Infinite Volume Relaxation in the Sherrington-Kirkpatrick Model

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Abstract

In a recent work [8] a numerical method has been proposed to simulate off-equilibrium zero-temperature parallel dynamics for the SK model without finite size effects. We study the extension of the method to non-zero temperature and sequential dynamics, and analyze more carefully the involved computational problems. We find evidence, in the glassy phase, for an algebraic relaxation of the energy density to its equilibrium value, at least at large enough temperatures, and for an algebraic relaxation of the magnetization to zero at non-zero temperatures, with an exponent directly proportional to the temperature.
1. Introduction

In the last years the study of off-equilibrium dynamics for spin glasses has become of great interest, experimentally, numerically and theoretically (as a subjective and non exhaustive list of references see, e.g., [1, 2, 3]). The analytical studies are based mostly on the dynamic functional integral method of de Dominicis [4] (DFM in the following) by which, in the infinite range limit where a mean field solution is exact, the dynamics can be expressed as a stochastic equation of motion of a single spin with self consistent nucleus of evolution and gaussian noise. In the equilibrium case these equations can be handled imposing time translation invariance and a suitable way of recovering partial validity of the fluctuation dissipation theorem, which is violated in the spin glass phase because of ergodicity breaking. For such an analysis we recall the fundamental work of Sompolinsky and Zippelius on the SK model [5] and recent works on the sSG model with p-spin interaction [6].

In spite of the great effort of the last years, nowadays the analysis of the off-equilibrium dynamics of mean field models has not been developed to the same extension as its equilibrium counterpart. From the numerical point of view the situation is reversed. An initial state for the dynamical evolution is very difficult to be realized at equilibrium, whereas it is easy in the off-equilibrium case: the archetypical off-equilibrium state can be the one in which all the spins of the system point in the same direction, or else the one in which the spins point independently in random directions. The dynamical equations obtained by DFM in the mean field case are single-spin equations at thermodynamical limit: this provides, in principle, a powerful tool to simulate by numerical methods off-equilibrium dynamics without finite-size effects. However, these equations are not suitable for a numerical simulation, as they represent the evolution of continuous spins with continuous time. A few years ago in [7] it has been developed an approach to the (parallel) dynamics of mean field models in the case of Ising spins and discrete times: this approach leads to single-spin equations completely analogous to the ones obtained by DFM in the continuous case. Recently, for the SK model at zero temperature, in [8] an implementation of these single-spin equations, written in the form of stochastic finite-difference equations with independent forcing Gaussian noises, has been presented.

The aim of this paper is to study more carefully the computational problem involved in the implementation, introducing a thermal noise at finite temperature, and discussing the application of the method to sequential dynamics too. We prove that the method is reliable for studying sequential dynamics at every temperature, as far as the relaxation of physical quantities of the SK model is concerned. As a first result, in the simplest experimental situation of an evolution at constant temperature and zero magnetic field, starting from an initial quench from the high-temperature paramagnetic state, we study the relaxation of the energy density of the model, which was ignored in [7, 8], together with the magnetization, in the whole range of temperature covering the glassy phase. We find evidence for an algebraic relaxation of the energy density to its equilibrium value, at least at large enough temperatures, and for an algebraic relaxation of the magnetization to zero at non-zero temperatures, with an exponent directly proportional to the temperature.
This behaviour for the magnetization is well established experimentally on real spin glasses (see, for instance, [14, 15]), but it has never been previously tested numerically for mean field models with sufficient reliability, since so far in all the numerical simulations it has been difficult to take finite-size effects into account (see, for instance, [2]).

The performance of the algorithm, in terms of CPU-time and memory requirements, is not so exceptional to qualify it as the panacea of the dynamical simulations for the SK model. However we believe that it is not a remote possibility to simulate situations directly comparable with the experimental ones [1], which present more delicate schedules of variation of the physical parameters (e.g. temperature and applied magnetic field) and make observable a phenomenology not confined to a simple relaxation of the physical quantities.

The outline of the paper is the following. In section 2 we discuss the generalization of the dynamical equations of [7, 8] to finite temperature, and we justify their use also for a sequential dynamics, in section 3 we enter in the details of implementation and precise the involved computational problems, in section 4 we present the results of our runs.

2. Dynamical equations and physical quantities of interest

The Sherrington-Kirkpatrick model for spin glasses ([9], SK model in the following) is a model for Ising spins, interacting via a disordered mean field Hamiltonian

$$H_J[\sigma] = -\frac{1}{2} \sum_{i \neq j} \sigma_i J_{i,j} \sigma_j$$

(1)

Here the (symmetric) couplings $J_{i,j}$ are Gaussian independent random variables, i.e.

$$J_{i,j} = J_{j,i}, \quad d\mu(J_{i,j}) = \sqrt{\frac{N}{2\pi}} e^{-N J_{i,j}^2 / 2} dJ_{i,j}$$

(2)

($N$ is the size of the sample; the variance of the $J$’s is $1/N$ in order to have finite Hamiltonian density). We denote by $\langle \cdot \rangle$ the thermal average with respect to the Hamiltonian (1) at fixed $J$, and by $\overline{\langle \cdot \rangle}$ the extra average over the couplings with the measure (2).

Our aim is to study a suitable dynamics for this model. The interesting physical quantities will be densities of time-varying extensive quantities. In order to avoid misunderstandings we recall that the couplings $J$ are constant along the dynamical evolution. Typically we shall consider the spin-spin correlation function

$$C(t, t') = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \overline{\langle \sigma_i(t) \sigma_i(t') \rangle}$$

and the magnetization

$$m(t) = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \overline{\langle \sigma_i(t) \rangle}$$
If $\sigma_i(t = 0) = 1$ for each site $i$ it is

$$m(t) = C(t, 0)$$

The energy density is obviously given by

$$e(t) = \lim_{N \to \infty} \frac{1}{N} \langle H_J [\sigma(t)] \rangle$$

We recall now the results of [7, 8]. At zero temperature a parallel dynamics for the model is defined by the equation

$$\sigma_i(t + 1) = \text{sign} \left[ \sum_{j \neq i} J_{i,j} \sigma_j(t) \right] \forall i$$

(3)

Averaging over the $J$'s in the limit $N \to \infty$, from equation (3) in [7, 8] the following stochastic single-spin equation is derived:

$$\sigma(t + 1) = \text{sign}[h(t)]$$

$$h(t) = \sum_{s \leq t} A_{t,s} \eta(s) + \sum_{s < t} K_{t,s} \sigma(s)$$

(4)

where $\eta$ is a temporary uncorrelated normal noise, i.e. the $\eta(s)$'s at every time $s$ are independent random variables, each of which is Gaussian distributed with zero mean and variance one. The nuclei $A$ and $K$ in (4) will be fixed by suitable self-consistency equations (see (5) below).

The equation (4) is equivalent to the (3) as far as mean values of density of extensive quantities are concerned, in a meaning that will be clarified in the following. In principle equation (4) can be solved for each realization of the noise $\eta$, thus giving the time evolution $\sigma(t)$ in function of the noise history $\eta(s)$. We denote by $\langle \ldots \rangle_\eta$ the average over the noise $\eta$. The nuclei $A$ and $K$ are fixed by the self-consistency equations

$$A_{t,t'} = 0 \text{ for } t' > t \text{ , } \sum_{s \leq \min(t,t')} A_{t,s} A_{t',s} = \langle \sigma(t) \sigma(t') \rangle_\eta$$

(5.1)

and

$$K_{t,t'} = 0 \text{ for } t' \geq t \text{ , } \sum_{t' \leq s < t} K_{t,s} A_{s,t'} = \langle \sigma(t) \eta(t') \rangle_\eta$$

(5.2)

Translated in the formalism of the single-spin equation (4) the spin-spin correlation function and the magnetization become

$$C(t, t') = \langle \sigma(t) \sigma(t') \rangle_\eta$$

$$m(t) = \langle \sigma(t) \rangle_\eta$$

(6)

Again, if $\sigma(t = 0) = 1$, it is

$$m(t) = C(t, 0)$$
A very high precision plot of the relaxation of $m(t)$ versus $t$ until $t = 100$ with initial condition $m(0) = 1$, is shown in [8]. The data in [8] can well be fitted with an algebraic relaxation of the type

$$m(t) \sim m_\infty + A t^{-\alpha}$$

and the quoted results for $m_\infty$ and $\alpha$ are

$$m_\infty = 0.184 \pm 0.002 \quad \alpha = 0.474 \pm 0.005$$

The result for $m_\infty$ agrees quite well with what is declared by [7]

$$m_\infty = 0.23 \pm 0.02$$

It is commonly believed that at $T \neq 0$ this relaxation form becomes

$$m(t) \sim C t^{-\delta}$$

with zero remanent magnetization and $\delta \propto T$. We shall come back to this point in section 4.

As far as the energy density is concerned, a direct translation in the formalism of the single-spin equation (4) would result in

$$e(t) = -\frac{1}{2} \langle \sigma(t) h(t) \rangle_\eta$$  \hspace{1cm} (7)$$

but this expression is identically zero. In fact, a peculiar characteristic of the dynamics (4), already pointed out in [7, 8], is that

$$\begin{align*}
\langle \sigma(t) \sigma(t') \rangle_\eta &= 0 & \text{if } |t - t'| \text{ is odd} \\
\langle \sigma(t) \eta(t') \rangle_\eta &= 0 & \text{if } |t - t'| \text{ is even} 
\end{align*}$$  \hspace{1cm} (8)$$

and it is easy to see that it implies that the form (7) for the energy density gives $e(t) \equiv 0$. In [7, 8] this inconsistency problem does not arise, because the energy density is ignored at all. We shall see soon that the correct expression is

$$e(t) = -\frac{1}{2} \langle \sigma(t) h(t - 1) \rangle_\eta = -\frac{1}{2} \langle \sigma(t - 1) h(t) \rangle_\eta$$  \hspace{1cm} (9)$$

The source of the problems is the fact that the parallel dynamics (3) is not a correct thermal dynamics, even at $T = 0$. In other words it does not drive the system to its thermal equilibrium, as does its sequential counterpart. The dynamics (3) is of practical interest for models of attractor neural networks, but at a first sight is not such for the SK model, considered as a thermodynamical model. Keeping this in mind it is not difficult to accept the fact that the energy density is identically constant in time, i.e. the dynamics is not dissipative. We can get rid of this unpleasant situation by considering a slightly different model, the Little model [10], for which a parallel dynamics too is a good thermal dynamics. We shall see soon that the dynamics defined by (3), which is a parallel (i.e. a bad) dynamics for the SK model, is instead a good thermal dynamics for the Little
model. In order to define the model we double the phase space considering, instead of $N$ Ising spins $\{\sigma_i\}_i$, $2N$ spins in two sets $\{\sigma_i\}_i$ and $\{\tau_i\}_i$, for $i = 1..N$, interacting via the disordered mean field Hamiltonian

$$H_J[\sigma, \tau] = -\sum_{i \neq j} \sigma_i J_{i,j} \tau_j$$

(10)

Again, the (symmetric) couplings $J$ are Gaussian random variables with the same measure (2). Now, it is easy to see that the (semi)parallel dynamics

$$\begin{align*}
\sigma_i(t+1) &= \text{sign}\left[\sum_{j \neq i} J_{i,j} \tau_j(t)\right], & \tau_i(t+1) &= \tau_i(t) \quad \forall i \\
\tau_i(t+2) &= \text{sign}\left[\sum_{j \neq i} \sigma_j(t+1) J_{j,i}\right], & \sigma_i(t+2) &= \sigma_i(t+1) \quad \forall i
\end{align*}$$

(11)

is equivalent to a sequential one, thus providing a good thermal dynamics.

In order to recover equation (3) we change slightly the notation. Starting from $t = 0$, (11) gives $\tau_i(t = 1) = \tau_i(t = 0)$, whereas the value of $\sigma_i(t = 1)$ is not trivial. Then $\sigma_i(t = 2) = \sigma_i(t = 1)$ and $\tau_i(t = 2)$ is not trivial, and so on. In general the value of the $\tau$’s at odd times and the value of the $\sigma$’s at even times is trivial, so these variables are not interesting, as far as the dynamical description of the system is concerned. Now, we rename tout court the remaining $\tau$’s (the ones at even times) simply by $\sigma$. Thus we are left with an unique set of dynamical variables $\sigma_i(t)$, and, rewritten in terms of it, the equation (11) is reduced to the previous (3).

At this point we are left with the following situation: the (formally) parallel dynamics (3) is a good thermal dynamics, at zero temperature, for the Little model. We shall see soon that the introduction of a finite temperature thermal noise does not present any difficulty. However, we must firstly justify why we feel us authorized to study the Little model instead of the SK model. In fact, the Little model in itself is of little physical interest, but it has ben shown [11], both by a replica approach and numerical simulations, that in the limit $N \to \infty$ the static properties of the two models are the same, i.e. their thermodynamical behaviours coincide. In particular, as far as the energy density is concerned, it is

$$e = \lim_{N \to \infty} \frac{1}{N} \langle H_J^{(SK)}[\sigma] \rangle = \frac{1}{2} \lim_{N \to \infty} \frac{1}{N} \langle H_J^{(Little)}[\sigma, \tau] \rangle$$

Now, with our notation, the dependence on time of the Little hamiltonian (10) is

$$H_J^{(Little)}[\sigma(t), \tau(t)] = -\sum_{i \neq j} \sigma_i(t) J_{i,j} \tau_j(t) = -\sum_{i \neq j} \sigma_i(t) J_{i,j} \sigma_j(t - 1)$$

Thus it is easy to see that, in the formalism of the single-spin equation (4), the energy density becomes

$$e_{Little}(t) = -\langle \sigma(t) h(t - 1) \rangle_\eta = -\langle \sigma(t - 1) h(t) \rangle_\eta$$

From this expression, and relation (12) between the energies in the Little and SK models, we recover the previously anticipated equation (9) for the correct form of the energy density.
(“correct” in the sense that we can compare correctly the dynamical results with the static ones for the SK model).

To extend the dynamical equations to finite temperature, it is sufficient to introduce in the equation (3) a temperature dependent local effective field which simulates the thermal agitation. This field, because of the fact that it does not depend on the J’s, is carried out without modifications during the derivation of the single-spin equation (4) starting from the (3). The resulting equation, which generalizes the (4) of [8], is

\[
\sigma(t+1) = \text{sign}[h(t)]
\]

\[
h(t) = \sum_{s \leq t} A_{t,s} \eta(s) + \sum_{s < t} K_{t,s} \sigma(s) - T \cdot \xi(t) \sigma(t-1)
\]  

(13)

where the nuclei A and K will again be fixed by the (5), and \( \eta \) is again a temporary uncorrelated normal noise. The thermal induced noise \( \xi \) is a new temporary uncorrelated noise with law

\[
P(\xi) = \theta(\xi) \cdot 2e^{-2\xi}
\]  

(14.1)

which represents a thermal dynamics of Metropolis type, or

\[
P(\xi) = \frac{1}{2}[1 - \tanh^2(\xi)]
\]  

(14.2)

which represents a thermal dynamics of heat-bath type. Obviously the presence of this second noise forces us to slightly change the notation in the above relations (5), (6) and (9), now denoting with \( \langle . \rangle_{\eta, \xi} \) the average over both noises.

Let us stress the fact that in (13) the thermal field is proportional to \( \sigma(t-1) \) and not to \( \sigma(t) \). This is a consequence of the fact that actually we are studying the dynamics of the Little model and not of the SK model: when we are updating a spin, deciding if we flip it or not, its previous value is actually \( \sigma(t-1) \), whereas \( \sigma(t) \) is only a short-hand notation for \( \tau(t) \). Obviously in the case of the heat-bath dynamics the thermal field can be reduced simply to \( T \cdot \xi(t) \), as in this case there is no need of a previous spin to flip: in fact, the distribution law of the heat-bath noise (14.2) is even in \( \xi \). For generality’s sake we maintain the form (13) for the dynamical equations, whereas for practical use it is better to pursue in each case simplicity in place of generality. In next section we shall see more carefully how to implement a simulation for the single-spin equation (13), and in section 4 we give the results of our runs.

3. Details of implementation and computational problems

To implement a simulation of the stochastic finite-difference equation (13) we follow the main lines of [8]. We generate randomly \( N_T \) different noise trajectories, and we define the average over the noise simply by

\[
\langle \sigma(t)\sigma(t') \rangle_{\eta, \xi} \equiv \frac{1}{N_T} \sum_{i=1}^{N_T} \sigma^{(i)}(t)\sigma^{(i)}(t')
\]
and by analogous expressions for the other interesting quantities. Here \( \sigma^{(i)}(t) \) denotes the evolution of \( \sigma \) in the \( i \)-th noise history. Let us stress that the run-time computation of certain averages is needed for the evolution itself, since the nuclei \( A \) and \( K \) are defined in terms of averages over the noise.

We shall be more explicit in a while, let us before anticipate two comments. Firstly, in the runs which we performed we kept the temperature fixed, and zero magnetic field. Changing \( T \) and \( h \) during the evolution would have been pointless, as our care was mainly devoted to test the reliability of the method.

Secondly, the choice of the initial conditions for the evolution is not straightforward. If in the equation (13) there was not the term \( \sigma(t - 1) \), as it is for \( T = 0 \) or for finite temperature heat-bath dynamics, then we would need only the initial condition at \( t = 0 \), i.e. \( \{\sigma^{(i)}(t = 0)\}_{i=1..N_T} \). In this case, as pointed out in [7], the choice of the initial condition is to a great extent arbitrary. In fact, because of the symmetry of the equation (13) under simultaneous inversion of \( \sigma \) and both noises \( \eta \) and \( \xi \), it is not difficult to see that the average of a product of an even number of fields (\( \sigma \) and/or the noises) does not depend on the initial conditions. The average of a product of an odd number of fields, on the other hand, depends on the initial conditions only through a factor which is simply given by the initial magnetization

\[
\begin{align*}
m(0) = & \frac{1}{N_T} \sum_{i=1}^{N_T} \sigma^{(i)}(t = 0) \\
\end{align*}
\]

From the physical point of view the initial condition for the evolution represents a sudden quench from a high temperature paramagnetic state which is in equilibrium in a field that sets the value of the magnetization.

In the general case the presence in (13) of the term \( \sigma(t - 1) \) forces us to impose two distinct initial conditions: besides \( \{\sigma^{(i)}(t = 0)\}_i \) we need also \( \{\sigma^{(i)}(t = -1)\}_i \). At this point it is not clear at all neither the exact physical meaning of this additional initial condition, nor how to keep \textit{a priori} under control the dependence of the evolution on the initial conditions. However, it is reasonable to argue that the additional initial condition at \( t = -1 \) has no real significance. We have therefore fixed the initial conditions in the way we believe to be the most natural one:

\[
\begin{align*}
\sigma^{(i)}(t = 0) = & 1 \quad \forall i = 1..N_T \\
\sigma^{(i)}(t = -1) = & 1 \quad \forall i = 1..N_T/2 \\
\sigma^{(i)}(t = -1) = & -1 \quad \forall i = N_T/2 + 1..N_T \\
\end{align*}
\]

We have not yet performed any systematic test on the dependence of the evolution on the initial conditions. Let us stress, by the way, that with the choice (15.2) the dynamics preserves the same property of selecting the parity (8) as in the zero temperature case.

We shall now sketch with some details the algorithm used in the simulation. Besides the already introduced notation, we denote respectively with \( S \) and \( X \) the spin-spin and the spin-noise correlation functions, \textit{i.e.} 

\[
S_{t,t'} = \langle \sigma(t)\sigma(t') \rangle_{\eta,\xi} \quad X_{t,t'} = \langle \sigma(t)\eta(t') \rangle_{\eta,\xi}
\]
The main steps are the following:

1.1) fix the values of:
   - type of thermal dynamics (Metropolis or heat-bath)
   - temperature \( T \)
   - number of noise histories \( N_T \)
   - terminal time point of the evolution \( t_{max} \)
   - initial seed of the random generator

1.2) for each history \( i = 1..N_T \), fix the initial conditions for \( \sigma(0) \) and \( \sigma(-1) \) as in (15)

1.3) for each history \( i = 1..N_T \), generate the \( t = 0 \) values of the noises \( \eta(0) \) and \( \xi(0) \) in according, respectively, to a normal law and to the law (14)

1.4) set the \( t = 0 \) values of the nuclei and of the correlation functions, i.e.

\[
S_{00} = 1 \quad A_{00} = 1 \quad X_{00} = 0 \quad K_{00} = 0
\]

1.5) set \( t = 0 \)

2) let \( t \) be the current value of the time step; if \( t \geq t_{max} \) then stop the main execution and go to step 8) (output of results)

3) for each history \( i = 1..N_T \), compute \( \sigma(t + 1) \) in according to the equation (13), by using the nuclei \( A \) and \( K \) already computed in the previous steps

4) compute

\[
S_{t+1,s} \equiv \frac{1}{N_T} \sum_{i=1}^{N_T} \sigma^{(i)}(t + 1)\sigma^{(i)}(s) \quad s < t + 1
\]

\[
\left( S_{s,t+1} = S_{t+1,s} , S_{t+1,t+1} = 1 \right)
\]

and

\[
X_{t+1,s} \equiv \frac{1}{N_T} \sum_{i=1}^{N_T} \sigma^{(i)}(t + 1)\eta^{(i)}(s) \quad s < t + 1
\]

\[
\left( X_{s,t+1} = 0 , X_{t+1,t+1} = 0 \right)
\]

(the correlation functions \( S_{s,s'} \) and \( X_{s,s'} \) for each \( s, s' \leq t \) are already known from the previous steps)

5.1) compute the nucleus \( A_{t+1,s} \) by inverting its defining equation (5.1); this gives the equation

\[
A_{t+1,t'} = \sum_{s \leq t'} S_{t+1,s} A_{t',s}^{-1} \quad t' \leq t
\]

\[
A_{t+1,t+1} = \sqrt{1 - \sum_{t' \leq t} (A_{t+1,t'})^2}
\]

which is well-posed since we already know from the previous steps \( A_{s,s'} \), for each \( s, s' \leq t \)
5.2) compute the nucleus $K_{t+1,s}$ by inverting its defining equation (5.2); this gives the equation

$$
K_{t+1,t'} = \sum_{t' \leq s < t+1} X_{t+1,s} A_{s,t'}^{-1}, \quad t' \leq t
$$

$K_{t+1,t+1} = 0$

which again is well-posed since we already know from the previous steps $A_{s,s'}$, for each $s, s' \leq t$

6) for each history $i = 1..N_T$, generate the values of the noises $\eta(t + 1)$ and $\xi(t + 1)$, in according, respectively, to a normal law and to the law (14)

7) set $t = t + 1$ and go to step 2)

8) output the results of the run:

- $S_{t,t'}$ and $X_{t,t'}$ for $t, t' \leq t_{\text{max}}$
- $m(t) = S_{t,0}$
- $e(t) = -1/2 \sum_{s<t} A_{t-1,s} X_{t,s} + A_{t,s} X_{t-1,s}$

Two technical remarks. Firstly, the random generator for the noises is the usual machine generator $RAN$ of the VAX-VMS systems. It is useful to generate two distinct random series for the two noises $\eta$ and $\xi$. The generator $RAN$ gives an uniform distribution between 0 and 1, but there is no difficulty to obtain, starting from it, the required distributions for $\eta$ and $\xi$. Secondly, in steps 5.1 and 5.2 the computation of $A^{-1}$ is easily made by the Gauss method thanks to the fact that $A$ is a (lower) triangular matrix.

As far as the CPU-time requiring is concerned, we note that the most expensive steps are the 3) and the 4), which cost $O(N_T t)$ multiplications and sums, and the 5)’s, which cost $O(t^2)$. Summing over $t$ until $t = t_{\text{max}}$ we have

$$
CPU \sim c \cdot N_T t_{\text{max}}^2 + c' \cdot t_{\text{max}}^3
$$

Our runs were performed on a DEC-VAX 6000, running VAX Fortran, where for $N_T = 1000$ and $t_{\text{max}} = 200$ the required CPU-time is about 1 minute. Concerning the memory occupation, the matrices $S$, $A$ and $X$ require $O(t_{\text{max}}^2)$ memory, whereas $K$ can be stored in a scratch array of $O(t_{\text{max}})$, since at time step $t$ we need only $\{K_{t,s}\}_{s<t}$. The main memory occupation stems however from the complete $N_T$ histories of $\sigma$ and $\eta$, whereas $\xi$ is needed only at current time step $t$. This gives an occupation of $O(N_T t_{\text{max}})$. In conclusion, reducing the memory occupation as much as possible, we have

$$
Mem/\text{bytes} \sim 5 \cdot N_T t_{\text{max}} + 3 \cdot t_{\text{max}}^2
$$

which gives an occupation of about 1.1 Mbytes for $N_T = 1000$ and $t_{\text{max}} = 200$.

Roughly speaking, the CPU-time sets a limitation for $t_{\text{max}}$, whereas the memory does it for $N_T$. If we want to reach a higher value of $t_{\text{max}}$ we only need to wait more time. At a first glance, the significance of $N_T$ is not so clear. It obviously affects the precision of the computation, but the error due to finite $N_T$ is not a purely statistical one, of the order of $1/\sqrt{N_T}$, because average quantities enter in the evolution itself throughout the nuclei $A$ and $K$. We cannot thus assume a priori that, repeating more times the same run with a low value of $N_T$, we shall obtain a higher precision.
It is therefore necessary to understand, at least empirically, the dependence of
the computation results on $N_T$. This for two reasons: the inherent limitations on a particular
machine force us to keep the value of $N_T$ relatively small ($N_T = 32,000$ at maximum, for
our runs); moreover, even if we would dispose of a bigger machine, we ought to control a
priori the reliability of a computation, in order to be confident of its results. Thanks to
the availability of a Cray, in fact, the authors of [8] could keep $N_T = 1,000,000$. Such
a value appears sufficiently high, although for no a priori reason): we shall come back to
this point in the next section. By the way, though it is not explicitly declared, probably
in [8] a slightly different implementation was used. In fact, $N_T = 1,000,000$ would impose
a memory occupation of about 1 Gbyte, which is enormous even for a Cray. To reduce
the memory occupation one could simply avoid to store in memory the complete $\sigma$ and
$\eta$ histories: one could maintain an array of $O(t_{\text{max}})$ with the initial conditions for $\sigma$ and
the initial seeds of the random generator for $\eta$, and at every time step $t$ one computes, or
generates, ex novo the $\sigma$ and $\eta$ histories until that time, by using the nuclei $A$ and $K$ already
computed and stored in memory. This makes the memory occupation independent on the
value of $N_T$, thus releasing any limitations on it, but increases the CPU-time requirement
by a factor $O(t_{\text{max}})$. On a VAX this would bring to about 25 days the amount of CPU-
time spent in a run with $N_T = 1,000,000$ and $t_{\text{max}} = 100$, but a Cray Y-MP could be
even 100 times faster than a VAX, thus reducing the time to about 6 hours, which is what
declared in [8].

We shall now anticipate what we regard as the main source of damage linked to
low values of $N_T$. Let us consider a given history $\sigma^{(i)}$. At each time step $t$ there is a
probability of spin flip which, in principle, can depend on the whole history $\{\sigma^{(i)}(s)\}_{s \leq t}$. Let us suppose, however, that this probability is even under global spin inversion. In this
case it is easy to see that
\[
\frac{dm}{dt} = -m(t)p(t)
\]
where $p(t)$ is the marginal spin flip probability at time $t$. Now, the probability that none
of the $N_T$ histories will flip at time $t$ is appreciable as soon as $p(t)N_T < 1$. At $T = 0$ it
is easy to see that, if at a certain time $\tilde{t}$ it is $\sigma^{(i)}(\tilde{t} + 1) = \sigma^{(i)}(\tilde{t})$ for each history $i$, then
it is $\sigma^{(i)}(t) \equiv \sigma^{(i)}(\tilde{t})$ for each $t \geq \tilde{t}$ and each history $i$, and the system freezes. At $T \neq 0$,
because of thermal fluctuations, this freezing can never happen, but we believe that a kind
of partial freezing forces the system to behave anomalously. In next section we shall show
such an anomalous behaviour, though we can not prove that this is due to a mechanism
of the type already described. For the time being, let us note that $p(t)$ is a function which
decreases to zero as $t$ goes to infinity, at least if the relaxation of $m(t)$ is slower than
exponential (an algebraic law or a stretched exponential one), as it is commonly believed.
Therefore it becomes $p(t)N_T \sim 1$ as soon as
\[
t \geq t_{\text{crit}}(N_T)
\]
and $t_{\text{crit}}$ is an increasing function of $N_T$. It is appealing to suppose that
\[
m(t) \sim t^{-\alpha}
\]
i.e. the relaxation of $m(t)$ is algebraic to zero, so that $p(t) \sim 1/t$ and

$$t_{\text{crit}}(N_T) \sim N_T$$

(16.1)

Probably there are some additional complications. In fact at $T = 0$, as we anticipated, it is [7, 8]

$$m(t) \sim m_{\infty} + At^{-\alpha}$$

i.e. the algebraic relaxation of $m(t)$ goes to a non-zero value, so that $p(t) \sim 1/t^{1+\alpha}$ and

$$t_{\text{crit}}(N_T) \sim N_T^{1+\alpha} \ll N_T$$

(16.2)

At $T \neq 0$ it is expected a relaxation to zero, but even if a kind of freezing mechanism works, it is not clear how to implement it. We shall see in the next section that, at least qualitatively, the numerical data give some evidence of the presence of a kind of “freezing time” which grows with $N_T$, though it is difficult to distinguish between a situation like the one of equation (16.1), where the freezing time grows quite fast with $N_T$, and the one of (16.2).

4. Numerical results

We made two series of runs. The first one was devoted to analyze the dependence of the results of a run on the value of $N_T$, in the case $T = 0.4$ and thermal dynamics of Metropolis type, while in the second one we measured the relaxation of the magnetization and of the energy density in the whole range of temperatures between 0.1 and 1.5, for both Metropolis and heat-bath dynamics. In both series the maximum time reached was $t_{max} = 200$, and the external magnetic field was kept equal to zero. We tried also to measure the relaxation at $T = 0$, but for the values of $N_T$ we used the system freezes before reaching $t_{max}$.

We discuss firstly the results of the first series. The choice of the Metropolis dynamics has no particular motivation. The value of the temperature has been chosen to be not too high, in order to have relevant effects of the breaking of the replica symmetry (we remember that with our choice of the normalization of the coupling (2) the glassy critical temperature is $T_g = 1$), and not too low, in order to avoid the very slow relaxation and the freezing effects of low temperatures. We made several runs for $N_T$ ranging from 1000 to 32,000. Apart from the systematic error due to $N_T$, which we would investigate, there is a natural statistical error of order $1/\sqrt{N_T}$, thus for each value of $N_T$ we made many independent runs, in order to have comparable statistical errors. More precisely

\[
\begin{array}{c|c|c}
N_T & \text{num. of indep. runs} \\
1000 & 80 \\
2000 & 40 \\
4000 & 20 \\
8000 & 10 \\
16,000 & 10 \\
32,000 & 10 \\
\end{array}
\]
Figure 1. Plot of the relaxation of the energy density $-2e(t)$ for Metropolis dynamics at temperature $T = 0.4$ and zero magnetic field. The horizontal dotted line represents the equilibrium value. Each curve corresponds to a different value of $N_T$, as it is shown in the inset, and it has been obtained by averaging the results of many independent runs, in order to have error bars of comparable magnitude.

In figure 1 we plot the energy density $-2e(t)$ versus $t$ for all the values of $N_T$. The time scale from 0 to 200 was divided in intervals of size proportionally scaled by a fixed factor (we have chosen 1.5 to have about ten intervals in the considered range), then for each run we averaged the data into each interval. In fact, the original data are strongly dependent at nearby times, so the form of the plot at small time scales has no significance. With our choice the reduced points are equally spaced in logarithmic time scale. This choice for the procedure of decimation of the data is due to the fact that we expect an algebraic relaxation, i.e. a linear dependence of $\ln(e - e_\infty)$ on $\ln t$, and such a functional form is invariant under such a transformation, up to an innocent logarithmic translation in the time scale. Finally, we made the arithmetic mean of the different runs, and we kept as error bars for each datum their standard deviation ($1\sigma$).

The horizontal dotted line is plotted as a reference and represents the equilibrium value for the energy density, computed by numerically solving the replica equations for the $SK$ model [12]. From figure 1 we see that at a certain time the plot of $-2e(t)$ starts to grow almost linearly and rapidly exceeds its equilibrium value. This anomalous effect is greatly
reduced by increasing $N_T$. It is useless to show a plot of the magnetization analogous to the one in figure 1, since in this case the various relaxation curves at different values of $N_T$ do not differ sufficiently to make the effect of $N_T$ directly observable. Anyway, if we consider the data at fixed $t$ versus $N_T$, a linear dependence on $1/N_T$ clearly appears. In fact, the data are very well fitted by

$$Y_{N_T}(t) \approx Y_\infty(t) + \frac{A(t)}{N_T}$$  \hspace{1cm} (17)$$

where $Y$ represents indifferently the energy density $-2e$ or the magnetization $m$. The curves $Y_\infty(t)$, i.e. the extrapolations to $N_T = \infty$, will be the subject of the next analysis.

Thanks to the very simple dependence (17) on $N_T$, to obtain a fairly reliable extrapolation of the data $N_T = \infty$, it is sufficient to produce two series of measures at two different values of $N_T$. In the following we shall choose $N_T = 8000$ and 16,000. The factor $A(t)$ in (17) depends roughly linearly on $t$, more precisely:

$$A_{\text{energy}}(t) \sim 0.6t$$
$$A_{\text{magn.}}(t) \sim 0.2t$$

In conclusion, the systematic error due to finite $N_T$, being $O(t/N_T)$, is fairly well manageable: at $N_T$ fixed we can be confident in the results of a run until $t$ remains smaller than a (not too small) fraction of $N_T$. It would be very interesting if we understood why the relaxation of the physical observables presents, for finite $N_T$, such an anomalous behaviour as in (17), particularly evident in figure 1 for the energy density. We believe that the underlying reason is a kind of freezing mechanism as it is sketched at the end of previous section, but we could not identify it.

In figure 2 we show the contour lines of the correlation matrix $S_{t,t'}$ in the plane $t-t'$, for the different values of $N_T$, measured in a randomly chosen run of each set. Obviously at low values of $N_T$ the plots are very noisy, because of the great statistical errors. Apart from this noise, the most evident feature of the plots, which gradually vanishes by increasing $N_T$, is the following. Let us consider the half plane $t > t'$, being the figure symmetric. As soon as $t$ is greater than a certain (not well identifiable) critical time, for each $t'$, $S_{t,t'}$ versus $t$ appears to freeze to a value which is almost constant with $t$. This behaviour is strongly reminiscent of the above mentioned freezing.

The main series of measures was devoted to explore systematically the relaxation curves of the energy density and the magnetization in the whole range of temperatures between $T = 0.1$ and $T = 1.5$. We recall that the glassy transition happens at $T_g = 1$. For each temperature value, and both dynamics (Metropolis or heat-bath) we performed two sets of independent runs at two different values of $N_T$, to extrapolate the data at $N_T = \infty$. More precisely

$$N_T = \begin{cases} 
8000 & \text{num. of indep. runs} = 20 \\
16,000 & 10 
\end{cases}$$

(with the exception of $T = 0.4$ with Metropolis dynamics, where we have already enough data). Now, we have pre-analyzed the data as follows. Firstly, for each run, we performed
\begin{align*}
N_T &= 1000 & N_T &= 2000 & N_T &= 4000 \\
N_T &= 8000 & N_T &= 16,000 & N_T &= 32,000
\end{align*}
on the data the previously described procedure of decimation, to obtain a reduced set of almost-independent time points. Then, for each value of \( N_T \), we averaged the data from the different runs, and the error bars were computed by the mean standard deviation (1\( \sigma \)). Secondly, we extrapolated to \( N_T = \infty \) assuming a linear dependence on \( 1/N_T \) as in (17), that is we computed, for each time point,

\[
Y_\infty = 2 \cdot Y_{16,000} - Y_{8000}
\]

where the error bars are the obvious ones. For uniformity’s sake we performed such an extrapolation even for \( T = 0.4 \) with Metropolis dynamics, instead of using the result of the previously described fitting procedure based on 6 different values of \( N_T \).

At this point we are left, for each temperature value and dynamics type, with a unique set of data giving the time relaxation of the magnetization and the energy density of the system. The data are very well fitted by the following functional forms, for \( T \leq T_g = 1 \): as expected, the magnetization shows an algebraic relaxation to zero

\[
m(t) \sim C t^{-\delta} \tag{18.1}
\]

and the energy density shows an algebraic relaxation to a well-defined non-zero value

\[
e(t) \sim e_\infty + C' t^{-\delta'} \tag{18.2}
\]

A few technical remarks. The fits were performed minimizing the (naturally defined) chi-square function. The one for the magnetization can be easily linearized and performed by standard methods, the one for the energy density, being highly non-linear, requires a package for non-quadratic function minimization and error analysis, in our case the package MINUIT of the CERN libraries. To test the reliability of the fits we impose a cutoff \( t_{\text{min}} \) at low times, we consider the relaxation only for \( t > t_{\text{min}} \), and we check if there is a systematic dependence of the fitted parameters on \( t_{\text{min}} \). The fits of the energy density show no evident dependence. The ones for the magnetization, for low temperature \( (T \leq 0.5) \), show a systematic decrease of the fitted exponent \( \delta \). This fact is commonly considered a sign of the presence of non-negligible corrections to the asymptotic behaviour (18.1). Thus we adopt, to take into account such (unknown) corrections, the Berretti-Sokal procedure, described in [13, sections 4.2 and 5.3]: we fit the data with the functional form

\[
m(t) = C t^{-\delta} \left( 1 + \frac{B}{t} \right)
\]

for various fixed values of \( B \), and we look for the range in \( B \) for which there is no systematic dependence of the fitted parameters \( \delta \) and \( C \) on \( t_{\text{min}} \). In this range of \( B \), for each fitted parameter we select the maximum and the minimum values: the best fit for the parameter will be simply the arithmetic mean of these values, whereas their difference will be considered as the systematic error due to unconsidered corrections to the leading behaviour, or to imperfect knowledge of the form of the corrections (95% subjective confidence limit
Figure 3. Plot of the asymptotic value $-2e_\infty$ of the energy density versus $T$ for Metropolis dynamics at zero magnetic field. The data where obtained by a fit with the algebraic relaxation form (18.2) for $T \leq T_g$, whereas in the paramagnetic phase for $T > T_g$ the energy density relaxes almost instantaneously to its asymptotic value. The full line is the plot of the energy density for the $SK$ model at equilibrium [12]; the tail for $T > T_g$ has the usual paramagnetic form $e = -1/2T$. The error bars from the fit are negligible with respect to the dimension of the dots.

as defined in [13, footnote 17]), in addition to the usual statistical error for the fit, at 95% confidence level $(2\sigma)$.

Now, the results of the whole analysis can be summarized, for both dynamics, by three functions of temperature: the exponents $\delta$ and $\delta'$ of the algebraic relaxation of the magnetization and the energy density, and the asymptotic value $e_\infty$ of the energy density. The interesting results are the following.

- The energy density relaxes to its equilibrium value, at least for high enough temperatures ($T > 0.2 \div 0.3$). The plot of $-2e_\infty$ versus $T$, for Metropolis dynamics, is shown in figure 3; the corresponding one for heat-bath dynamics is very similar. The full line is the plot of the energy density for the $SK$ model at equilibrium, obtained by an exact numerical solution of the replica equations [12]. Recall that for $T > T_g$ an exponential relaxation is expected, instead of the algebraic one of equation (18.2), and this can not be observed, since the procedure of decimation we followed to reduce the data does not leave invariant an exponential relaxation. However, the asymptotic value is almost instantaneously reached, so there is no need for a fit. Let us remark that, in fact, our estimate for the asymptotic value of the relaxation is slightly lower than the equilibrium value (in figure 3 minus two times the energy is plotted, so the experimental points appear above the equilibrium curve). This is very probably due to some inaccuracy in the extrapolation to $N_T = \infty$.
- The exponent $\delta'$ of the relaxation of the energy density is almost constant with $T$.  

17
Figure 4. Plot of the exponent $\delta'$ of the algebraic relaxation of the energy density versus $T$, for both Metropolis (■) and heat-bath (□) dynamics at zero magnetic field. The data were obtained by a fit with the form (18.2) for $T \leq T_g$, whereas in the paramagnetic region the relaxation is exponential. The two series of data hereby displayed are slightly shifted for mere convenience of representation. The error bars from the fit are at 95% confidence level (2σ).

A plot of $\delta'$ versus $T$, for both dynamics, is shown in figure 4; let us remark that for Metropolis dynamics it is $\delta' \sim 1$, slowly increasing with $T$, whereas for heat-bath dynamics it is $\delta' \sim 0.7$, again slowly increasing with $T$, but with a jump at $T = T_g = 1$ where it is $\delta' \simeq 1$. This behaviour of the exponent $\delta'$ is somewhat anomalous, since it differs from one dynamics to the other, whereas we expect an universal behaviour. Moreover, though our results agree qualitatively with previous simulations [2], it would be nice if the exponent of the relaxation go to zero with $T$. We shall come back to this point in a while.

- The exponent $\delta$ of the relaxation of the magnetization is proportional to $T$. This can be seen from a plot of $\delta$ versus $T$, which is shown, for both dynamics, in figure 5. Moreover, the data for $\delta$ are very well compatible with a dependence on $T$ of the simple form

$$\delta(T) = T/T_g$$

though we have not scrupulously tested this by a fit. Noticeably, this feature has been observed in experiments on real spin glasses since a long time (see, for instance, [14, 15]). Strong indications for the validity of this fact also for the mean-field $SK$ model come from recent numerical simulations [2], but it has never been previously tested numerically with sufficient reliability, since so far in all the numerical simulations it has been difficult to take finite-size effects into account. Let us stress that the exact numerical solution of the $SK$ dynamics at equilibrium gives an exponent $\nu$ for the algebraic relaxation of the magnetization which tends to a non-zero value when $T$
Figure 5. Plot of the exponent $\delta$ of the algebraic relaxation of the magnetization versus $T$, for both Metropolis ($a$) and heat-bath ($b$) dynamics at zero magnetic field. The data were obtained by a fit with the form (18.1) for $T \leq T_g$, whereas in the paramagnetic region the relaxation is exponential. The dashed line $\delta(T) = T$ is drawn as a guide for the eye. The error bars are the systematic ones of the Berretti-Sokal procedure for $T \leq 0.5$ (95% subjective confidence limit as defined in [13, footnote 17]), whereas for $T > 0.5$ they are the usual statistical ones from the fit, at 95% confidence level ($2\sigma$).

goes to zero [12]. This implies that what is observed cannot be explained by the equilibrium features of the $SK$ dynamics.
As a concluding remark, a few words of caution are necessary. Though from our data we do not observe a strong evidence for the presence of subleading terms in the relaxation form of the energy density (18.2), nevertheless there are some anomalies in the behaviour of the energy that could be explained by the underlying presence of such subleading corrections. In fact, we have already pointed out that at low temperatures \( T < 0.3 \) our estimate of the asymptotic value of the energy density is definitely higher than the true equilibrium value. Our data (see figure 3) show a clear trend to the value \(-2e_\infty \simeq 1.4\) at zero temperature, in agreement with what was observed in previous simulations [2]. It is expected that at \( T \neq 0 \) this value relaxes again very slowly to the true equilibrium value, with an exponent which goes to zero with \( T \). However, due to the fact that this further relaxation at finite temperature is only a few percent of the main relaxation at zero temperature, one could argue that at low temperatures and not sufficiently long times the observed exponent of the relaxation is an effective exponent, with three consequences: the effective exponent is not universal, and it is different in Metropolis and heat-bath dynamics; it is almost constant with \( T \), and remains different from zero even at low temperatures (in [2] it was observed \( \delta' \simeq 0.6 \div 0.8 \) for \( T \) ranging from 0.2 to 0.4); we miss the estimate for the asymptotic value, which at low temperatures remains higher than the true equilibrium value. All those troubles are not present in the relaxation of the magnetization, since its zero-temperature asymptotic value is \( m_\infty \simeq 0.2 \) [7, 8], so its further finite temperature relaxation is much more impressive and much more easy to observe.

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