, Y, Z$ to be finite. In figure 3, 4, 5 we show $NX, Y, Z$ (where $N = L^4$) as a function of temperature for four different lattice sizes $L = 3, 5, 7, 9$.

![FIG. 2. Mean value $[q]$ as a function of temperature. From bottom to top $L = 3, 5, 7, 9$. Data for $L = 9$ is hardly distinguishable from $L = 7$.](image)

Figure 3 is quite interesting. We observe the presence of a cusp in the spin-glass susceptibility for sizes $L = 5, 7$. This cusp moves to higher temperatures as the size increases (for $L = 3$ such a cusp is not observed in the range of temperatures explored). The observation of this effect already for $L = 5, 7$ reveals that it is a real trend of the data and not a mere fluctuation. Unfortunately for $L = 9$ we have not been able to confirm or disprove this tendency (we have not succeeded in thermalize $L = 9$ at low temperatures). According to the droplet picture, the spin-glass susceptibility in the $\pm J$ model at zero temperature should be positive at finite field due to the ground state degeneracy (see the discussion in [27]). According to the mean-field picture, the susceptibility should diverge below the AT line.

![FIG. 3. Spin glass susceptibility $NX$ as a function of temperature. From bottom to top $L = 3, 5, 7, 9$.](image)

Figures 4 and 5 show the parameters $Y, Z$ for the different sizes. What should be the manifestation of the existence of a second order transition line? For large enough sizes, one expects the adimensional quantities $Y, Z$ to scale like $Y \equiv Y(L(T - T_c)\nu)$ (the same for $Z$). Consequently they should display a crossing point for different sizes at $T = T_c$ like happens at zero magnetic field [13]. The lines in figures 4 and 5 corresponding to $L = 5, 7, 9$ sizes have been indicated by full symbols in order to distinguish the general trend of the data from the results for $L = 3$. Figure 4 shows that the skewness is negative for finite sizes and above $T \approx 1.5$ it goes to zero when the size increases as expected in the paramagnetic phase. The same tendency is also observed in figure 5 for the kurtosis. It is interesting to note that the curves for $L = 5, 7$ for both the skewness and the kurtosis cross at the same temperature $T \approx 1.5$ which is an upper bound for of an hypothetical critical temperature. Unfortunately, we have not covered a large enough range of sizes ($L = 3$ is too small) in order to have clear evidence of such a crossing point. Our results suggest the existence of paramagnetic ordering at least above $T \approx 1.5$ and we cannot exclude the existence of crossing point and hence a phase transition below that temperature.
From our data we reach the following three conclusions: 1) From figures 4 and 5 we can conclude that a phase transition, if existing, appears below $T_c(h = 0) \simeq 2.0$. Hence the transition temperature is pushed down by the magnetic field. 2) We clearly observe a change of behavior above $L = 5$ where the trend of the skewness and kurtosis as a function of the size changes. This crossover length is in agreement with the estimated chaos correlation length $\xi_c \simeq 5$ for the value of the magnetic field $h = 0.4$ and should correspond to the size $L$ such that the tail of the $P(q)$ extending down to negative values is suppressed. 3) Most interestingly, figure 3 shows the existence of a cusp which does not grow very fast with the size of the system and which has to be appropriately interpreted, since it is in disagreement with the mean-field picture. If the spin-glass susceptibility is finite at zero temperature this cusp is then to be expected. This result suggests that if a transition exists, it should have non trivial finite-size effects.

A word of caution is essential at this point. Spin glasses are extremely difficult to thermalize and this is probably the reason why small progress has been done in the understanding of their equilibrium properties. The cusp observed in figure 3 can indeed be suppressed in the presence of non equilibrium effects. The presence of this cusp was not observed in [13] but in that case the magnetic field was larger ($h = 0.6$) and thermalization was achieved by simulated annealing which is a less effective procedure than tempering.

It is important to note that the results we are presenting here are probably seen in a very narrow range of fields. For fields larger than $h = 0.4$, the cusps in $X$ will move to lower temperatures and hence it is difficult to see them numerically since tempering does not work efficiently for very low temperatures. On the other hand, for smaller fields, the chaos correlation length would be larger and this would require to simulate much larger lattices in order to start to see the trend of the data.

Our data can then be interpreted in the framework of two scenarios: 1) The transition is absent 2) The transition exists and the cusp in the spin glass susceptibility is a finite size effect not incompatible with a divergence in the thermodynamic limit. In this case the transition should be above $T \simeq 1.25$ (where the cusp of $X$ in fig. 3 for the largest size is located) and below $T \simeq 1.5$ (where the crossing point for the skewness and the kurtosis is observed). It is difficult to go beyond such a conclusion and extremely careful work (full thermalization in each sample is compulsory) has to be done in order to discern among these possibilities. A similar work on the Gaussian case (to avoid the ground state degeneracy) using the replica exchange method recently proposed by Hukushima, Takayama and Nemoto [19] would be welcome in order to check the main conclusions of this work.

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