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A Bivariate Multicanonical Monte Carlo of the 3D $\pm J$ Spin Glass

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Abstract. A bivariate multicanonical Monte Carlo simulation of the three-dimensional $\pm J$ Ising spin glass is described. The autocorrelation time is approximately proportional to the system size, which is a great improvement over previous spin-glass simulations. The Binder plot indicates the critical temperature $T_c \simeq 1.3$. The order-parameter distribution function $P(q)$ exhibits a feature of the droplet picture of the low-temperature phase.

1 Introduction

It has been a few decades since spin glasses first attracted much attention [1]. Although there have been many extensive studies, theoretical, numerical, and experimental, there still remain a few unsettled fundamental problems. In the present paper, we report the results of our recent Monte Carlo simulation of the three-dimensional $\pm J$ Ising spin glass, focusing on two issues: estimation of the spin-glass transition temperature and the nature of the low-temperature phase [2].

First, in the next section, we give a short review of the current status of spin-glass studies. In Sect. 3, we describe our simulation method, namely a bivariate multicanonical Monte Carlo method. Monovariate multicanonical methods [3,4] have been applied to spin glasses before [5–7]; we found, however, that using a bivariate version is essential in reducing the correlation time of the simulation. We show that the autocorrelation time is approximately proportional to the system size. Since the output of multicanonical simulations is the density of states, we can access to any temperatures in principle. Thus we were able to explore low-temperature regions which have been hard to access by other Monte Carlo methods. We present our Monte Carlo results in Sect. 4. Our Binder plot clearly indicates the existence of a spin-glass transition at the critical temperature $T_c \simeq 1.3$. In addition, the order-parameter distribution function $P(q)$ exhibits a feature of the droplet picture of the low-temperature phase: $P(0)$ decreases at $T = 0.3$ as the system size is increased. The both results are not completely consistent with previous Monte Carlo results. We discuss possible reasons of the inconsistency in the last section.

2 Spin Glass

2.1 The $\pm J$ model and the overlap order parameter

Spin glasses are realized typically in alloys of a magnetic metal and a non-magnetic metal [1]. Because the RKKY exchange interaction between the magnetic moments alternates in sign as a function of the distance, some of the magnetic-moment pairs interact ferromagnetically, some antiferromagnetically.

A simple theoretical model to which we focus our attention is the $\pm J$ Ising spin glass. Its Hamiltonian is given by [8]

$$\mathcal{H} \equiv - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j. \quad (1)$$

Here the Ising spins σ_i fluctuates thermodynamically, while each exchange interaction J_{ij} is quenched to $\pm J$ randomly. The summation runs over the nearest-neighbor pairs of a cubic lattice.

If all the exchange interactions were positive, there would be a ferromagnetic phase transition at a finite temperature, below which the system falls into one of the two global minima of the free energy, namely the ordered states. "Frustration" of the interactions drastically changes the situation [9]. The random interactions generate many local minima in the free energy landscape, each of which may represent a seemingly random configuration of the spins. However, the spins may be frozen into such a configuration at low temperatures: this spin freezing is the essence of the spin-glass "order."

A theoretical measure of the spin-glass phase is called the overlap order parameter [8]. To define it, we duplicate the random exchange interactions in (1) and change the Hamiltonian to

$$\mathcal{H} \equiv - \sum_{\alpha=1,2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i^{(\alpha)} \sigma_j^{(\alpha)}, \quad (2)$$

where the superscript of the spin variables indicates each replica of the system. The spins of one replica and those of the other are thermodynamically independent. Nonetheless, we can expect that the spin configurations of the two replicas are similar to each other at low temperatures, if there is a thermodynamic state which the system is frozen into. Thus we define the order parameter as the Hamming distance of the spin configurations of the replicas [8]:

$$q = \frac{1}{N} \sum_{i=1}^N \sigma_i^{(1)} \sigma_i^{(2)}. \quad (3)$$

Here N is the number of the lattice sites. One may regard that the two replicas represent the same system at two moments in time with infinite interval [8];

hence the parameter q measures how strongly the spins are frozen into a configuration.

The thermodynamic average $\langle \dots \rangle$ in the following is calculated with respect to the replica Hamiltonian (2). In addition, we calculate the random average $[\dots]_{\text{av}}$ to obtain the final estimates of physical quantities.

2.2 Theoretical issues

Because of the very nature of the spin-glass order, it is generally hard to equilibrate spin glasses in simulations and in experiments. After a few decades of research, there are still unresolved issues on equilibrium properties of spin glasses. Fundamental theoretical questions that we address here regarding spin glasses in equilibrium are: (i) what is the critical temperature T_c , below which $[\langle q \rangle]_{\text{av}} \neq 0$? (ii) what is the nature of the low-temperature phase?

It is now widely accepted that there is no spin-glass phase transition in two dimensions. It has been harder to determine the existence of the transition in three dimensions.

A well-used method of estimating the critical temperature of various systems, and particularly spin glasses, is the Binder parameter given by [10]

$$g_L \equiv \frac{3}{2} \left[1 - \frac{\langle q^4 \rangle}{3 \langle q^2 \rangle^2} \right]_{\text{av}}, \quad (4)$$

where L denotes the linear system size. Because of the dimensionless combination of the second moment and the fourth moment, the Binder parameter is expected to be independent of the system size at fixed points, *i.e.* $T = 0, T_c, \infty$. The order-parameter distribution is a Gaussian at $T = \infty$; hence $\langle q^4 \rangle = 3 \langle q^2 \rangle^2$ and $g_L = 0$. If the order parameter can take only two values $\pm q_0$ at $T = 0$ as in usual ferromagnets, we have $\langle q^4 \rangle = \langle q^2 \rangle^2 = q_0^4$ and hence the Binder parameter is $g_L = 1$. At $T = T_c$, the Binder parameters for different system sizes are expected to cross at a nontrivial value. In the high-temperature phase, $g_L(T)$ decreases towards zero as $L \rightarrow \infty$, while it increases towards unity in the low-temperature phase. Thus the crossing point of $g_L(T)$ should give the critical temperature.

Unfortunately, in earlier studies of spin glasses, the numerical results for the Binder parameter did not show the expected behavior; the Binder parameter $g_L(T)$ for different L appeared to collapse into one curve at low temperatures [1,11], which made one even doubt the applicability of the Binder plot to spin glasses. The issue was settled only when two independent Monte Carlo studies several years ago yielded the expected behavior of the Binder parameter [12,13]. (In other words, the earlier numerical results turned out to be inaccurate at low temperatures, probably owing to slow dynamics of the simulations.) The crossing point of the new studies was $T_c \simeq 1.1$. We stress, however, that the Binder-parameter crossing in these studies was still subtle

compared to our result. As we describe below, our results show a clearly visible crossing point near $T_c \simeq 1.3$. The crossing point is clearer even than in the two new studies.

The other theoretical issue is the nature of the low-temperature phase. This is the subject of a long-standing and unresolved controversy between the mean-field picture and the droplet picture. The mean-field picture maintains the existence of an infinite number of global minima of the free energy, which is called the replica symmetry breaking [14]. This is true for the mean-field (Sherrington-Kirkpatrick) model [15,16]; the question is whether this also applies to finite-dimensional models. The droplet picture, on the other hand, claims that only two global free-energy minima exist, although there must be many local minima [17,18]. According to this picture, the nature of the spin-glass transition is less exotic in three dimensions than in the mean-field model.

While many numerical simulations appear to support infinite degeneracy [19–21], a recent analytic treatment argues against it [22,23]. Note that the droplet picture actually is a theory concerning the *zero*-temperature fixed point; if the droplet picture is correct, it might be seen only near $T = 0$. Unfortunately, the slow dynamics of spin glasses has hindered numerical simulations from approaching the zero-temperature fixed point. A recent numerical study [24] demonstrated that results of the Migdal-Kadanoff approximation appear to indicate the mean-field picture near and below the critical point, but eventually come to support the droplet picture as $T \rightarrow 0$. Uncertainty, however, comes from the fact that the Migdal-Kadanoff approximation produces the droplet picture even for the mean-field model.

One way of distinguishing the two pictures is to measure the order-parameter distribution $P(q)$, which is given by

$$P(q) \equiv [\langle D(E, q) \rangle]_{av} \quad (5)$$

where $D(E, q)$ denotes the density of states with respect to the energy and the order parameter. If the droplet picture is correct, $P(q)$ should converge to two delta functions as $T \rightarrow 0$ and $L \rightarrow \infty$, because only two thermodynamic states are available at $T = 0$ according to this picture. If the mean-field picture, on the other hand, is correct, $P(q)$ should maintain a nontrivial form even as $T \rightarrow 0$. Hence many numerical simulations focus onto the size dependence of $P(0)$. The droplet picture predicts that $P(0)$ decreases as $L \rightarrow \infty$ at low enough temperatures, while the mean-field picture predicts that it converges to a finite value.

As was mentioned above, many simulation studies suggest the mean-field picture on the basis of their numerical estimates of $P(0)$ at as low as $T = 0.7$. Again, because of the slow dynamics of the simulations, it has been hard to lower the temperature further and to explore the vicinity of the zero-temperature fixed point. Using a multicanonical Monte Carlo method, we managed to reduce the difficulty of the slow dynamics significantly. Multicanonical simulations produce the density of states as output, from which

we can calculate expectation values at any temperatures in principle. Our estimation of $P(0)$ at low temperatures suggests the droplet picture, as shown in the next section.

Let us add a few words regarding the correspondence between theories and experiments of spin glasses. As was stressed above, it generally takes very long time to equilibrate experimental samples. Hence many experiments nowadays feature nonequilibrium behavior of spin glasses. One might then say that the above theoretical issues regarding equilibrium properties, particularly the second one, are pedantic, if the equilibrium is not achievable in reality. However, the above issues are in fact linked to many different subjects of complex systems beyond spin glasses [14], and hence worth resolving. Furthermore, there are also efforts on the experimental side to quicken the equilibration process (*e.g.* with quantum fluctuation from transverse magnetic fields [25]) in the hope of achieving the true equilibrium of samples.

2.3 Simulation methods

Attempts to resolve the above theoretical issues have been closely tied to the development of simulation methods. A simulation method that reduces the difficulty of the slow dynamics will be also useful in studying other complex systems.

One may classify the existing Monte Carlo methods for complex systems into two categories: cluster algorithms and extended-ensemble approaches. Swendsen and Wang [26] applied a cluster algorithm to spin glasses first in 1986 and saw successful results in two dimensions. However, cluster algorithms have been less successful in three dimensions.

In the last decade, many studies found extended ensembles useful in simulations of complex systems. Here the extended ensemble refers to an ensemble other than the canonical and micro-canonical ensembles. In spin glasses, canonical-ensemble simulations tend to be trapped in metastable states because of its strong emphasis on low-energy states at low temperatures. The main purpose of using extended ensembles is to provide paths out of metastable states via high-energy states without giving up sufficient statistics of low-energy states.

Among various extended-ensemble approaches is the multi-canonical Monte Carlo method [3,4]. In this method, the ensemble is defined so that any *macrostates* appear at the same frequency in the course of the simulation. Berg and others [5-7] have applied this method to spin glasses, taking the weight of each spin configuration $\{\sigma\}$ either as

$$W(\{\sigma\}) \propto 1 / D(E(\{\sigma\})) \quad (6)$$

or

$$W(\{\sigma\}) \propto 1 / D(q(\{\sigma\})), \quad (7)$$

where $D(E)$ is the density of states with respect to the energy and $D(q)$ is the one with respect to the overlap order parameter. It has been argued [27] that "simulated tempering [28]," where replicas at different temperatures have an equal weight, is mathematically similar to taking the weight (6).

As we show in the following, we used for our simulation the bivariate weight

$$W \propto 1 / D(E, q). \quad (8)$$

Bivariate multicanonical Monte methods have been used in different contexts, *e.g.* protein simulations [29,30]. In preliminary runs, we found that the use of both E and q for spin-glass simulations is essential in improving the slow dynamics [2].

3 Multicanonical Monte Carlo Method

In this section, we describe the multicanonical Monte Carlo method in more detail. Let us first compare it with micro-canonical and canonical methods in the following way. Suppose that we carry out a simulation with the importance weight $W(E)$, keeping the histogram of the states with respect to E . After equilibration of the simulation, each microstate (spin configuration) is generated in the course of the simulation at a rate proportional to $W(E)$. The rate at which a *macrostate* (thermodynamic state) with the energy E appears is proportional to $D(E)W(E)$, where $D(E)$ is the density of states.

In the micro-canonical simulation, we generate all microstates at the same rate. In other words, we set $W(E) = \text{const.}$, and hence the resulting histogram is proportional to the density of states: $h(E) \propto D(E)$ (see Fig. 1). In

Fig. 1. A schematic of the histograms of states that would be generated in the micro-canonical, canonical, and multicanonical simulations.

many cases, the density of states becomes very small in low-energy regions. Hence simulations based on the micro-canonical ensemble are generally not suitable for investigating low-temperature properties; low-energy states that

dominate the thermodynamic average at low temperatures are not generated frequently.

Algorithms of importance sampling, or the canonical method, were developed to overcome this difficulty. In the canonical method, states are generated with the importance weight $W(E) \propto e^{-\beta E}$, and hence the energy histogram is $h(E) \propto e^{-\beta E} D(E)$. Thus, in ideal cases, low-energy states appear at great frequency at low temperatures. In spin-glass simulations, however, the simulation tends to fall into a local minima of the free-energy landscape and stay there, because the system would have to be excited to a higher-energy state to go to the global minima.

In the multicanonical simulations, the importance weight is set to $W(E) \propto 1/D(E)$, and hence the histogram should become flat. (Of course, we cannot set $W(E) \propto 1/D(E)$ from the beginning, since we do not know the density of states *a priori*. However, there is a procedure that makes the importance weight converge to the reciprocal of the density of states [31].) The aim is to ensure better statistics of low-energy states than in the micro-canonical method and, at the same time, generate more high-energy states than in the canonical method so that the system can escape local free-energy minima.

In the ideal situation, the multicanonical simulation generates a free random walk in the macroscopic phase space, since all the macrostates should appear with the same probability. We can deduce from this that the autocorrelation time of the thermodynamic variable (E in the above case) should be proportional to the volume (the number of the sites). In the simulation of the $\pm J$ model, the energy change after each spin flip is of the order of J . On the other hand, the upper and lower bounds of the energy are of the order of NJ , where $N = L^3$ is the number of the sites. Hence the number of spin flips necessary for the random walk to cover the entire energy phase space is of the order of N^2 . Thus the measured energy should decorrelate after N^2 Monte Carlo steps, or N Monte Carlo sweeps.

This was not achieved, however, in the previous attempts of the multicanonical simulations of spin glasses [5-7]. Berg *et al* reported $\tau \propto N^{2.8}$ for the importance weight (6) [5] and $\tau \propto N^{2.24}$ for the importance weight (7) [7]. (Here τ is measured in the unit of Monte Carlo *sweep*.) This suggests that the slow dynamics in the low-energy region was not removed completely in these monovariate multicanonical simulations. (Note, however, that Berg *et al* did not use the conventional definition of the autocorrelation time in measurement of τ . This might be another source of the above power laws.)

In the present study, we carried out the simulation using the bivariate importance weight (8). As shown in Fig. 2 (a), we almost achieved the ideal situation $\tau \propto N$. The random walk in the two-dimensional phase space is exemplified in Fig. 2 (b). The drawback of the bivariate simulation, on the other hand, is the need for large memory in the computation. The number of bins in the energy phase space is of the order of L^3 , and so is that in the q phase space. Hence an array of the size L^6 is necessary to store each of

Fig. 2. (a) The system-size dependence of the autocorrelation time τ with respect to E and q . The dotted line represents the power law $\tau \propto N^{2.24}$, which was reported in [7]. (b) An example of the random walk in the phase space (E, q) . The system size simulated here is $L = 4$. The time series of 2500 Monte Carlo sweeps after equilibration is plotted.

the density of states $D(E, q)$, the histogram $h(E, q)$, and a work space. This amounts to about 30MB per sample for $L = 10$ and 400MB per sample for $L = 16$.

The actual algorithm of the multicanonical method has the following structure:

- (A) Take a guess at the density of states, $D_0(E, q)$. Start the following loop with $i = 0$.
- (B) The outer loop (multicanonical-iteration loop):
 - (a) Set the importance weight as $W_i = 1/D_i$. Calculate the energy and the order parameter of the initial spin configuration, E_0 and q_0 . Start the following loop with $j = 0$.
 - (b) The inner loop (spin-update loop):
 - (i) Choose a spin to be updated. Calculate the energy and the order parameter, E'_j and q'_j , assuming that the spin is actually flipped.
 - (ii) Calculate the spin-flip probability as

$$P_{\text{flip}} = \min \left(1, \frac{W_i(E'_j, q'_j)}{W_i(E_j, q_j)} \right) \quad (9)$$
 - (iii) Draw a random number $R \in [0, 1]$. If $R < P_{\text{flip}}$, flip the spin and make the substitution $E_{j+1} = E'_j$ and $q_{j+1} = q'_j$. Otherwise, keep the current spin configuration and make the substitution $E_{j+1} = E_j$ and $q_{j+1} = q_j$.
 - (iv) Increment the histogram bin $h_i(E_{j+1}, q_{j+1})$ by one.
 - (v) Increment the number of steps, j , by one and go to the step (i) until j exceeds a pre-determined number.
 - (c) Measure a physical quantity as

$$\langle Q \rangle_i = \frac{1}{Z_i} \int dE \int dq Q(E, q) e^{-\beta E} h_i(E, q) D_i(E, q), \quad (10)$$

where the partition-function estimate is given by

$$Z_i = \int dE \int dq e^{-\beta E} h_i(E, q) D_i(E, q). \quad (11)$$

- (d) Update the guess of the density of states as follows: [31]

$$D_{i+1}(E, q) = \frac{D_i(E, q) (h_i(E, q) + 1)}{\text{Normalization}}. \quad (12)$$

The normalization constant is chosen so that the integration of the density of states becomes unity. (An extra count is added to the histogram in (12) in order to avoid zero division in setting the next importance weight $W_{i+1} = 1/D_{i+1}$ [31].)

- (e) Increment the number of multicanonical iterations, i , by one and go to the step (a), until the histogram meets certain conditions of being flat.

The step (iv) should be skipped until the simulation reaches the "equilibrium" for the importance weight W_i . In our simulation, we devoted to equilibration Monte Carlo sweeps of a few times as long as the correlation time.

It is also best to skip the step (c) until the histogram h_i becomes practically flat. In principle, the estimator (10) should be applicable even before the histogram becomes flat. With sufficient statistics, the histogram h_i would be proportional to $W_i(E, q) D(E, q) = D(E, q)/D_i(E, q)$, where $D(E, q)$ is the true density of states. Thus the estimator (10) would give

$$\langle Q \rangle_i \simeq \frac{1}{Z_i} \int dE \int dq Q(E, q) e^{-\beta E} D(E, q), \quad (13)$$

with the partition function

$$Z = \int dE \int dq e^{-\beta E} D(E, q). \quad (14)$$

In practice, however, a limited number of Monte Carlo steps can cause large errors wherever h_i is small.

In the convergence process, the histogram is usually concentrated first in the mid part of the density of states and expands towards the upper and lower bounds of the energy until it becomes flat. Hence we determined that the histogram became flat, whenever the histogram count of the bin at the center of the density of states and that at the edges of the density of states are both close to the average histogram count.

As another remark, all physical quantities could be calculated after the whole simulation is over, if we stored the density of states itself on the storage disk. This would, however, require a huge disk space after simulating large number of random samples.

4 Numerical Results

We have carried out the bivariate multicanonical simulation of the systems of size $L = 4$ (838 samples), $L = 6$ (767 samples), $L = 8$ (719 samples) and

Fig. 3. The Binder plot for the 3D $\pm J$ Ising spin glass.

$L = 10$ (365 samples). The temperature dependence of the Binder parameter is shown in Fig. 3. The Binder-parameter crossing in this figure is much more prominent than in other numerical results. Although it is hard at this point to analyze the data including finite-size corrections, we can safely say that critical temperature is higher than 1.2.

The order-parameter distribution $P(q)$ at $T = 0.3$ is shown in Fig. 4. Although the statistical errors are still large, we can see the tendency of decreasing $P(0)$, which is the behavior predicted from the droplet picture. At $T = 0.7$, on the other hand, $P(0)$ does not show a definite tendency to decrease (Fig. 5), which may spuriously indicate the mean-field picture.

In the algorithm described in the previous section, we repeated the outer loop five times after we determined that the histogram became practically flat, so that we could detect erroneous estimates of the density of states. We also divide the inner loop into a few sections, from which we calculated the statistical errors. Note that errors of data at different temperatures of the same sample are generally correlated in multicanonical simulations.

5 Discussions

As we have seen, the results of our multicanonical Monte Carlo calculation are in disagreement with some of previous results. First, $P(q)$ near $q \simeq 0$ appears to be much smaller at low temperatures. Second, the Binder parameter

Fig. 4. The order-parameter distribution $P(q)$ at $T = 0.3$. The error bars are shown only for a part of the data points.

Fig. 5. The order-parameter distribution $P(q)$ at $T = 0.7$. The error bars are shown only for a part of the data points.

appears to be greater in the low-temperature phase and this disagreement grows as the system size is increased.

These disagreements may be understood by the following scenario: If there are many local free-energy minima with small q , simulations may be trapped by them and thus overestimate $P(q)$ near $q = 0$, particularly when the system size is increased. This would result in underestimating the Binder parameter of large systems at low temperatures. This scenario is supported by a recent study, where Sandvik[32] carried out a series of simulated annealing calculations with different annealing rates and estimated $P(q)$ in each annealing. He showed that the ground-state estimate of $P(0)$ is greater for faster annealing than for slower annealing (which must be more precise). His results suggest that simulations without substantial equilibration could overestimate $P(0)$.

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References

1. Binder, K., Young, A. P. (1986) Spin-Glasses: Experimental Facts, Theoretical Concepts, and Open Questions. *Rev. Mod. Phys.* **58**, 801-976
2. Preliminary results have been reported in the 8th Tohwa University International Symposium. See the proceedings, Hatano, N., Gubernatis, J. E., Bivariate Multicanonical Monte Carlo of the 3D $\pm J$ Spin Glass. In: Tokuyama, M. (Ed.) *Slow Dynamics in Complex Systems*. American Institute of Physics, Maryland, to be published
3. Berg, B., Neuhaus, T. (1991) Multicanonical Algorithms for First Order Phase Transitions. *Phys. Lett. B* **267**, 249-253
4. Berg, B., Neuhaus, T. (1992) Multicanonical Ensemble: A New Approach to Simulate First Order Phase Transitions. *Phys. Rev. Lett.* **68**, 9-12
5. Berg, B.A., Hansmann, U., Celik, T. (1994) Ground-State Properties of the Three-Dimensional Ising Spin Glass. *Phys. Rev. B* **50**, 16444-16452
6. Berg, B.A. (1996) Multicanonical Recursions. *J. Stat. Phys.* **82**, 323-342
7. Berg, B.A., Janke, W. (1998) Multioverlap Simulations of the 3D Edwards-Anderson Ising Spin Glass. *Phys. Rev. Lett.* **80**, 4771-4774
8. Edwards, S. F., Anderson, P. W. (1975) Theory of Spin Glasses. *J. Phys. F: Metal Phys.* **5**, 965-974

9. Toulouse, G. (1977) Theory of the frustration effect in spin glasses: I. *Comm. Phys.* **2**, 115-119
10. Binder, K. (1981) Finite Size Scaling Analysis of Ising Model Block Distribution-Functions. *Z. Phys. B* **43**, 119-140
11. For example, Bhatt, R. N., Young, A. P., Numerical Studies of Ising Spin Glasses in 2, 3, and 4 Dimensions. *Phys. Rev. B* **37**, 5606-5614
12. Kawashima, N., Young, A. P. (1996) Phase Transition in the Three-Dimensional $\pm J$ Ising Spin Glass. *Phys. Rev. B* **53**, R484-R487
13. Hukushima, K., Takayama, H., Nemoto, K. (1996) Application of an Extended Ensemble Method to Spin Glasses. *Int. J. Mod. Phys. C* **7**, 337-344
14. For a review, Mézard, M., Parisi, G., Virasoro, M. (1987) *Spin Glass Theory and Beyond*. World Scientific, Singapore
15. Sherrington, D., Kirkpatrick, S. (1975) Solvable Model of a Spin-Glass. *Phys. Rev. Lett.* **35**, 1792-1796
16. Parisi, G. (1979) Infinite Number of Order Parameters for Spin-Glasses. *Phys. Rev. Lett.* **43**, 1754-1756
17. Fisher, D. S., Huse, D. A. (1986) Ordered phase of Short-Range Ising Spin-Glasses. *Phys. Rev. Lett.* **56**, 1601-1604
18. Fisher, D. S., Huse, D. A. (1988) Equilibrium behavior of the Spin-Glass Ordered Phase. *Phys. Rev. B* **38**, 386-411
19. Marinari, E., Parisi, G., Ruiz-Lorenzo, J., Ritort, F. (1996) Numerical Evidence for Spontaneously Broken Replica Symmetry in 3D Spin Glasses. *Phys. Rev. Lett.* **76**, 843-846
20. Iñiguez, D., Marinari, E., Parisi, G., Ruiz-Lorenzo, J. (1997) 3D Spin Glass and 2D Ferromagnetic XY Model: A Comparison. *J. Phys. A: Math. Gen.* **30**, 7337-7347
21. Marinari, E. (1999) Numerical Evidence for Continuity of Mean Field and Finite Dimensional Spin Glasses. *Phys. Rev. Lett.* **82**, 434-437
22. Newman, C. M., Stein, D. L. (1996) Non-Mean-Field Behavior of Realistic Spin Glasses. *Phys. Rev. Lett.* **76**, 515-518
23. Newman, C. M., Stein, D. L. (1998) Simplicity of State and Overlap Structure in Finite-Volume Realistic Spin Glasses. *Phys. Rev. E* **57**, 1356-1366
24. Moore, M. A., Bokil, H., Drossel, B. (1998) Evidence for the Droplet Picture of Spin Glasses. *Phys. Rev. Lett.* **81**, 4252-4255
25. Wu, W., Ellman, B., Rosenbaum, T. F., Aeppli, G., Reich, D. H. (1991) From Classical to Quantum Glass. *Phys. Rev. Lett.* **67**, 2076-2079
26. Swendsen, R. H., Wang, J.-S. (1986) Replica Monte Carlo Simulation of Spin-Glasses. *Phys. Rev. Lett.* **57**, 2607-2609
27. Hansmann, U., Okamoto, Y. (1996) Monte-Carlo Simulations in Generalized Ensemble: Multicanonical Algorithm versus Simulated Tempering. *Phys. Rev. E* **54**, 5863-5865
28. Marinari, E., Parisi, G. (1992) Simulated Tempering: A New Monte Carlo Scheme. *Europhys. Lett.* **19**, 451-458
29. Higo, J., Nakajima, N., Shirai, H., Kidera, A., Nakamura, H. (1997) Two-component Multicanonical Monte Carlo Method for Effective Conformation Sampling. *J. Comp. Chem.* **16**, 2086-2092
30. Iba, Y., Chikenji, G., Kikuchi, M. (1998) Simulation of Lattice Problems with Multi-Self-Overlap Ensemble. *J. Phys. Soc. Jpn.* **67**, 3327-3330
31. Smith, G.R., and Bruce, A.D. (1995) A Study of the Multi-Canonical Monte Carlo Method. *J. Phys. A: Math. Gen.* **28**, 6623-6643

32. Sandvik, A. (1999) Comment on "Evidence for Nontrivial Ground-State Structure of $3d \pm J$ Spin Glasses." Europhys. Lett., to be published