MA/UC3M/10/95

Analytical solution of the Monte Carlo dynamics of a simple spin-glass model

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(August 6, 1995)

Abstract

In this note we present an exact solution of the Monte Carlo dynamics of the spherical Sherrington-Kirkpatrick spin-glass model. We obtain the dynamical equations for a generalized set of moments which can be exactly closed. Only in a certain particular limit the dynamical equation of the energy coincides with that of the Langevin dynamics

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There has been in recent years a renewal of the interest in the study of the dynamics in spin glasses. The main motivation is based upon the fact that real spin glasses (and also real glasses) are always off equilibrium during the experimental time window, the most clear signature being the existence of aging [1]. Two main approaches have been put forward very recently to understand this problem. In the first approach, special emphasis is put on the behavior of two-time quantities (like the correlation or the response function at two different times) for a specific microscopic dynamics [2]. This has been complemented by the study of several phenomenological models which try to capture the main essentials of the slow dynamical process [3]. In the second approach, one tries to find the time evolution of some macroscopic observables (one-time quantities) and, eventually in a latter stage, the evolution of the two-time quantities [4]. While less ambitious than the first approach, this line of thought allows one to obtain fairly good results in simple cases.

The major part of these approaches have focused their attention in the solution of the Langevin or Glauber dynamics [5]. In this letter we analytically solve the Monte Carlo dynamics in a simple spin glass model. There are two reasons why this study should be of interest. First, there is no special reason to privilege a particular type of dynamics over others, and it is important to understand why other dynamics may yield different results and how different these results may be. The second reason is more practical and relies on the fact that the major part of numerical simulations use the Monte Carlo algorithm. Consequently, more direct comparisons between theory and numerics can be done.

While the results we will show are based on a very simple spin-glass model, it would be interesting to extend our approach to more complex cases (for instance where replica symmetry is broken). We will also show that the Monte Carlo dynamics is different from the Langevin dynamics although the same dynamical equation for the energy is obtained in a certain limit.

The model and the dynamics. The model we are considering is the two-spin spherical spin-glass model [6], defined by

$$E\{\sigma\} = -\sum_{i<j} J_{ij}\sigma_i\sigma_j \tag{1}$$

where the indices i, j run from 1 to N (N is the number of lattice sites) and the spins σ_i satisfy the spherical global constraint

$$\sum_{i=1}^{N} \sigma_i^2 = N. \tag{2}$$

The interactions J_{ij} are Gaussian distributed with zero mean and $1/N$ variance. This model has been extensively studied in the literature in all its details (the statics and the Langevin dynamics [7]) and is an useful starting point for our approach.

We will consider the Monte Carlo dynamics with the Metropolis algorithm (another algorithm would yield the same qualitative results). The dynamics is done in this way: we take the configuration $\{\sigma_i\}$ at time t and we perform a small random rotation of that configuration to a new configuration $\{\tau_i\}$ where

$$\tau_i = \sigma_i + \frac{r_i}{\sqrt{N}} \tag{3}$$

and the r_i are random numbers extracted from a Gaussian distribution $p(r)$ of finite variance δ,

$$p(r) = \frac{1}{\sqrt{2\pi\delta^2}}\exp(-\frac{r^2}{2\delta^2}) \quad . \tag{4}$$

We impose the new configuration $\{\tau_i\}$ to satisfy the spherical constraint eq.(2). Let us denote by ΔE the change of energy $\Delta E = E\{\tau\} - E\{\sigma\}$. According to the Metropolis algorithm we accept the new configuration with probability 1 if $\Delta E < 0$ and with probability $exp(-\beta\Delta E)$ if $\Delta E > 0$ where $\beta = \frac{1}{T}$ is the inverse of the temperature T.

We have chosen the particular equation of motion (3) because it makes the dynamics invariant under rotations. There are other types of motions, for instance moving only one randomly chosen component $\tau_i = \sigma_i + r_i$, but they do complicate much more the analytical treatment (details will be shown elsewhere [8]).

The joint probability $P(\Delta h_k, \Delta E)$. Because the dynamics eq.(3) is invariant under rotations we will work in what follows in the diagonal basis of the interaction matrix J_{ij}. In that basis the energy reads,

$$E\{\sigma_\lambda\} = -\sum_\lambda J_\lambda \sigma_\lambda^2 \tag{5}$$

where the σ_λ are the eigenvectors and the J_λ are distributed according to the Wigner semi-circular law [9],

$$w(\lambda) = \frac{\sqrt{4-\lambda^2}}{2\pi}. \tag{6}$$

We also define the generalized k-moments,

$$h_k = \sum_{(i,j)} \sigma_i (J^k)_{ij} \sigma_j = \sum_\lambda J_\lambda^k \sigma_\lambda^2 \tag{7}$$

where $h_0 = 1$ (spherical constraint) and $h_1 = -2E$. The basic object we want to compute is the joint probability $P(\Delta h_k, \Delta E)$ to have a certain variation Δh_k of the k-moment given that the energy E has also varied by a quantity ΔE. This is a quantity which gives all the information about the dynamics. The variation of the quantities h_k and E in an elementary move eq.(3) are given by

$$\begin{aligned} \Delta E^* &= -\frac{1}{\sqrt{N}} \sum_\lambda J_\lambda \sigma_\lambda r_\lambda - \frac{1}{2N} \sum_\lambda J_\lambda\, r_\lambda^2 \\ \Delta h_k^* &= \frac{2}{\sqrt{N}} \sum_\lambda J_\lambda^k\, \sigma_\lambda\, r_\lambda + \frac{1}{N} \sum_\lambda J_\lambda^k\, r_\lambda^2. \end{aligned} \tag{8}$$

The joint probability $P(\Delta h_k, \Delta E)$ is,

$$P(\Delta h_k, \Delta E) = \int \delta(\Delta h_k - \Delta h_k^*) \delta(\Delta E - \Delta E^*) \delta(\Delta h_0) \prod_\lambda \Big(p(r_\lambda) dr_\lambda \Big) \tag{9}$$

where the last delta function in the integrand accounts for the spherical constraint and the variations $\Delta h_k^*, \Delta E^*$ are given in eq.(8).

Using the integral representation for the delta function

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\alpha x} d\alpha \tag{10}$$

and substituting in (8) we get

$$\begin{aligned} P(\Delta h_k, \Delta E) = \int d\alpha\, d\mu\, d\eta\, \exp\Big(& i\alpha \Delta h_k + i\mu \Delta E - \\ & \frac{\delta^2}{2N} \sum_\lambda \frac{\sigma_\lambda^2 \gamma_\lambda^2}{(1 - \frac{i\gamma_\lambda^2 \delta^2}{N})} - \frac{1}{2} \sum_\lambda \log(1 - \frac{i\gamma_\lambda^2 \delta^2}{N}) \Big) \end{aligned} \tag{11}$$

where $\gamma_\lambda = -2\alpha J_\lambda^k + \mu J_\lambda + 2\eta$. Expanding the logarithm and retaining the first $1/N$ correction we get (after some manipulations)

$$P(\Delta h_k, \Delta E) = P(\Delta E)\, P(\Delta h_k|\Delta E) \tag{12}$$

where $P(\Delta E)$ is the probability distribution to have a change of energy ΔE and $P(\Delta h_k|\Delta E)$ is the conditional probability of Δh_k given ΔE. The final expressions are,

$$P(\Delta E) = \frac{1}{\sqrt{2\pi\delta^2 B_1}} \exp\Big(-\frac{(\Delta E + \delta^2 E)^2}{2\delta^2 B_1}\Big)$$
$$P(\Delta h_k|\Delta E) = \frac{1}{\sqrt{8\pi(C_k - (B_k^2/B_1))}} \exp(-\frac{\Delta h_k + \delta^2(h_k - << J^k >>) + 2\frac{B_k}{B_1}(\Delta E + \delta^2 E)^2}{8\delta^2(C_k - B_k^2/B_1)}\Big) \tag{13}$$

with

$$C_k = h_{2k} - h_k^2; \quad B_k = h_{k+1} + 2Eh_k; \quad (h_0 = 1; h_1 = -2E);$$
$$<< f(J) >>= \int_{-2}^{2} d\lambda w(\lambda) f(\lambda); \tag{14}$$

Before showing the dynamical equations for the moments we will prove that equilibrium is a stationary solution of the Monte Carlo dynamics. The equation for the energy is obtained by considering the average variation of energy in an elementary move,

$$\overline{\Delta E} = \int_{-\infty}^{0} \Delta E\, P(\Delta E) d\Delta E + \int_0^\infty \Delta E \exp(-\beta\Delta E) P(\Delta E) d\Delta E \quad . \tag{15}$$

A direct calculation shows that this variation is zero when $B_1 = h_2 - 4E^2 = -2ET$. It can be easily shown (using standard static calculations [10]) that this is the condition satisfied at equilibrium.

Also one can compute the acceptance rate as a function of time, which is given by

$$A(t) = \int_{-\infty}^{0} P(\Delta E) d\Delta E + \int_0^\infty \exp(-\beta\Delta E) P(\Delta E) d\Delta E \quad . \tag{16}$$

In what follows we will consider the zero temperature case, the computations being straightforward in case of finite temperature. A straightforward computation shows,

$$A(t) = \frac{Erf(\alpha)}{2} \tag{17}$$

where $Erf(\alpha)$ is the error function $Erf(\alpha) = \frac{2}{\sqrt{\pi}} \int_\alpha^\infty dx \exp(-x^2)$ and the parameter α is given by,

$$\alpha = -\frac{\delta E}{\sqrt{2B_1}} \tag{18}$$

Now we can understand qualitatively how the dynamics goes on. Suppose we start at zero temperature with a random initial configuration $\sigma_i = \pm 1$ such that $E(t=0) = 0$ and $B_1(t=0) = 1$. The energy monotonically decreases to the ground state energy $E = -\frac{J_{max}}{2} = -1$ while B_1 decreases also to zero. In the large time limit α diverges and the acceptance rate goes to zero (we are at zero temperature). There are two different regimes in the dynamics. The first one is an initial regime where α is small and the acceptance rate is nearly 1/2. This corresponds to a gaussian $P(\Delta E)$ (eq.(13)) with width $\delta\sqrt{B_1}$ larger than the position of its center ($\delta^2 E$). In this case, the changes of configuration which increase or decrease the energy have the same probability. The energy decreases fast in this regime because the acceptance is large. The second regime appears when B_1 is so small in order that α becomes large. In this case the acceptance is very small (it goes like $\frac{exp(-\alpha^2)}{\alpha}$) and the dynamics is strongly slowed down. The system goes very slowly to the equililibrium.

In order to obtain the time evolution of the acceptance rate we need to know the energy E and B_1 at time t. In the next paragraph we will show that all k-moments only depend on these two quantities. In figure 1 we show the results for the acceptance rate obtained in a self-consistent way using expression (17). The two regimes (separated by a drastic fall of the acceptance rate $A(t)$) can be clearly appreciated.

Analytical solution of the hierarchy. In order to obtain the dynamical evolution of the k-moments h_k we have to compute its average variation in a Monte Carlo step over the accepted changes of configuration. In this case one Monte Carlo step corresponds to N elementary moves. In the thermodynamic limit we can write the continuous equations,

$$\frac{\partial h_k}{\partial t} = \overline{\Delta h_k} = \int_{-\infty}^{\infty} \Delta h_k \, d\Delta h_k$$
$$\Big(\int_{-\infty}^{0} d\Delta E P(\Delta h_k, \Delta E) + \int_{0}^{\infty} d\Delta E \, \exp(-\beta \Delta E) P(\Delta h_k, \Delta E)\Big) \tag{19}$$

In the zero-temperature case one obtains,

$$\frac{\partial h_k}{\partial t} = -\frac{\delta^2 (h_k - << J^k >>) Erf(\alpha)}{2} - \frac{2}{\sqrt{\pi}} \alpha B_k E \exp(-\alpha^2) \tag{20}$$

where the average $<< .. >>$ has been previously defined in eq.(14). In particular one gets, for $k = 0$, $\frac{\partial h_0}{\partial t} = 0$ which is the spherical constraint. For the energy $E = -\frac{h_1}{2}$ we get the equation,

$$\frac{\partial E}{\partial t} = \frac{B_1}{E} K(\alpha) \tag{21}$$

where $K(\alpha) = \frac{\alpha \exp(-\alpha^2)}{\sqrt{\pi}} - \alpha^2 \, Erf(\alpha)$ and $B_1 = h_2^2 - 4E^2$, where h_2 is the squared local field. In the first dynamical regime (α small) we get $\frac{\partial E}{\partial t} = -\frac{\delta \sqrt{B_1}}{\sqrt{2\pi}}$ and in the slow dynamical regime (α large) we find $\frac{\partial E}{\partial t} = \frac{B_1 exp(-\alpha^2)}{2E\alpha\sqrt{\pi}}$. In the last case, if we redefine the time $\tau = tA(t)$ then we obtain the expression $\frac{\partial E}{\partial \tau} = \frac{B_1}{E} = -B_1$ (because $E = -1$ for large enough times). In this limit we get the equation for the energy in the Langevin dynamics ([8]).

$$g(x,t) = \sum_{(i,j)} \sigma_i \, (e^{xJ})_{ij} \, \sigma_j = \sum_{\lambda} e^{\lambda x} \sigma_\lambda^2(t). \tag{22}$$

This function yields all the moments $h_k = \left(\frac{\partial^k g(x,t)}{\partial x^k}\right)_{x=0}$.

It is easy to check that $g(x,t)$ satisfies the following differential equation

$$\frac{\partial g(x,t)}{\partial t} = a(t) \frac{\partial g(x,t)}{\partial x} + b(t) g(x,t) + c(x,t) \tag{23}$$

where the coefficients are given by,

$$a(t) = -\frac{2 \, \alpha \, e^{-\alpha^2}}{E\sqrt{\pi}} \tag{24}$$

$$b(t) = -(\frac{\delta^2 \, Erf(\alpha)}{2} + \frac{4\alpha \, \exp(-\alpha^2)}{\sqrt{\pi}}) \tag{25}$$

$$c(x,t) = \frac{\delta^2 \; << e^{xJ} >> \; Erf(\alpha)}{2} \tag{26}$$

where $a(t)$ is a positive quantity. Note the difference with the Langevin case in which $a(t) = 2$, $b(t) = 4E$, $c(x,t) = 0$ [8]. The solution of this partial differential equation with the initial conditions $g(0,t) = 1$, $g(x,0) =<< \exp(x\lambda)\,\sigma^2(\lambda, t = 0) >>$ and subject to the self-consistency conditions (24-26) where α is given by

$$\alpha = \frac{\delta \frac{\partial g}{\partial x}(0,t)}{2\sqrt{\frac{\partial^2 g}{\partial x^2}(0,t) - \left(\frac{\partial g}{\partial x}(0,t)\right)^2}} \tag{27}$$

is

$$g(x,t) =<< \exp^{(x+\int_0^t a(t')dt')\lambda}\,\sigma^2(\lambda, t=0) >> \exp(\int_0^t b(t')dt') + \delta^2 \int_0^t dt' c(x + \int_{t'}^t a(t'')dt'', t') \exp(\int_{t'}^t b(t'')dt''). \tag{28}$$

¿From this function we can readily obtain all moments as a function of time. In particular, we show in figure 2 the energy obtained (at zero temperature) in a real Monte Carlo simulation as a function of time compared to the theoretical prediction obtained from the previous equation.

We note the following differences between Monte Carlo and Langevin dynamics. In the Langevin dynamics one can show that the time evolution of all k-moments is completely determined only by the energy (the first moment). In the Monte Carlo case we have seen the time evolution of the moments is determined by the time dependent parameter α which is a function of the energy E and the second cumulant as shown in eq. (28). In this sense the dynamics is slightly more complicated than the Langevin case but simple enough to be governed by two (time dependent) quantities.

Now we can summarize our results. We have analytically solved the Monte Carlo dynamics of a simple spin-glass model (without replica symmetry breaking). The method consists in constructing the joint probability eq.(9) of having a certain change of the generalized moments h_k for a given change ΔE of energy. Once this probability is constructed it is possible to derive the dynamical evolution equations for all moments. The hierarchy of equations can be closed by introducing the generating functional $g(x,t)$. While we have applied this method in a very simple case we expect it to be aplicable to other more interesting cases where replica symmetry is broken. The philosophy of the method is very close to that devised by Coolen and Sherrington [4] but applied in our case for the the specific Monte Carlo dynamics. It is interesting to note that the hierarchy of equations (20) is different from that obtained in case of Langevin dynamics. Only in the large time limit, and renormalizing the time by the acceptance ratio, the equation for the energy coincides in both cases (but higher moments do not coincide). It would be also interesting to try to derive the correlation functions and the response function in this framework.

We are indebted to Silvio Franz for useful discussions on these subjects. (F.R.) and (L.B.) acknowledge Ministerio de Educación y Ciencia and European Comunity for finacial support through grant PB92-0248.

REFERENCES

[1] L. Lundgren, P. Svedlindh, P. Nordblad and O. Beckman; Phys. Rev. Lett. **51**, 911 (1983). E. Vincent, J. Hammann and M. Ocio; in 'Recent progress in Random Magnets', ed. D. H. Ryan (Singapore: World Scientific) (1992), and references therein.

[2] A. Crisanti, H. Horner and H.-J. Sommers, Z. Phys. **B92** (1993) 257; L. F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. **71** (1993) 173; S. Franz and M. Mézard, Physica **A210** (1994) 48.

[3] J. P. Bouchaud, J. Physique I (Paris) **2** (1992) 1705; J. P. Bouchaud and D. Dean, J. Physique I (Paris) **5** (1995) 265;

[4] A. C. C. Coolen and D. S. Sherrington, J. Phys. A (Math. Gen.) **27** (1994) 7687 ; A. C. C. Coolen and S. Franz, J. Phys. A (Math. Gen.) **27** (1994) 6947; A. C. C. Coolen, S. Laughton and D. Sherrington *Dynamical Replica Theory for Disordered spin systems* Preprint cond-mat/9507101

[5] H. Sommers, Phys. Rev. Lett. **58** (1987) 1268;

[6] J. M. Kosterlitz, D. J. Thouless and R. C. Jones; Phys. Rev. Lett. **36** (1976) 1217;

[7] G. A. Rodgers and M. A. Moore , J. Phys. A (Math. Gen.) **22** (1989) 1085; S. Ciuchi and F. De Pasquale, Nucl. Phys. **B300** (1988) 31; L. F. Cugliandolo and D. S. Dean, *Full dynamical solution for a spherical spin-glass model* Preprint cond-mat 9502075.

[8] L. L. Bonilla, F. G. Padilla, G. Parisi and F. Ritort, in preparation

[9] M. L. Mehta, *Random Matrices and the Statistical theory of Energy levels* (Academic, New York, 1967)

[10] M. Mézard, G. Parisi and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore 1987); K. H. Fischer and J. A. Hertz, *Spin Glasses* (Cambridge University Press 1991);

FIGURES

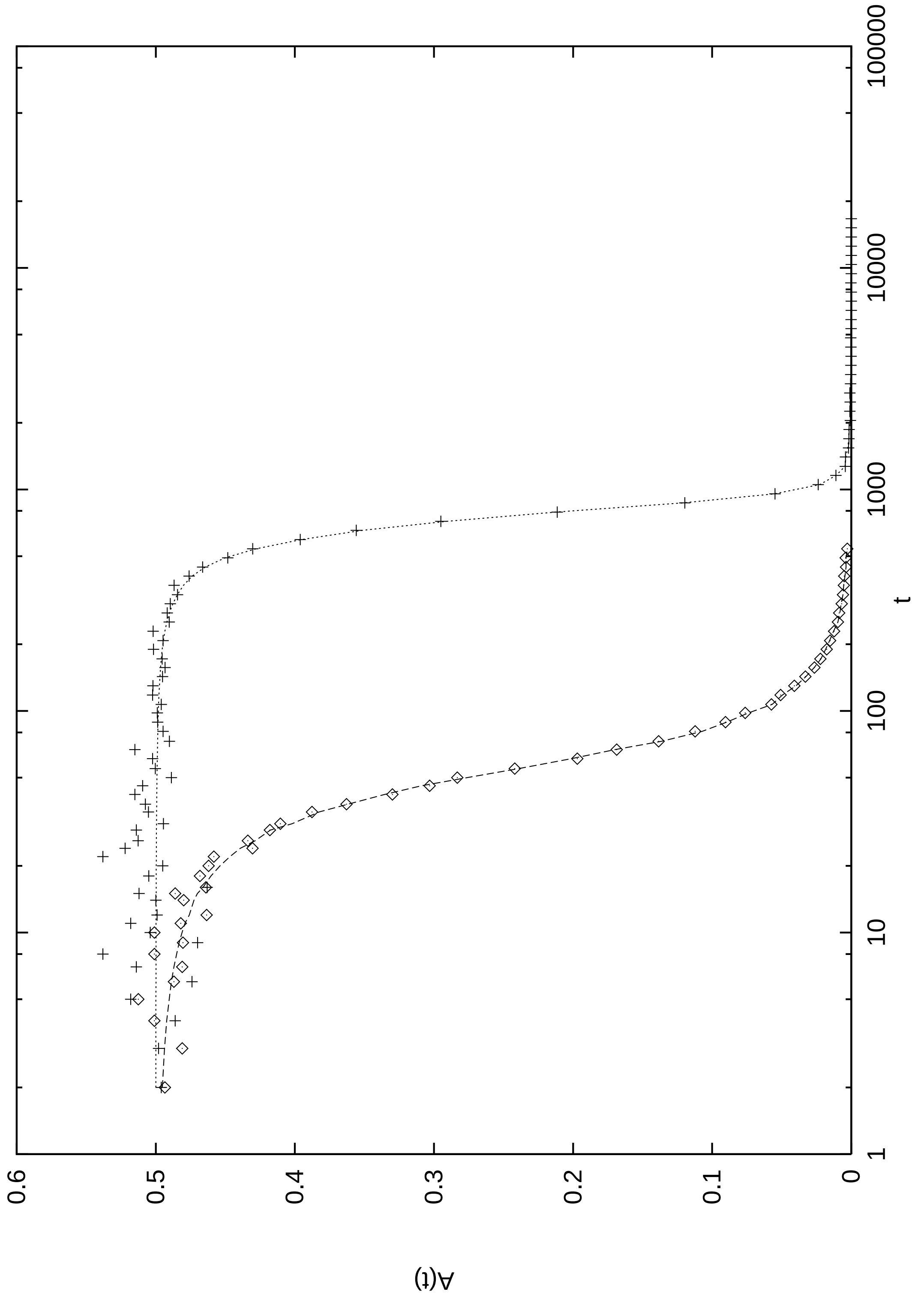

FIG. 1. Acceptance rate $A(t)$ calculated self-consistently using eq.(17) compared to Monte Carlo results at zero temperature for two different values of $\delta = 0.1$ (rhombs) and 0.01 (crosses) for $N = 2000$ and $N = 500$ respectively.

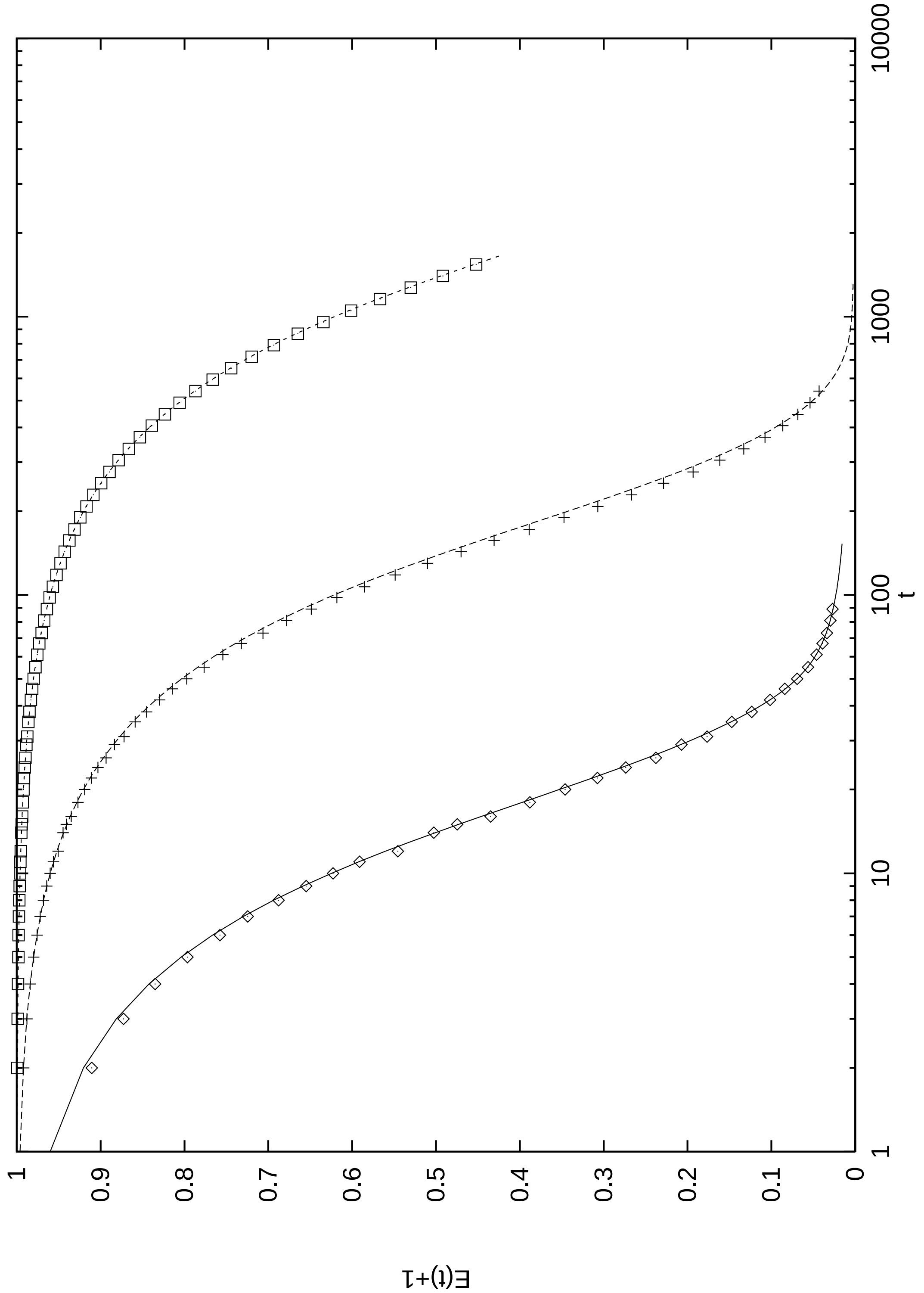

FIG. 2. Relaxation of the internal energy as a function of time for three different values of δ (0.1 (rhombs),0.01(crosses), 0.001 (boxes)) and $N = 2000$ at zero temperature compared with the analytic prediction eq.(28).