UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

SMR/1003 - 9

SUMMER COLLEGE IN CONDENSED MATTER ON
" STATISTICAL PHYSICS OF FRUSTRATED SYSTEMS "

(28 July - 15 August 1997)

" Numerical methods in glassy systems "

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Numerical methods in Glassy systems

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August 6, 1997

Lectures given in the Summer School on "Statistical Physics of Frustrated Systems" in Trieste (Italy), August 1997

Abstract

In these lectures I describe some theoretical tools and numerical techniques to investigate glassy systems. The discussion is centered on spin glasses where there has been a large amount of theoretical as well as numerical work during the recent years. After discussing the utility of introducing real replicas in numerical simulations, I analyze topics such as equilibration methods and the analysis of the critical point. Improved Monte Carlo methods like simulated tempering and parallel tempering are also discussed.

1 Introduction

The reliability of numerical simulations to successfully investigate glassy behavior is an open problem in modern statistical physics. To numerically investigate equilibrium properties in real glassy systems we face very hard problems related to the existence of relaxation processes with very long time scales. Indeed, the main problem which distinguishes *glasses* from usual systems (for instance, ferromagnets, liquids, gases,...) is the impossibility to reach thermodynamic equilibrium within available computer time at low temperatures as soon as the size of the system starts to be large. Then, to investigate and to discern the physical behavior and properties of such a system much skill is needed. It is not enough to have a very powerful computer or even to have a very fast code program but to really understand what is worth to look at when doing numerical simulations.

Trying to understand what is worth to look at with the aid of numerical simulations is the primary scope of the present lectures. I will try to convey you the main concepts and tools to investigate the underlying physics and scenario in glassy systems. I do not pretend to present an exhaustive collection of numerical methods and tricks but to present what I think are the most general ideas needed to start a numerical research. Consequently, the spirit of my lectures will be at a very introductory level. Those who are interested in a more detailed description can find in the literature an exhaustive list of references which deal with these and other related topics [1].

To investigate glassy systems we have to take into account the main difficulty which characterizes them, i.e. the existence of a large number of metastable configurations due to the frustrated character in the Hamiltonian. For instance, in spin glasses the frustration emerges directly from the disordered nature of the exchange couplings between the spins. These couplings are quenched, i.e they do not change in time and induce a frustration in the ground state of the system which translates into extremely large relaxation times at low temperatures. But disorder is not the only way to generate a frustrated Hamiltonian. For instance, structural glasses do not have intrinsic disorder and frustration can emerge directly from the dynamics. Although the ground state of a glass is the solid crystalline phase a new type of phase transition can be induced by the existence a very large number of metastable states.

Note that the main difference between glassy systems and usual ordered systems relies on the frustrated character of the Hamiltonian which induces a very slow relaxation towards equilibrium at low temperatures. In other systems (for instance ferromagnets) the relaxation to equilibrium is slow in the vicinity of the critical point T_c but it can be approached, always being in equilibrium, not only from above T_c but also from below T_c. In glassy systems equilibrium is impossible to achieve (for large systems) below the glass transition and only can be explored coming from high temperatures in the disordered phase.

To start any research in glassy systems it is convenient to understand as much as possible the equilibrium properties. But sometimes it is difficult to claim that the system has reached full thermal equilibrium. In a general situation it can be difficult to assure that the system has jumped over all intermediate metastable configurations and reached a stationary state where only the low lying free energy states are explored. Note that thermalization is required to investigate the equilibrium properties of the system and, in particular, to identify thermodynamic singularities. Unfortunately, to reach full thermalization is a very difficult problem in numerical simulations. In fact, if we take a system large enough and the thermalization time (i.e. the time spent before starting to compute thermodynamic observables) is not large enough then quite probably the system will not be thermalized. Consequently we cannot analyze data with the conventional predictions used for equilibrium systems (for instance, scaling laws based on renormalization group methods).

If we want to reach equilibrium for a finite system we need a thermal noise strong enough for the system to overcome the different energy barriers which can lead the system to the stationary state. This can be achieved in two different ways. We can study small systems (note that usually energy barriers grow with system size) or otherwise we study (for large sizes) high temperatures. How far we are able to go out of these limiting cases is largely unclear.

In this lectures, we will center our discussion on Monte Carlo methods for disordered systems like spin glasses for which there has been a large amount of numerical work in the last decade. We have chosen spin glasses also for reasons of simplicity. Quite probably spin glasses are the most simple glassy systems where questions like the existence or not of a phase transition can still be answered. Also these are systems in which a large quantity of notions and tools have been borrowed from theory (in particular, mean-field theory) and where numerical methods can also be checked. Nevertheless the concepts and tools described in these lectures are not restricted to spin glasses and can be also used for a large variety of systems. Furthermore, we will concentrate our study on Monte Carlo methods which can be applied to nearly any system. There are other powerful numerical methods like ground-state calculations or transfer matrix calculations. Because they are of little aid to investigate large dimensional systems (they are indeed very useful for low dimensional systems) we will not treat them here.

Our presentation will start in section 2 with a general description of the Monte Carlo method. Then we will introduce the order parameter for spin glasses and discuss the structure of mean-field theory. After discussing some of the open problems in spin-glasses (where numerical simulations can be very helpful) we discuss thermalization techniques as well as the different approaches commonly used to analyze the critical point. Section 3 is devoted to more sophisticated Monte Carlo methods specially suited to reach equilibrium in a more efficient way. There we will discuss simulated annealing, simulated tempering and parallel tempering.

2 Basic tools for glassy systems

We have already said that at low temperatures the relaxation time in spin glasses grows very rapidly due to the presence of a large number of states separated by large energy barriers. The disordered character of spin glasses reveals that there is no macroscopic long range order at low temperatures, i.e. no magnetization. But still it is worth to ask if there is a thermodynamic phase transition. Indeed spin glasses do have a phase transition but the order parameter associated with the transition is not the magnetization but a new type of order parameter (the Edwards-Anderson order parameter). In next subsections we will deal with the following question, how to numerically observe a thermodynamic phase transition in spin glasses? This implies to numerically measure the order parameter. Even if we will always refer to disordered spin glasses our discussion has a quite general character and can be certainly applied to other families of systems (disordered or not).

2.1 The Monte Carlo method

Suppose we deal with a Hamiltonian system described by the following set of variables or fields σ_i ($1 \leq i \leq N$) which can be discrete or continuous. The Hamiltonian of the system gives the energy of any configuration $\{\sigma_i\}$ via the relation $E = \mathcal{H}(\{\sigma\})$.

The basic idea behind the Monte Carlo method [3] is that Gibbs averages can be substituted by temporal averages of a Markov process if transition probabilities among different configurations satisfy detailed balance. Consequently, the Monte Carlo method has an inherent dynamics such that temporal averages directly yield the equilibrium expectation values. Note that this does not mean that Monte Carlo dynamics is a real time dynamics. To define such a Monte Carlo dynamics we need to specify the Monte Carlo step. There is a complete freedom to choose which is the best move. The only requirement for the set of moves is that the system is ergodic, i.e. all configurations of the finite system need to be visited in a finite time. The Monte Carlo move is specified by the following rule,

$$\sigma_i \to \sigma_i' = \sigma_i + \delta_i \tag{1}$$

If the σ_i are continuous variables so are the δ_i. But if the σ_i are discrete variables then the δ_i will be also discrete (for instance if the spins σ_i can take the values + or - 1 then δ_i is given by $\delta_i = -2\sigma_i$). In this last case the proposed move is the inversion of a given spin. In general the move can be local (changing a small set of variables) or global (changing a large number of them). As we will see, the only requirement for the move is that the change in energy $\Delta E = \mathcal{H}(\{\sigma'\}) - \mathcal{H}(\{\sigma\})$ is finite. If $\sigma(t) = \sigma$ and the proposed move (1) is accepted then $\sigma(t+1) = \sigma'$

Consider the master equation for any dynamical process,

$$\frac{\partial P(\{\sigma\},t)}{\partial t} = \sum_{\sigma'} W(\sigma' \to \sigma) P(\{\sigma'\},t) - P(\{\sigma\},t) \sum_{\sigma'} W(\sigma \to \sigma') \tag{2}$$

where $P(\sigma,t)$ is the probability that the system is in the configuration $\{\sigma\}$ at time t and $W(\sigma' \to \sigma)$ is the transition probability to go from $\{\sigma'\}$ to $\{\sigma\}$. A sufficient condition for stationarity (i.e. the $P(\{\sigma\},t)$ does not depend on time) is that detailed balance holds,

$$W(\sigma' \to \sigma) P(\{\sigma'\},t) = P(\{\sigma\},t) W(\sigma \to \sigma') \tag{3}$$

for any pair of configurations (σ, σ'). The Boltzmann equilibrium distribution is given by,

$$P(\{\sigma'\}) = \frac{\exp(-\beta\mathcal{H}(\sigma))}{Z} \tag{4}$$

where $Z = \sum_\sigma \exp(-\beta\mathcal{H}(\sigma))$ is the partition-function. In order that time averages over the Monte Carlo dynamics (in the stationary state) coincide with equilibrium averages the following condition needs to be satisfied,

$$\frac{W(\sigma' \to \sigma)}{W(\sigma \to \sigma')} = \exp(\beta\Delta E) \tag{5}$$

where $\Delta E = \mathcal{H}(\{\sigma'\}) - \mathcal{H}(\{\sigma\})$. Note that ΔE needs to be finite in order that the ratio of probabilities to be also finite. Two types of algorithms are commonly used in Monte Carlo simulations, the Metropolis algorithm

$$W(\sigma \to \sigma') = min(1, \exp(-\beta\Delta E)) \tag{6}$$

and the heat-bath algorithm

$$W(\sigma \to \sigma') = \frac{1}{1 + \exp(\beta\Delta E))} \tag{7}$$

Concerning glassy systems the performance of both algorithms is quite similar and they do not yield much different results.

There is one relevant point concerning the general performance of the Monte Carlo method. It can be generally shown that if the system is ergodic then the Monte Carlo dynamics asymptotically reaches the Boltzmann distribution. Certainly this does not happens at zero temperature (for finite sizes) or systems (in the thermodynamic limit) in a broken symmetry phase. Because we will only deal with finite sizes we expect that Monte Carlo dynamics will eventually reach equilibrium although the times needed for that can be extremely large.

2.2 Spin-glass models

As an example of glassy systems we are now interested in studying spin glasses [2]. These are systems where frustration is a direct consequence of the quenched disorder. Spin glasses appear in nature as a host material (metallic or insulator) doped with magnetic impurities. The essential idea is that the interaction between the magnetic impurities can be ferromagnetic or antiferromagnetic depending on the distance between the spins. The simplest model for spin glasses was proposed a long time ago by Edwards and Anderson [4]. In this model spins occupy all sites of a finite dimensional lattice and interact with disordered but quenched (i.e. unchanged in time) couplings which can take positive and negative values. The Edwards-Anderson model is described by a Hamiltonian,

$$\mathcal{H} = -\sum_{(i,j)} J_{ij}\sigma_i\sigma_j \tag{8}$$

where the J_{ij} are symmetric ($J_{i,j} = J_{j,i}$) and taken from a distribution $P(J_{ij})$. For simplicity we will consider here the case where $P(J_{ij}) = P(-J_{ij})$ (average zero coupling) and Ising spins $\sigma_i = \pm 1$. It is common to consider a Gaussian or binary distribution of couplings $P(J_{ij})$. In the former case

$$P(J_{ij}) = (2\pi\Delta^2)^{-1/2} \exp(-J_{ij}^2/(2\Delta^2)) \tag{9}$$

while in the later case,

$$P(J_{ij}) = \frac{1}{2}(\delta(J_{ij} - J_0) + \delta(J_{ij} + J_0)) \tag{10}$$

It is also common that the interaction in the Hamiltonian eq.(8) is between nearest-neighbor spins only (although more complicated interactions can be devised, for instance, next-nearest neighbors, plaquettes in the lattice, ...). A particular case of the Edwards-Anderson model is the mean-field limit where $D \to \infty$. This limit converges to the well-known SK model introduced in 1975 by Sherrington and Kirkpatrick [5]. In the SK model all spins interact one to each other and can be exactly solved.

In the following sections we will carefully analyze the SK model as well as the Edwards-Anderson model in $D = 4$ with binary couplings ((10) with $J_0 = 1$). These models will be the laboratory to check our numerical algorithms.

2.3 Introducing replicas

Now we face the problem (and this is something specific to disordered systems) that some kind of disorder average is needed. Usually extensive quantities (like energy, entropy, specific heat, magnetic susceptibility) are self-averaging. While intensive quantities like the order parameter q in eq.(13) depend on the disorder distribution.

In general, one would expect that indications of a phase transition could be obtained from extensive quantities like the specific heat or the magnetic susceptibility,

$$c = \frac{\beta^2}{N}\overline{(< H^2 > - < H >^2)} \tag{11}$$

$$\chi = \frac{\beta}{N}\overline{(< M^2 > - < M >^2)} \tag{12}$$

where $M = \sum_i \sigma_i$ is the total magnetization and H the total energy. Unfortunately these quantities are not very useful (compared to the case when ordered systems are studied) to determine if there is a phase transition or not. The reason is that quite generally they do not show any singularity at the glass transition. For instance, in spin glasses, the phase transition is continuous but only high order derivatives of the free energy are discontinuous.

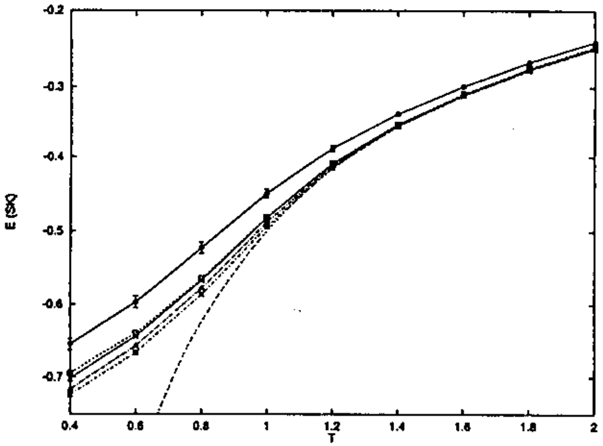

Figure 1: Energy of the SK model. From top to bottom $N = 32, 64, 128, 256, 512$. Data has been averaged over 50 samples. The dashed line is the high temperature behavior $E = -1/(2T)$.

So, for instance, the specific heat does not show any singularity like a jump or a divergence (note that the specific heat is the second derivative of the free energy).

In figures 1, 2 and 3 we show the energy, specific heat and magnetic susceptibility in the SK model versus temperature. Note that there is no singularity in the specific heat but a cusp. Figure 4 shows the specific heat for the 4D Ising spin glass model. Also in this case no singularities are observed in the specific heat.

Up to now we have discussed the interest of measuring thermodynamic extensive quantities. But we still need to define an appropriate order parameter. What is the correct order parameter for spin glasses? Edwards and Anderson [4], within a mean-field theory approach, showed that at low temperatures the spins freeze pointing along random directions. In the low temperature phase spatial correlations between spins are therefore negligible but temporal correlations are very important. This ordered phase corresponds to a new thermodynamic phase very different from usual ordered phases in normal systems. The order parameter which correctly describes such a transition is given by,

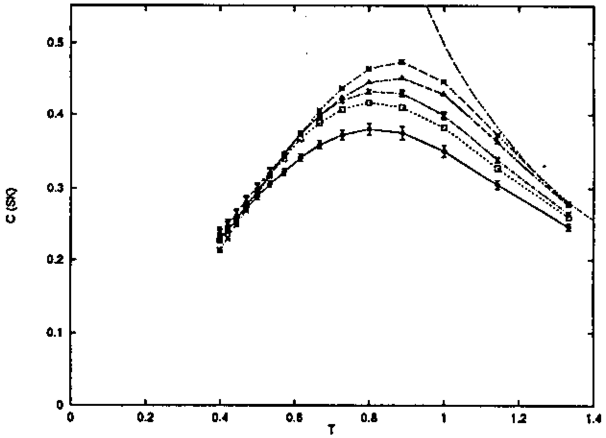

Figure 2: Specific heat of the SK model eq.(11). From bottom to top $N = 32, 64, 128, 256, 512$. Data has been averaged over 50 samples. The dashed line is the high temperature behavior $C = 1/(2T^2)$.

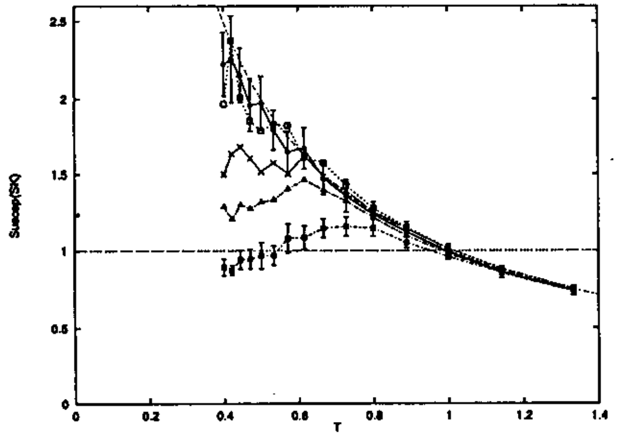

Figure 3: Magnetic susceptibility of the SK model eq.(12). From top to bottom $N = 32, 64, 128, 256, 512$. Data has been averaged over 50 samples. The horizontal dashed line is the low temperature behavior $\chi = 1$ valid for $T \leq T_c = 1$ while $\chi = 1/T$ for $T > T_c$.

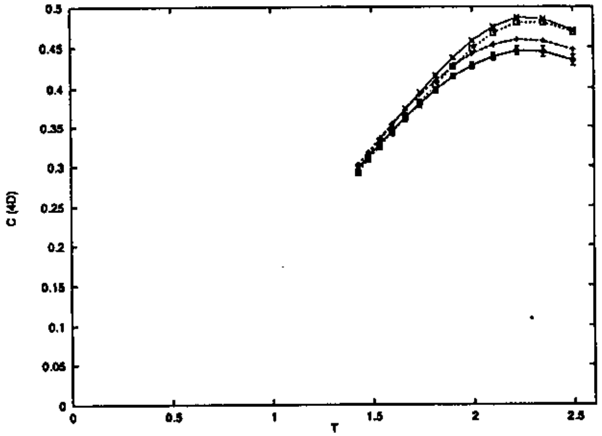

Figure 4: Specific heat of the 4D model eq.(11). From bottom to top $L = 3, 4, 5, 6$. Data has been averaged over 50 samples. At zero temperature the specific heat vanishes.

$$q = \frac{1}{N}\sum_i \overline{< \sigma_i >^2} \tag{13}$$

where $\overline{(..)}$ and $< .. >$ are disorder and Boltzmann-Gibbs averages respectively. In the high temperature (disordered) phase the spins can take any value and $q = 0$. In the cold phase instead, the spins freeze in random directions and $< \sigma_i >^2$ is finite. The value of q is a measure of the how frozen the spins are in the equilibrium state. Note that $< \sigma_i >$ can take any positive or negative finite value (between -1 and 1) . Consequently in the spin glass phase there is no macroscopic magnetization (i.e. $\sum_i < \sigma_i > = 0$). Now, the average $< \sigma_i >^2$ can be written as $< \sigma_i \tau_i >$ where the Boltzmann-Gibbs average is taken over the set of configurations (σ, τ) with Hamiltonian $\mathcal{H} = H(\sigma) + H(\tau)$. This last Hamiltonian is the sum of two Hamiltonians describing two identical systems (we will call them replicas). The Hamiltonians corresponding to different replicas have the same realization of quenched disorder.

The spin-glass order parameter is generally described by the two replica overlap

$$q = \frac{1}{N}\sum_{i=1}^{N} \sigma_i \tau_i \tag{14}$$

The get more information about all the possible values of the overlap q it is convenient to define the order parameter distribution,

$$P_J(q) = < \delta(q - q^*) > \qquad q^* = \frac{1}{N}\sum_i \sigma_i \tau_i \tag{15}$$

While the extensive quantities like the energy or the entropy are self-averaging this is not true for the order parameter. For this reason we have kept in the definition eq.(15) the subindex J in the $P(q)$. The moments of the distribution $P(q)$ give a lot of information to locate a possible phase transition. Here we will mainly concentrate our analysis to spin-glass models with a Hamiltonian with time reversal symmetry, i.e. $H(\sigma) = H(-\sigma)$. This is not true, for instance, in spin glasses in the presence of a magnetic field. When the Hamiltonian is time reversal symmetric then all odd powers of the order parameter q vanish, i.e. $\int_{-1}^{1} q^{2k+1} P(q) dq = 0$ for any $k \geq 0$. The even moments of the $P(q)$ do not vanish and, as we will see later, yield information about the phase transition. In figure 5 we show the expectation value $< q^2 >$ for the SK model. Note that below $T_c = 1$ the value of $< q^2 >$ becomes nearly finite-size independent while above T_c it decreases to zero like $1/N$ signaling the existence of a spin-glass phase transition.

The reason why the order parameter q is so important in spin glasses (and also in other glassy systems, disordered or not) lies in its physical meaning [6]. It tells how many equilibrium states are in the system. In fact, the partition function for a statistical system is given by

$$Z = \sum_\sigma \exp(-\beta H(\sigma)) \tag{16}$$

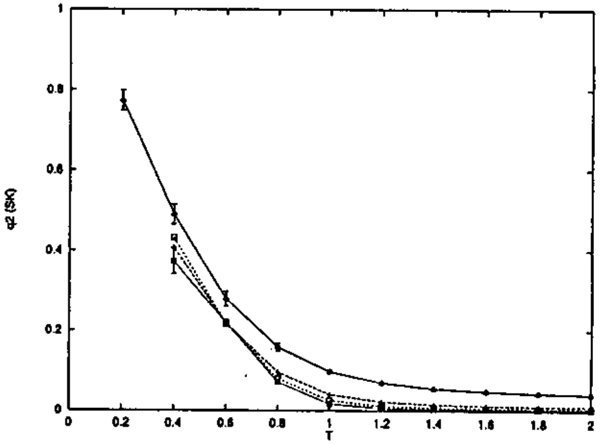

Figure 5: Spin-glass order parameter $< q^2 >$ in the SK model. From top to bottom $N = 32, 128, 256, 512$. Data has been averaged over 50 samples.

Following mean-field theory, let us assume that the phase space splits into different states α (also called ergodic components or phases). Each state comprises a set of configurations such that correlation functions restricted to configurations within that state decay to zero at very large distances. The partition function can then be rewritten,

$$Z = \sum_{\alpha} \sum_{\sigma \in \alpha} \exp(-\beta H(\sigma)) = \sum_{\alpha} \exp(N\beta f_\alpha) \tag{17}$$

where

$$\beta f_\alpha = \frac{1}{N} \log\Big(\sum_{\sigma\in\alpha} \exp(\beta H(\sigma))\Big) \quad . \tag{18}$$

Now we define the statistical weight of a given state by $\omega_\alpha = \frac{\exp(N\beta f_\alpha)}{Z}$. The weights ω_α corresponding to different states are finite and satisfy $\sum_\alpha \omega_\alpha = 1$. Let us now suppose that states are not exponentially degenerate (i.e. its number does not increase like $\exp(\alpha N)$ with N). Then we can say that all those states α which contribute to the partition function with a finite weight ω_α differ in their free energies (per site) f_α by a quantity smaller than $1/N$. Consequently all equilibrium states have the same intensive free energies f_α (in the $N \to \infty$ limit) but different weights ω_α. This does not exclude the possibility of existence of other states with free energy per site larger than the equilibrium state by a quantity of order N^γ with $\gamma < 1$. These states would have the same free energy but they would be exponentially suppressed (like $\exp(-\lambda N^{(1-\gamma)})$ in the large N limit.

The decomposition of Gibbs averages into pure states implies that the expectation value of any observable O can be written as,

$$< O >= \sum_{\alpha} \omega_\alpha < O >_\alpha \tag{19}$$

where $< .. >_\alpha$ is the Boltzmann-Gibbs average restricted to those configurations belonging to the state α,

$$< O >_\alpha = \frac{\sum_{\sigma\in\alpha} O(\sigma) \exp(-\beta H(\sigma))}{\sum_{\sigma\in\alpha} \exp(-\beta H(\sigma))} \tag{20}$$

The $P(q)$ contains information about this set of equilibrium phases with finite statistical weights. Taking the definition eq.(15) and considering that the Boltzmann-Gibbs statistical average is a linear superposition of averages over ergodic components, i.e $< .. >= \sum_\alpha \omega_\alpha^J < .. >_\alpha$ we obtain,

$$P_J(q) = \sum_{\alpha\beta} \omega_\alpha \omega_\beta \delta(q - q_{\alpha\beta}) \tag{21}$$

with $Nq_{\alpha\beta} = \sum_i < \sigma_i >_\alpha < \sigma_i >_\beta$. Each pair of states α, β contributes to the $P_J(q)$ with a weight $\omega_\alpha\omega_\beta$ if the overlap $q = q_{\alpha\beta}$. A very simple particular case corresponds to disordered or paramagnetic phase where there is only a unique thermodynamic state with zero overlap $q_{\alpha\alpha} = 0$. In this case $P(q) = \delta(q)$. Another simple case corresponds to ferromagnetic systems which stay in two thermodynamic phases. In those cases, in the presence of a time reversal symmetry, a unique state (and its time reversal) contribute to the partition sum. Then $\omega_\alpha = \omega_{-\alpha} = 1/2$ for a single state α ($-\alpha$ means the reversed state of the α , i.e. $\sigma_i^{-\alpha} = -\sigma_i^\alpha$). The $P(q)$ is given by,

$$P(q) = \frac{1}{2}(\delta(q - q_{\alpha\alpha}) + \delta(q + q_{\alpha\alpha})) \tag{22}$$

where $Nq_{\alpha\alpha} = \sum_i < \sigma_i >_\alpha^2$. The $P(q)$ has two peaks corresponding to the two unique ferromagnetic states. In general, for mean-field disordered systems, the $P_J(q)$ is not self-averaging (the validity of this assertion is still discussed in finite D systems) and strongly depends on the set of couplings. Evidence in favor of this result is shown in figure 6 where the $P_J(q)$ for three different realizations of the disorder is shown in case of the SK model. In this case, some kind of disorder average is needed. Numerically then one simulates different realizations of the disorder and averages all different distributions $P_J(q)$. So one has,

$$P(q) = \overline{P_J(q)} \tag{23}$$

Is there any quantity contained in the $P(q)$ which is self-averaging ? Within mean-field theory it can be shown that all moments of the $P(q)$ are not self-averaging and that only the self-overlap $q_{\alpha\alpha}$ is self-averaging. Moreover the overlap $q_{\alpha\alpha}$ does not depend on the state α. The self-overlap is nothing else than the Edwards-Anderson parameter eq.(13) restricted to an equilibrium state,

$$q_{EA} = \frac{1}{N} \sum_i \overline{< \sigma_i >_\alpha^2} \tag{24}$$

Note that the order parameter defined in eq.(13) is given by,

$$q = \frac{1}{N} \sum_i \overline{< \sigma_i >^2} = \int_0^1 qP(q)dq \tag{25}$$

which is different from from q_{EA} (except when there is a single thermodynamic phase or two of them related by spin inversion symmetry). In particular, for mean-field spin glasses it can be shown that the $P(q)$ consists of two delta functions (peaked around the self-averaging value $q_{EA} = q_{\alpha\alpha}$) plus a continuous part between the two singularities,

$$P(q) = P_0(q) + c\delta(q - q_{EA}) \quad q \geq 0 \ ; \qquad P(q) = P(-q) \qquad . \tag{26}$$

Note that the Edwards-Anderson order parameter corresponds to the maximum value of the support of the function $P(q)$ such that $P(q) \neq 0$. Figures 7 and 8 shows the $P(q)$ in the SK model in two different regimes: paramagnetic phase $T > T_c = 1$ and spin-glass phase $T < T_c = 1$. Having discussed the meaning of the order parameter $P(q)$ we can now explain how to investigate the critical behavior.

Before it is convenient to discuss what are the main open problems in spin-glass theory

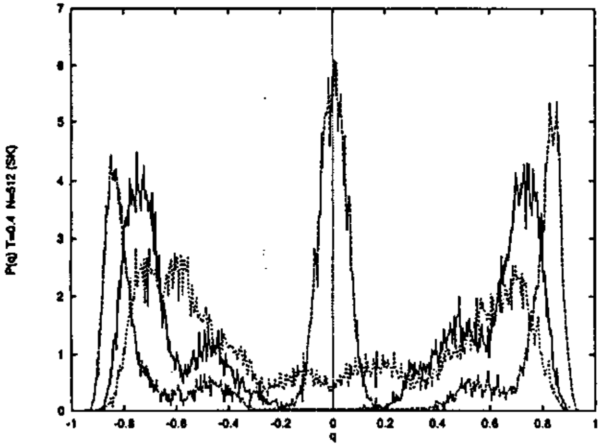

Figure 6: $P_J(q)$ for three different samples in the SK model with $N = 512$. Note that $P_J(q) = P_J(-q)$ is symmetric.

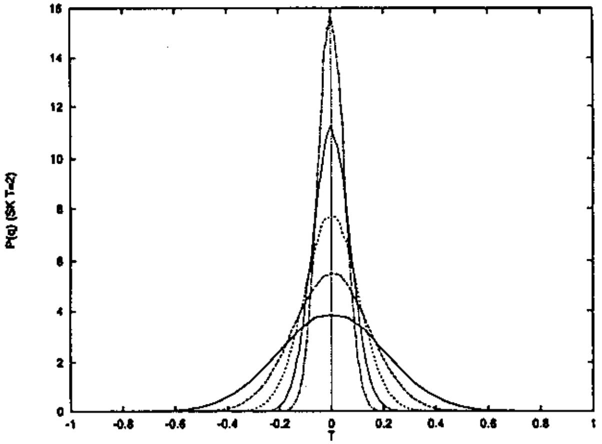

Figure 7: $P(q)$ in the SK model $T = 2$. From bottom to top, $N = 32, 64, 128, 256, 512$. Data has been averaged over 50 samples.

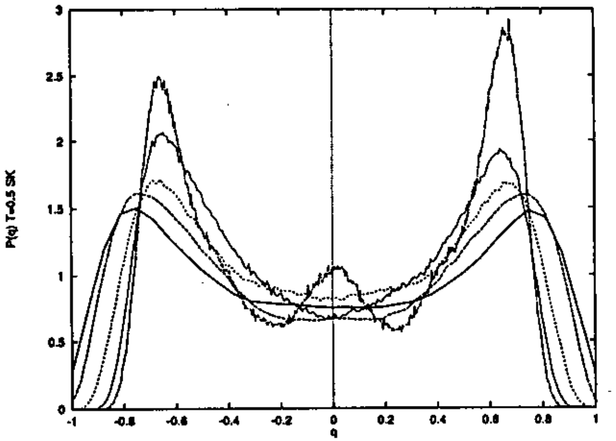

Figure 8: $P(q)$ in the SK model $T = 0.5$. From bottom to top, $N = 32, 64, 128, 256, 512$. Data has been averaged over 50 samples.

2.4 Open problems in spin glasses

The previous discussion has been centered around mean-field spin glasses where the low temperature phase is described by spontaneous replica symmetry breaking. The low temperature phase is described by a large number of pure states or phases. These phases are separated by infinite energy barriers. On the other hand, connected correlation functions within states decay to zero for large distances,

$$< \sigma_i \sigma_j >_\alpha \to < \sigma_i >_\alpha < \sigma_j >_\alpha \quad ; \quad |i-j| \to \infty \quad . \tag{27}$$

Now we would like to know whether mean-field theory, as described by the Parisi replica symmetry breaking solution, is the correct description of the low temperature phase. Also it is of much interest to understand what is the structure of the theory in finite dimensions and whether the mean-field picture is valid in finite dimensions. In what follows we briefly discuss these and other related open questions.

- *Is the Parisi ansatz the correct solution to Mean-Field theory?* It is well known that below T_c the replica symmetric solution found by Sherrington-Kirkpatrick is unstable [7]. In particular, it gives a negative entropy at low temperatures. The Parisi solution was shown to be marginally stable by De Dominicis and Kondor [8] and there are few doubts that it correctly describes the low temperature phase in mean-field spin glasses. On the other hand, numerical simulations are a good test of the theory (see the discussion in [2] as well as figure 8 in previous subsection). From figure 8 it is clear that the $P(q)$ is developing a growing peak close to $q_{max} \simeq 0.63$ (as the theory predicts) if the size of the system grows. On the other hand, the $P(q)$ has a tail extending to low values of q and is not suppressed as the size of the system increases. Certainly it is difficult to claim what is the limit of the $P(q)$ in figure 8 when $N \to \infty$. To do such extrapolation it is necessary to know what are the finite-size corrections to the thermodynamic solution $N \to \infty$. Some finite-size corrections around the Parisi solution have been analytically calculated [9] and they provide a direct check of the validity of the Parisi ansatz. In particular, finite-size corrections to the $P(q)$ have been analytically computed for the right hand side of the peak of the $P(q)$, that is, the region of the $P(q)$ for values of q such that $q > q_{max}$. One finds,

  $$P(q) \sim N^{\frac{1}{3}} \hat{P}(N(q-q_{max})^3) \tag{28}$$

  Numerical simulations show that this scaling behavior nicely reproduces the numerical data [9].

- *What is the structure of the theory in finite dimensions?* Here there are several questions we would like to understand. In particular, what is the lower critical dimension of the theory. A Migdal-Kadanoff approximation yields $D_l = 2.46$ revealing that 3 is quite close to the lower critical dimension. On the other hand, a mean-field calculation shows that $D_l = 2.5$ [10] in quantitative agreement with the previous result.

While the issue of existence or not of a phase transition in $D = 3$ has been a debated subject [16] recent numerical results [13] strongly suggest that there is indeed phase transition in three dimensions.

Another interesting open problem concerns the validity of the mean-field approach in finite dimensions. Is there spontaneous replica symmetry breaking in finite dimensions? An alternative description (droplet model [15]) of the low temperature phase has been proposed in the 80's were spontaneous replica symmetry breaking does not survive in finite dimensions. The essential idea of this approach is that true ergodicity breaking due to the breaking of the replica symmetry is suppressed in finite dimensions because the free energy barriers (which separates the pure phases in mean-field theory) become finite as soon as interactions are short-ranged. This is quite similar to the mechanism by which metastable states in mean field-theory (which have an infinite lifetime) decay in a finite time in short-range systems.

To answer this question it would be relevant to understand the shape (in the thermodynamic limit) of the $P(q)$ in finite dimensions. There have been extensive numerical works on this subject, in particular for D=4 (a dimension far enough from D_l such that there is clear evidence in favor of a spin-glass transition). Recent numerical simulations in 3D tend to support the mean-field picture for the low temperature phase [11]. In any case, the question is far from being settled, mainly because the structure of the finite D theory is not completely understood [8]. In figure 9 we show the $P(q)$ obtained in $D = 4$ for several sizes. Note that figure 9 is quite similar to figure 8. One would be tempted to conclude that the structure of mean-field theory is preserved in finite dimensions. But it is dangerous to make such a conclusion since the nature of the finite size corrections (necessary to reach definite assessments about the thermodynamic limit) is not known.

In this context it would be also convenient to understand whether a phase transition in a field does or does not exist . This is quite relevant since a phase transition with spontaneous replica symmetry breaking should exist also in the presence of a field. On the contrary, if the system is similar to a disordered ferromagnet, like the droplet model predicts, this transition would disappear and only a dynamical crossover transition line would be left. This problem still remains open and no conclusive evidence in favor or against this transition has been found (for recent results see [21, 12]).

2.5 Thermalization criteria

Up to now we have discussed the Monte Carlo technique, the family of models we are interested in as well as the quantities it would be worth to look at, in particular the order parameter $P(q)$. But, as we have already stressed in the introduction, one of the big problems with numerical simulations of frustrated systems is the large amount of computer time needed to reach thermal equilibrium. If we are looking for singularities which can

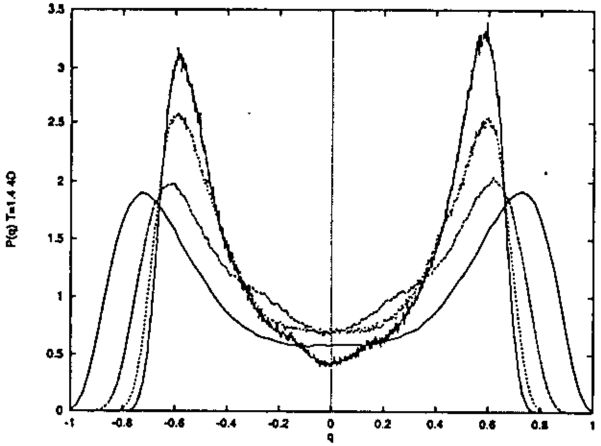

Figure 9: $P(q)$ in the 4D model $T = 1.4$. From bottom to top, $L = 3, 4, 5, 6$. Data has been averaged over 50 samples.

reveal the existence of a phase transition, then it is certainly crucial to reach thermal equilibrium in numerical simulations. In fact, non equilibrium effects can smear or even make disappear any trace of thermodynamic singularity. This is particularly true for instance in real glasses. In those systems any trace of an equilibrium singularity is smeared as soon as the system goes off-equilibrium and, for instance, experimental evidence for a divergent correlation length still has not been established.

Now, what are the most common criteria used to know whether finite systems have reached thermal equilibrium? There is not a unique criteria and here we will consider three of the most important which have been proposed in the literature.

- One of the best criteria for thermalization was proposed initially in the middle 80's by Bhatt and Young [14]. In this case one makes two runs evolve independently for a time t_0 starting from different initial conditions. Then one measures the two replica overlap,

$$q_{\sigma\tau}(t) = \frac{1}{Nt}\sum_{t'=t}^{2t}\sum_i \sigma_i(t')\tau_i(t') \tag{29}$$

  This overlap is equal to 0 for small values of t (because the replicas are initially uncorrelated) and grows with time t reaching the equilibrium value q_{eq} after the equilibration time t_{eq}.

  On the other hand one can make the replica σ evolve up to a time t, store the values of $\sigma_i(t)$ from time t up to time $2t$ and then compute the autocorrelation overlap,

$$Q_{\sigma\tau}(t) = \frac{1}{Nt}\sum_{t'=t}^{2t}\sum_i \sigma_i(t')\sigma_i(t'+t) \tag{30}$$

  Now, for small values of t we have that $Q_{\sigma\tau}(t) = 1$ and then decreases with t until it reaches the equilibrium time independent value q_{eq}. Obviously we do not know what the value of q_{eq} is. The criteria for reaching thermal equilibrium is that the two overlaps $Q_{\sigma\tau}(t), q_{\sigma\tau}(t)$ coincide in equilibrium,

$$Q_{\sigma\tau}(t_{eq}) \simeq q_{\sigma\tau}(t_{eq}) \simeq q_{eq} \tag{31}$$

  This method is efficient but requires some work to be implemented. For this reasons, some other methods have been looked for.

- *The Bray and Moore formula [2].* Another method which is useful relies on a well know relation known in mean-field theory which relates the energy to the order parameter,

$$E = -\frac{\beta}{2}(1 - \overline{< q^2 >}) \tag{32}$$

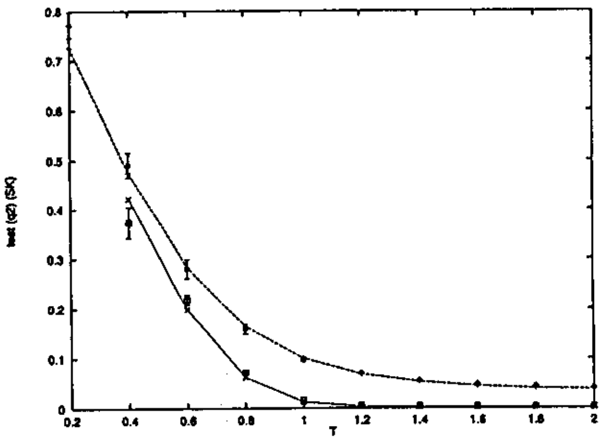

Figure 10: Test of the relation eq.(32) for the SK model. The lines are the values for $< q^2 >$ obtained from the energy and using relation (32). The points are the direct calculation of the second moment. From top to bottom $N = 32, 512$. Data has been averaged over 50 samples.

  where E is the energy. This relation is easily obtained in mean-field theory doing an integration by parts. It is exact in the limit $N \to \infty$ and it has some $1/N$ finite corrections (which can be easily computed). On the other hand, this relation is only valid once all samples have been averaged and not for a given sample in particular. Figure 10 shows the result of this test for the SK model.

  For finite dimensional spin-glass systems a similar formula can be derived in case of a Gaussian distribution of couplings. Then, it can be shown that

$$E = -\beta D(1 - G(1)) \tag{33}$$

  where $G(1) = \overline{< \sigma_x \sigma_{x+e_\mu} >^2}$ is the disorder average of the correlation function between neighboring spins in the lattice.

  This criteria of thermalization is practically useful but not extremely safe because rare samples which are also badly thermalized cannot be distinguished in the averaged data. On the other hand this criteria, for finite range systems, depends on thermalization at short distances as previous equation reveals. This is a serious drawback if growth processes take place during the equilibration procedure.

- *Symmetry of the $P(q)$.* Finally, there is a very simple criteria which relies on the symmetry property ($P(q) = P(-q)$) of the order parameter distribution. Mackenzie and Young showed in 1980 [2] that the time needed to jump over the energy barrier which separates the reflected states $\sigma \to -\sigma$ in the SK models grows much faster than the time needed to jump over all different states (the former one grows approximately like $\exp(aN^{1/2})$ while the latter increases approximately like $\exp(aN^{1/3})$). Then, the time needed to reach a symmetric $P(q)$ should be enough to reach full thermal equilibrium. As we will see later, this is not true when one devises special methods (like tempering methods) which explicitly allow the system to jump over energy barriers.

2.6 Analysis of the critical point

As said in the introduction, a numerical study of spin glasses can only be safely done in the high temperature phase. At low temperatures full equilibration can be reached only with small sizes. In what follows we analyze both possibilities,

2.6.1 Large sizes.

One possible way to analyze glassy systems is to investigate large sizes in the high temperature phase. In this case, thermalization times are not very large and equilibrium properties can be computed.

For large systems, it is convenient to introduce the $q-q$ correlation function which takes into account how spin correlations decay in space,

$$G(x) = \frac{1}{N}\sum_{i=1}^{N}\overline{<q_i q_{i+x}>} \quad ; \quad q_x = \sigma_x \tau_x \tag{34}$$

While the magnetization correlations $\sigma_0\sigma_x$, $\tau_0\tau_x$ decay exponentially fast to zero in the spin-glass phase, the $G(x)$ does not. In fact, at large distances, above the critical point we expect that,

$$G(x) \sim \frac{\exp(-x/\xi)}{x^{D-2+\eta}} \tag{35}$$

where D is the dimension of the lattice. An estimate of the correlation length above the critical point can be obtained under the assumption that η is small compared to $D-2$ and finding an estimate estimate $\xi = log(((x+1)^{D-2}G(x+1))/(x^{D-2}G(x)))$ for large values of x (usually this is done taking values of x up to one third of the lattice size due to the usual boundary conditions $G(x) = G(L-x)$ imposed to the system). For an analysis of this type see [16].

In the simplest scaling scenario, as we approach the critical point the correlation length $\xi(T)$ grows and eventually diverges at the critical temperature T_c,

$$\xi(T) \sim (T-T_c)^{-\nu} \tag{36}$$

The correlation length exponent ν and the anomalous dimensions η determine (via scaling relations) the rest of the exponents. In particular, when the correlation length diverges also does the spin-glass susceptibility defined by,

$$\chi_{SG} = \sum_x G(x) = N\overline{<q^2>} \sim (T-T_c)^{-\gamma} \tag{37}$$

The critical exponent γ for the spin-glass susceptibility can be written in terms of the exponents ν and η following standard manipulations. In fact, using definitions eq.(37,35) we have,

$$\chi_{SG} = \int d^D x G(x) \sim \int_0^\infty d^D x \frac{\exp(-x/\xi)}{x^{D-2+\eta}} \sim \xi^D \xi^{2-D-\eta} \int_0^\infty \frac{\exp(-y)}{y^{D-2+\eta}} \sim \xi^{2-\eta} \tag{38}$$

Using relation(36) we obtain $\chi_{SG} \sim (T-T_c)^{-\nu(2-\eta)}$. This yields the critical exponents relation $\gamma = (2-\eta)\nu$. On the other hand, the critical exponent β for the Edwards-Anderson parameter q (an in general, for any finite moment of the order parameter function $P(q)$) can be obtained using the definition (37) with the relation $q \sim |T-T_c|^\beta$ (valid only below the critical point). The following chain of relations holds,

$$(T-T_c)^{-\gamma} \sim \chi_{SG} = N\overline{<q^2>} \sim \xi^D (T-T_c)^{2\beta} \tag{39}$$

which yields the scaling relation,

$$\frac{\beta}{\nu} = \frac{D-2+\eta}{2} \tag{40}$$

Finally, the specific heat exponent can be found from the hyperscaling relation $\alpha = 2 - D\nu$. As we will discuss later the exponent α is negative. Hence no singularity of the specific heat is expected.

2.6.2 Finite-size scaling

Since it is impossible to equilibrate large systems in the cold phase, to get information about the low T equilibrium behavior (i.e. within the glassy phase) it is convenient to study small sizes. This is big large source of information below and above the critical point. Close to the critical point the scaling relations, valid for usual continuous phase transitions, can be used. Much information can be obtained with reasonable numerical effort by studying the following quantities,

- *The Binder parameter.* The Binder parameter or kurtosis gives information about the Gaussianity properties of the order parameter distribution in the critical point. It can be successfully used for ordered systems as well as for spin-glasses. In this last case the only difference relies on the disorder average which can be taken in several ways. It is common to use the following expression for the Binder parameter is used,

  $$g = \frac{1}{2}\left(3 - \frac{\overline{<q^4>}}{(\overline{<q^2>})^2}\right) \tag{41}$$

  The behavior of this quantity is quite illuminating. Above T_c, due to the Gaussianity property of the $P(q)$ in the disordered phase, the g vanishes in the infinite size-limit. While below T_c the g is finite. Above T_c the g decreases when the size increases. While below T_c the g increases as N increases. At the critical point g does not depend on the size. This is not true if sub-dominant corrections to the leading scaling behavior are large. Subdominant corrections to the main scaling behavior are important but they can be always skipped in a preliminary research.

  Because the g is adimensional, it is expected to scale as

  $$g = \hat{g}(L(T - T_c)^{\nu}) \tag{42}$$

  At $T = T_c$ the values of g for different sizes should cross at a finite value $g_c = \lim_{L\to\infty} g(L, T_c)$ which should take a universal value, independent of the disorder distribution (continuous or discrete couplings). Moreover g_c should increase with the dimensionality of the system (at $D = D_l$ the value of g_c should be 1 for continuous couplings with non degenerated ground state). Numerical estimates for g_c are $g_c = 0.3, 0.42, 0.75$ for mean-field, $D = 4$ and $D = 3$ respectively.

  In figures 11 and 12 we show the Binder parameter in the SK model as a function of the temperature for different sizes.

- *Spin-glass susceptibility.* Suppose we have a finite size $N = L^D$. In this case, from the spin-glass susceptibility eq.(38) we have

  $$\chi_{SG} = \int d^D x G(x) \sim \int_0^L d^D x \frac{\exp(-x/\xi)}{x^{D-2+\eta}} \sim \xi^{2-\eta}\hat{\chi}(L/\xi) \tag{43}$$

  Using relation (36) we get,

  $$\chi_{SG} = N\overline{<q^2>} \sim L^{2-\eta}\hat{\chi}(L(T - T_c)^{\nu}) \tag{44}$$

  Figures 13 and 14 show the scaling behavior of the spin-glass susceptibility in the SK and 4D model.

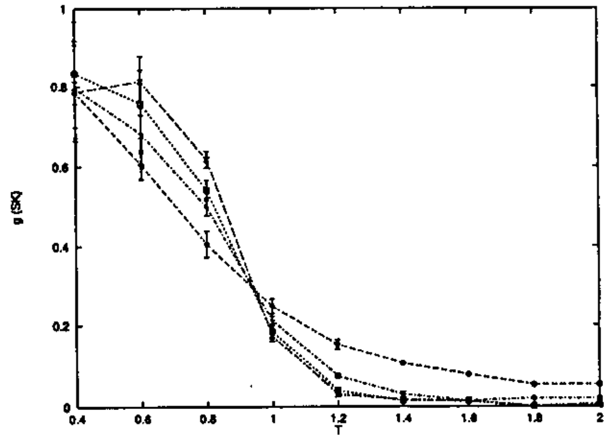

Figure 11: g as a function of T for different sizes (bottom to top in the low T phase $N = 32, 128, 256, 512$). They cross at T in the vicinity of $T_c = 1$. Doing a larger number of samples (here we have done only 50 samples) and larger sizes the crossing point should converge to $T_c = 1$ (see [17]).

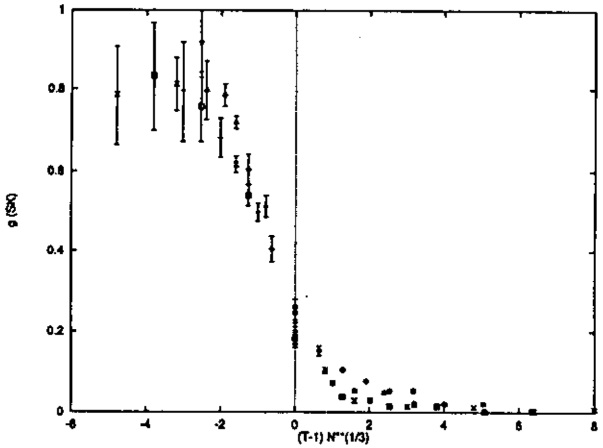

Figure 12: Scaling behavior of the g in the SK model for different sizes ($N = 32, 64, 128, 256, 512$). Because $\nu_{MF} = 1/2$ and $d_u = 6$ the scaling argument is $N(T - T_c)^3$.

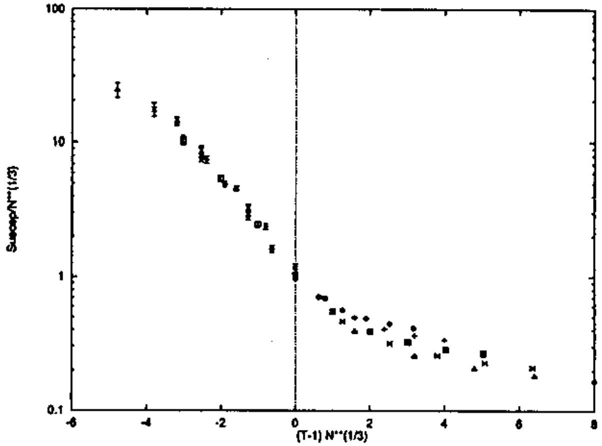

Figure 13: Scaling plot $\chi_{SG}/N^{1/3}$ versus $N^{1/3}(T - T_c)$ in the SK model. The sizes are $N = 32, 64, 128, 256, 512$ and data has been averaged over 50 samples.

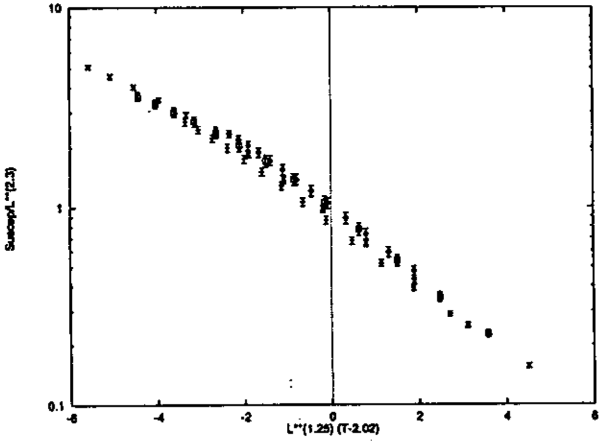

Figure 14: Scaling plot $\chi_{SG}/L^{2-\eta}$ versus $(T-T_c)L^{1/\nu}$ in the 4D model. The sizes are $L=3,4,5,6$ and data has been averaged over 50 samples. The parameters of the scaling are $T_c \simeq 2.02$, $\eta \simeq -0.3$, $\nu \simeq 0.85$

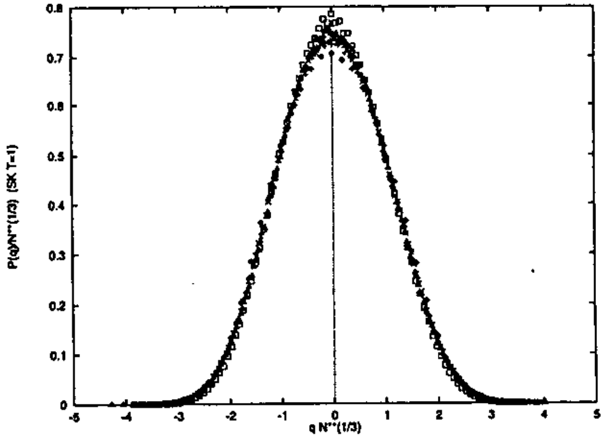

Figure 15: Scaling plot $P(q)/N^{1/3}$ versus Nq^3 in the SK model. The sizes are $N=32,64,128,256,512$ and data has been averaged over 50 samples.

- *Scaling of the* $P(q)$ *[17].* The $P(q)$ scales in the vicinity of T_c. In particular, the leading scaling correction to the $P(q)$ at $T=T_c$ is given by,

$$P(q) \simeq L^{\frac{\beta}{\nu}}\hat{P}(qL^{\frac{\beta}{\nu}}) \tag{45}$$

This result is consequence of the general scaling behavior of all different moments $< q^k >$ which is explicit in the argument of the scaling function $\hat{P}(x)$. The factor $L^{\frac{\beta}{\nu}}$ which multiplies the scaling function $\hat{P}(x)$ assures that the $P(q)$ is a probability distribution normalized to 1. Figure 15 shows the scaled $P(q)$ in the SK model at $T=T_c$.

- *The specific heat exponent.* Because α (the specific heat exponent) is negative there is no singularity or jump in the specific heat but only a broad maximum in the vicinity of T_c. In particular $\alpha=-1$ in mean-field theory, $\alpha \simeq -1.2$ for $D=4$ and $\alpha \simeq -1.6$ for $D=3$. In mean-field theory only the third derivative of the free energy has a jump (or the first derivative of the specific heat) while for $D=3,4$ there is a singularity in the fourth derivative of the free energy (or a divergence in the second derivative on the specific heat).

2.7 Critical or activated slowing down?

One of the major technical problems when approaching the critical point is the fast grow of the relaxation time. This is particularly true for finite dimensional spin glasses where the relaxation time grows so fast that it can be difficult to discern an algebraic divergence ($\tau \sim (T-T_c)^{-\lambda}$) from an activated behavior (for instance, a Vogel-Fulcher law $\tau \sim \exp(a/(T-T_c))$). For standard critical dynamics (valid for continuous phase transitions) we find the following asymptotic behavior in the vicinity of T_c,

$$\tau \sim \xi^z \sim (T-T_c)^{-z\nu} \tag{46}$$

where τ is the decorrelation time. Note that τ is the relaxation time for processes in thermal equilibrium. Although it is a dynamical quantity it has full meaning only in equilibrium. Generalizations to the non equilibrium case (kinetic growth) have been considered and can yield some information regarding non-equilibrium dynamical exponents.

For Ising spin glasses z can take considerably large values ($z = 4$ in mean-field, $z \simeq 5$ in $D = 4$ and $z \simeq 6$ in $D = 3$). Note that relaxation in mean-field theory is slower than for simple diffusive systems where $z = 2$. Because z is large it can be extremely difficult to thermalize large simples close to the critical temperature where thermalization time can grow with the size in the same way as the equilibrium decorrelation time $\tau \sim L^z$. The situation we are discussing here is valid for spin-glasses where in principle we do not expect that activated behavior is present. The situation is much worse in real glasses or spin-glass models with a discontinuous transition where it is suspected that the relaxation time grows with L much faster than a power law. This happens in a very narrow range of temperatures and there is little hope that equilibrium can be reached with moderately large sizes.

The best we can do is to investigate new algorithms which can improve the efficiency of the thermalization schedule. Unfortunately there is no algorithm which can do that for glassy systems. The design of powerful numerical algorithms to thermalize glassy systems is a promising field of research which will grow in the forthcoming years. A short introduction to some of these methods is the subject of the next chapter.

3 Tempering algorithms

The main purpose of this chapter is to consider new algorithms which take into account the critical slowing down as well as the presence of activated processes over energy barriers. A family of new algorithms which deals with this problem has been proposed in the recent years. They go under the name of multicanonical algorithms [19]. There is real hope that the implementation of these methods will help in understanding the low temperature

properties of spin glasses (for other type of glassy systems there are only quite few works and much research needs still to be done).

One of the simplest methods which allows the system to jump over energy barriers is the simulated annealing. Due to its importance for optimization problems we will also describe it here. Closely related to the multicanonical methods are the tempering methods like the simulated and parallel tempering. We will describe them in some detail here. In all these methods the temperature plays the role of a dynamical variable which is changed in real time during the simulation. The main difference between tempering methods and simulated annealing is that in the last case the temperature is changed when equilibrium at a given temperature has been achieved. If the temperature is changed suddenly the system is off-equilibrium and a thermalization process is again required. While in former methods the Monte Carlo dynamics itself decides when the temperature is changed always being in equilibrium. This is achieved by enlarging the space of variables in the Markov process associated to the Monte Carlo dynamics. As we will see tempering methods are a real improve over simulated annealing methods specially when energy barriers need to be overcome. Apparently, in the presence of entropy barriers all methods fail to achieve equilibrium in an efficient way.

3.1 Simulated annealing

This method was developed more than 10 years ago by S. Kirkpatrick and collaborators [18] to improve search-algorithms in combinatorial optimization. Suppose we want to find optimal solutions of a given cost function. The ideal method would be to do an exhaustive search looking for the value of the cost function for all the possible configurations of the system and finally taken the optimal one. This is unpractical because the number of possible configurations or solutions grows very fast with the size of the system. Another possible solution would be to try different solutions within a given set and finally choosing the best solution. Because there is no reason why the optimal one should be include in a random set then quite probably we will never find the optimal one. The idea of simulated annealing is to appeal to statistical mechanics and apply a similar reasoning which explains why the Monte Carlo method finally reaches thermal equilibrium (i.e. the Boltzmann distribution) at finite temperature. An efficient way to go close to the ground state is to allow the system to jump over energy barriers looking for the solutions with the largest basin of attraction. Then, the idea of the method is to start a Monte Carlo simulation at a high temperature and slowly cool down the system. As temperature is lowered the system is able to explore new low energy configurations, hence it reaches the equilibrium more efficiently. The main drawback of this method is that sooner or later the system will remain trapped in a low energy configuration and will not go out from that state for very long times. This is what happens in simulations. While the major part of simulations done in glassy systems during the past have used this method this is still one of the most efficient ones due to its inherent simplicity.

3.2 Simulated tempering

If one continuously cools and heats the system then we expect that the system will converge to the equilibrium much faster than by doing a sudden quench at a given temperature. Then, why do not implement a numerical method in which the system itself performs a continuous cooling and heating procedure? Simulated tempering accomplishes this goal by allowing the system to change the temperature being always in thermal equilibrium. The method was proposed by Marinari and Parisi [20] with the purpose to study disordered systems like random field or spin-glass models. But how the system decides to change the temperature in such a way that it is always in thermal equilibrium ?

Suppose we compute the specific heat at a given temperature,

$$C = \frac{\beta^2}{N}(< H^2 > - < H >^2) \tag{47}$$

The specific heat measures the fluctuations of the energy which (at not very low temperatures) we can suppose to be distributed accordingly to a Gaussian which is approximately centered around the equilibrium value $< H >$. For a finite size the variance of the Gaussian is finite, hence probability energy distributions corresponding to neighboring temperatures will superimpose. Configurations which lie within the superposition region can be considered to belong to the basins of attractions of equilibrium states corresponding to neighboring temperatures. Figure 16 shows the typical qualitative shape of energy histograms at different temperatures.

Let f_β be the free energy per site at temperature $1/\beta$. The partition function at that temperature is given by,

$$Z_\beta = \sum_C \exp(-\beta\mathcal{H}(C)) \sim \exp(-N\beta f_\beta) \tag{48}$$

and the probability of a configuration C is given by,

$$P_\beta(C) = \frac{\exp(-\beta\mathcal{H}(C))}{Z_\beta} \tag{49}$$

Now we propose two types of changes. We can change the configuration C at a fixed temperature $(C,\beta) \to (C',\beta)$ or we can change the temperature for a fixed configuration $(C,\beta) \to (C,\beta')$. In the first case, detailed balance implies

$$\frac{W((C,\beta) \to (C',\beta))}{W((C',\beta) \to (C,\beta))} = \frac{P_\beta(C')}{P_\beta(C)} = \exp(-\beta(\mathcal{H}(C') - \mathcal{H}(C))) \tag{50}$$

while the second move implies,

$$\frac{W((C,\beta) \to (C,\beta'))}{W((C,\beta') \to (C,\beta))} = \frac{P_{\beta'}(C)}{P_\beta(C)} = \exp(-(\beta - \beta')\mathcal{H}(C) - N(\beta f_\beta - \beta' f_{\beta'})) \tag{51}$$

In this last case, using the relation

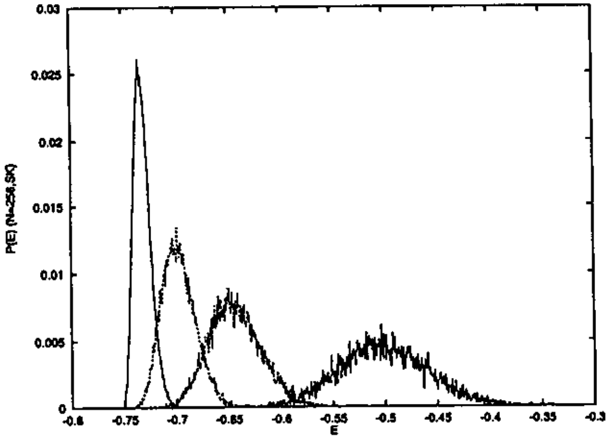

Figure 16: Energy equilibrium histograms in the SK model (one sample $N = 256$) at different temperatures ($T = 1, 2/3, 1/2, 1/3$).

$$\beta F_\beta - \beta' F_{\beta'} \simeq \frac{\partial \beta F_\beta}{\partial \beta}(\beta - \beta') = (\beta - \beta')(\frac{E_\beta + E_{\beta'}}{2}) \qquad (52)$$

we finally obtain,

$$\frac{W((C,\beta) \to (C,\beta'))}{W((C,\beta') \to (C,\beta))} = \exp\Big(-(\beta - \beta')(\mathcal{H}(C) - (\frac{E_\beta + E_{\beta'}}{2}))\Big) \qquad (53)$$

It suffices to estimate the internal energy as a function of the temperature to make run the algorithm. Note that if the free energies at different temperatures are correctly estimated the system spends the same time at each temperature. If the free energies are not correctly estimated the probabilities of occupying the different temperatures is not uniform. Even if detailed balance is then violated in eq.(51) this does not change the stationary probability distribution at a given temperature (i.e. the Boltzmann distribution at a given temperature) but the probabilities $P_\beta = \sum_C P_\beta(C)$ which are not normalized to unity.

The method is obviously better than simulated annealing but it finally fails if the system finds states with energy much lower than the estimated energy E_β. The simulated tempering algorithm has been used to investigate short-ranged spin glasses as well as some optimization problems. While simulated tempering represents an improve over standard simulated annealing procedures still it has some drawbacks. These are the following,

- To make simulated tempering run we need to know what are the free energy differences between neighboring temperatures. We have seen that it suffices to estimate the internal energies of different temperatures. But still some error in the determination of the free energy differences is introduced since the energy is never accurately known.
- The system can be trapped at low temperatures in low energy configurations during the simulation. In this case, much care needs to be taken to check whether and when this happens. Those runs where the system is trapped need to be repeated again until good performance of the algorithm is achieved. In figures 17 and 18 we show two different histories of the same system with the same realization of disorder and the same determination of free energies. One dynamical history (figure 18) remains trapped at low temperatures in some states while the other one (figure 17) does not [21].
- From a technical point of view simulated tempering has another inconvenience. If you take two replicas evolving independently and you want to compute what the overlap is then you need to consider those configurations belonging to different replicas but staying at the same temperature. The simplest way to do that would be to store the configurations of the two replicas and then compute the corresponding overlaps between configurations at equal temperatures. This is impractical because you need to save a lot of configurations and this implies a lot of memory. The best solution is

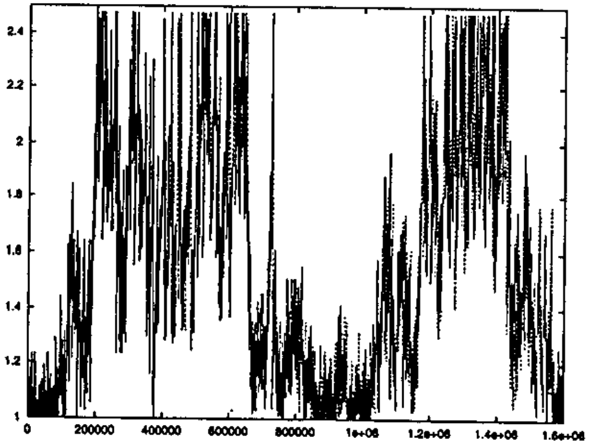

Figure 17: Dynamical history for one sample in a simulated tempering run. We plot the temperature of the system as a function of time in an interval of nearly 2 Million MC steps. The simulated system is the 4D spin glass in a magnetic field, extracted from [21].

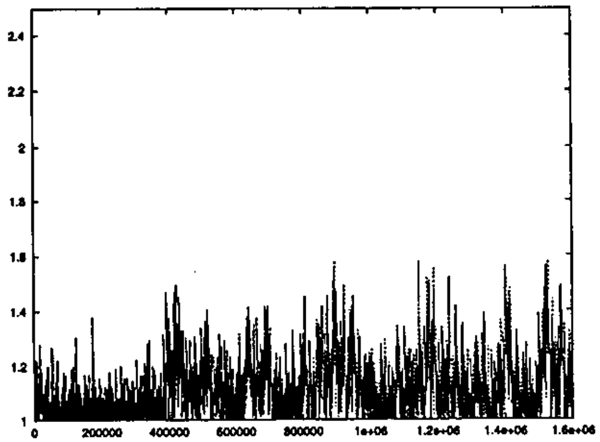

Figure 18: The same as in figure 17 for another dynamical history

then to move simultaneously both replicas when changing the temperature in such a way that they are always at the same temperature. This induces a larger thermalization time (as if the system were at half the real temperature) and consequently slows down very much the equilibration process.

3.3 Parallel tempering

The method of parallel tempering was introduced by Hukushima and Nemoto [22] (they called it replica exchange Monte Carlo method) in the same spirit as the simulated tempering method previously described.

The main difference of both methods is that parallel tempering is much more easy to implement than simulated tempering. In this new method the problems 1) and 3) described in the previous subsection are automatically solved while the second problem is improved (but not completely solved).

In this method we consider M copies of the system each one lying at a different temperature. Similarly to what happens in the simulated tempering both temperatures need to be close enough in such a way that neighboring equilibrium states have an exponentially large number of configurations in common. In this method, each one of the M copies or replicas is specified by a configuration C and a label number (which denotes the temperature β at which the replica stays). Then, at a given time two replicas staying at neighboring temperatures are exchanged. The exchange operation is extremely simple: the labels are exchanged.

Like in the simulated tempering method we propose two types of changes. We can change the configuration C at a fixed temperature $(C_1,\beta) \to (C_2,\beta)$ or we can change two replicas staying at neighboring temperatures $(C_1,\beta_1;C_2,\beta_2) \to (C_1,\beta_2;C_2,\beta_1)$ where β_1 and β_2 are neighboring temperatures. The first type of move is described like in the case of the simulated tempering by the usual transition probability eq.(50) while the second move is specified (for instance, in the Metropolis algorithm) by the following transition probability,

$$W((C_1,\beta_1;C_2,\beta_2) \to (C_1,\beta_2;C_2,\beta_1)) = min(1,\exp((\beta_2-\beta_1)(\mathcal{H}(C_2)-\mathcal{H}(C_1)))) \quad (54)$$

For the algorithm to be efficient the acceptance of changing the temperature needs to be not very large and also not very small. Figure 19 shows the acceptance in exchanging replicas for the SK model. This transition probability satisfies detailed balance and consequently the system reaches equilibrium as expected. Like simulated tempering, this method has been used to study short-range spin glasses and represents a quantitative improve over standard methods.

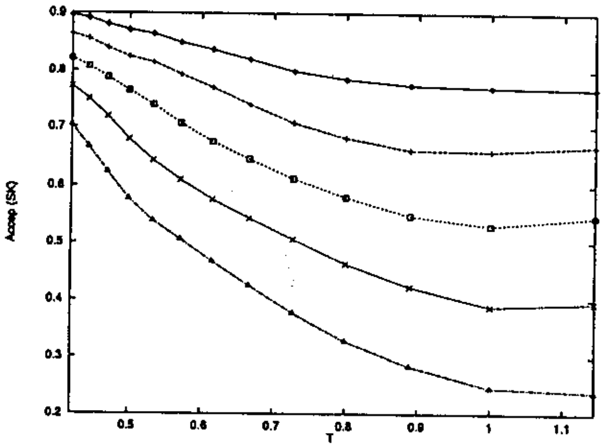

Figure 19: Acceptance of exchanging replicas in the parallel tempering. From top to bottom $N = 32, 64, 128, 256, 512$. If the size of the system increases the acceptance decreases as expected.

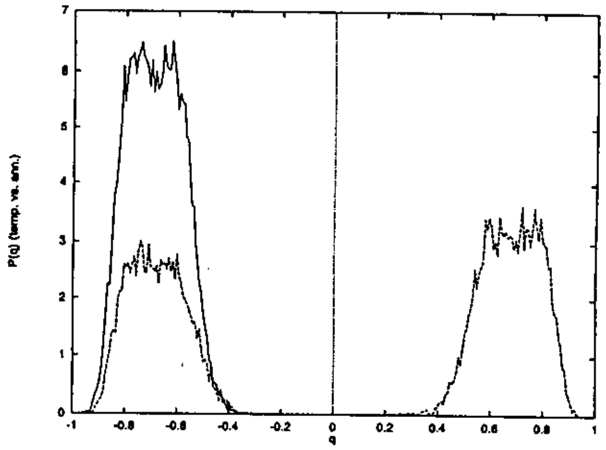

Figure 20: $P(q)$ for a give sample in the SK model ($N = 256$) obtained with the same statistics with the two methods: the parallel tempering (the symmetric curve around $q = 0$) and the simulated annealing (the non symmetric curve). Simulated tempering thermalizes quite effectively over large energy barriers.

3.4 Efficiency of the tempering methods

How much efficient are tempering methods compared to usual simulated annealing (i.e. repeated cooling and heating) procedures? We have already seen that the advantages of the tempering methods (and in particular, of the parallel tempering method) is that the system can change temperature always being in thermal equilibrium. This represents an improve over the standard simulated annealing method where the change of temperature is decided by the cooling schedule which definitely violates detailed balance. If statistics needs to be collected at a new temperature then the system needs to equilibrate again at the new temperature. For the purpose of collecting statistics at different temperatures the tempering methods (and in particular, the parallel tempering) are specially good. There are no doubts on the improved efficiency of the tempering methods to collect statistics.

What happens concerning thermalization? Is the tempering method better to thermalize systems than the standard simulated annealing? Intuitively one expects that tempering

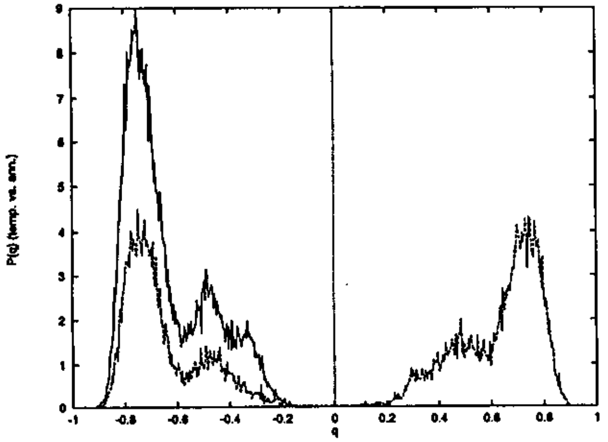

Figure 21: The same as in figure 20 for another sample and $N = 512$

methods should be better because they allow the system to jump over energy barriers reaching new configurations at low temperatures uncorrelated from the initial ones. Then the system should be more effective sampling the phase space. This assertion is correct if energy barriers are involved in the process of equilibration. But if entropy barriers were involved in the equilibration process this would be no longer true (for a recent discussion on that see [23]). Intuitively this can be easily understood. Entropy barriers are insensitive to temperature and the typical time to cross them depends on the ratio of volumes in phase space at higher and lower energies. In the presence of entropy barriers tempering methods would be as ineffective as standard simulated annealing. In figures 20 and 21 we show the $P(q)$ obtained for the SK model obtained with the parallel tempering and the simulated annealing. Both simulations have taken the same total amount of Monte Carlo time. While the $P(q)$ in the tempering method is symmetric the one in the simulated annealing is not. With parallel tempering the system jumps more effectively over energy barriers. In particular, the energy barriers which separates the ergodic components belonging to different time reversal classes have been thermalized with the tempering and not with the simulated annealing.

Still tempering methods are very powerful to numerically investigate glassy systems and quite probably we will see a growing increase of activity in the development of new algorithms in the forthcoming years.

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