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Dynamical behaviour of low autocorrelation models

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Abstract. We have investigated the nature of the dynamical behaviour in low autocorrelation binary sequences. These models do have a glass transition T_G of a purely dynamical nature. Above the glass transition the dynamics are not fully ergodic and relaxation times diverge like a power law $\tau \sim (T - T_G)^{-\gamma}$ with γ close to 2. Approaching the glass transition the relaxation slows down, in agreement with the first-order nature of the dynamical transition. Below the glass transition the system exhibits aging phenomena, as in disordered spin glasses. We propose the aging phenomena as a precise method to determine the glass transition and its first-order nature.

1. Introduction

There has been much interest recently in the field of condensed matter physics concerning the study of frustrated models without explicit disorder [1–5]. These models (also called deterministic models) show a very similar behaviour to spin glasses [6], i.e. there exists a very large number of metastable configurations where the system remains trapped and it is very difficult to reach the global equilibrium state in a dynamical process starting from a random initial configuration.

The main difference between these frustrated models and spin glasses is that in the case of deterministic models the quenched disorder is not present. Because some symmetries are preserved in the deterministic model, in some cases it is possible to explicitly construct the ground state. This possibility is generally forbidden in disordered systems because no symmetry is preserved. Also, in disordered systems, each realization of the randomness yields a different ground state, implying that there is much difficulty in devising any kind of algorithm to identify the ground state.

Recently, it has been shown that the application of techniques initially devised for this random systems promises to be a powerful tool in the understanding of the deterministic models [1]. In particular, much effort has been devoted recently to the study of the Bernasconi model [10]. This is an optimization problem in which one searches for strings of binary digits with minimal autocorrelation. The high-temperature phase of this model has been solved exactly in the particular case of periodic boundary conditions ([1], hereafter referred to as paper I). The system shows a static transition to a frozen phase where the entropy is nearly zero. In the original Bernasconi model with open boundary conditions an exact solution for the high-T phase is still lacking, but some approximations suggest that a similar static transition also takes place in that case. This static transition is different

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from the dynamical transition one observes in a real system. The dynamical transition is higher than the static transition and corresponds to the situation in which the system remains trapped in metastable configurations. Below this dynamical transition temperature, thermal fluctuations are very small and very reminiscent of what happens in real glasses [9]. In the context of models without explicit disorder this transition has been called the *glass transition*. Starting a dynamical evolution from the high-temperature region, a large enough system is unable to see the static transition because it gets trapped in the metastable phase at a higher temperature. For all purposes, it is always this higher temperature transition which governs the dynamics. Within the realm of disordered systems this dynamic transition can be computed using the *marginality condition* [11]. This condition corresponds to the search for certain saddle points of the free energy (not true maxima as in the static case) such that one particular eigenvalue of the stability matrix vanishes (the so-called replicon eigenvalue). This condition corresponds to the temperature at which dynamical stability disappears. The dynamical transition temperature has been obtained by several authors using the dynamic mean-field theory of spin glasses initially studied by Sompolinsky and Zippelius for the study of the SK model [12]. In the framework of disordered systems, the studies of Kirkpatrick and collaborators on the p-spin Ising models [13] and the Potts glass [14] have always shown that this dynamical temperature is above that predicted by the statics. Recent studies of the off-equilibrium dynamics of the p-spherical spin-glass model by Cugliandolo and Kurchan have shown that the energy of the dynamics in the low-temperature phase, below the dynamical transition, is higher than that predicted by the statics [15]. As the dynamical transition temperature is approached, the off-equilibrium dynamics slows down and aging effects start to appear. Similar aging phenomena have been found in the context of random manifolds [16].

In some cases the glass transition for the models without disorder can also be predicted using the replica approach. A concrete test of all these theoretical results for a deterministic model and its disordered version (defined as the disordered model which has the same high-T expansion as the deterministic model) has been performed very recently for the sine model [2] (hereafter referred to as paper II). In this case, the dynamical transition can be computed exactly and compared to the numerical results. We stress the fact that this dynamical transition, in the context of disordered systems, corresponds to the glass transition for the deterministic case.

The purpose of this work is to show how several numerical techniques in spin glasses can be used for the determination of the glass transition temperature for deterministic models. Because this glassy transition is, as we have already indicated, purely dynamical, this will also be the essence of the techniques we will use. Now the reader will realize that the main advantage of the study of deterministic models relies on the fact that one does not need to average over different realizations of disorder. Because of the dynamical nature of the transition one should average over different initial conditions. Anyway, comparing to the spin-glass case, we have eliminated one source of strong fluctuations. In this work we will concentrate on the case of low autocorrelation binary sequences. These models have received a lot of attention very recently because they are the simplest prototype of ordered systems with a very complex energy landscape; we refer the reader to the different works on this subject. Migliorini has performed extensive numerical simulations using the tempering method [21] and Krauth and Mezard [22] and Krauth and Pluchery [23] have applied a modified version of the BKL algorithm (due to Bortz *et al* [24]) which allows the investigation of dynamical properties for very large times.

This paper is divided as follows. Section 2 introduces the low autocorrelation models we will investigate and presents the main theoretical results in this case. Section 3 is devoted

to the study of different thermodynamical quantities during an annealing cooling process which clearly displays the existence of the glassy transition. Section 4 is the main nucleus of our work, which is the study of off-equilibrium properties of this model and particularly of aging. The discontinuous nature of the glass transition will enable us to use this property for an accurate prediction of the glass temperature.

2. Low autocorrelation models

By low autocorrelation models we denote a large class of deterministic one-dimensional models with long-range interactions. In this work we have focused our attention on the periodic and open models (so-called depending on the type of boundary conditions). These models have their own interest as optimization problems in the field of communication systems. Let us suppose there is a one-dimensional chain of Ising spins $\{\sigma_i; i = 1, N\}$ which can take the values ± 1 and the following Hamiltonian:

$$H = \frac{1}{N} \sum_{k=1}^{N} C_k^{2\nu} \tag{1}$$

where the C_k are correlation functions which connect spins at distance k. The case $\nu = 1$ is the problem we are generally interested in but nothing prevents us from considering different models for a generic value of ν. For the periodic model we have

$$C_k = \sum_{i=1}^{N} \sigma_i \sigma_{i+k} \tag{2}$$

and in the case of the open model

$$C_k = \sum_{i=1}^{N-k} \sigma_i \sigma_{i+k} \tag{3}$$

so, in this case, there is no translational symmetry in the model.

It was shown by Golay [25] and later by Bernasconi [10] that one could approximate the thermodynamics of the open model by supposing that the different correlation functions C_k are uncorrelated Gaussian distributed random variables. This is the Golay–Bernasconi (GB) approximation and predicts the existence of a phase transition at a low temperature where the entropy vanishes. The same conclusion is valid for the periodic model where one expects the existence of a phase transition at low temperatures.

The interested reader can find most of the results of this section for the periodic model in paper I. Now we will recall some of the main results obtained in that work. In the case of the periodic model it can be shown that for prime values of N of the type $(4k+3)$, k being an integer, there exists an explicit ground state of finite global energy (and energy per spin zero in the thermodynamic limit because (1) has to be normalized by N). This construction does not exist in the open case. This ground state has a very low entropy up to a finite temperature where the entropy experiences a sudden jump. This finite temperature is the crystallization transition. Starting at zero temperature from the ground-state configuration and slowly increasing the temperature, the entropy also increases very slowly (always remaining very close to zero). At the crystallization temperature the entropy jumps to a finite value and the system enters the high-temperature regime. To account for this situation it is sometimes said that the phase space has *'golf course'*-like properties. As regards the dynamical behaviour of these models, the existence of a ground state of very low energy is of no relevance because we are interested in the behaviour of large systems. In fact, during a usual dynamical

relaxation process, the system is unable to find the ground state because this state has very low entropy. In this situation, the particular mathematical features of the selected number N (prime of the type $4k+3$ or not) are irrelevant. As has been shown in 1, the high-temperature phase of the periodic model can be solved exactly. Due to the translational symmetry of the model one can write the Hamiltonian in terms of the Fourier-space components

$$B(p) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \exp\left(\frac{2\pi i j p}{N}\right) \sigma_j \tag{4}$$

where i stands for the imaginary unit. The Hamiltonian (2) now reads

$$H = \frac{2}{N} \sum_{p=1}^{N/2} |B(p)|^4 . \tag{5}$$

Because σ_i are real functions (i.e. $B(p) = \overline{B(-p)}$) half of the Fourier components can be neglected. Writing the Hamiltonian in the Fourier space one can show that only certain kind of connected diagrams contribute to the free energy allowing for a Hartree–Fock resummation of the full series. In another way one can demonstrate, by introducing in equation (4) a generic unitary matrix, that the replica approach can be used to find the free energy of the model. In the replica-symmetric approximation one recovers the Hartree–Fock resummation. For our purposes it is important to note that the free energy of the periodic model is given by

$$f = \frac{1}{\beta} \log \int_0^\infty r \exp\left(-\beta r^4 - \mu r^2\right) dr \; - \frac{1}{\beta} \log(2) - 1 \tag{6}$$

where the value of μ is determined by the equation

$$\int_0^\infty r^3 \exp\left(-\beta r^4 - \mu r^2\right) dr = \int_0^\infty r \exp\left(-\beta r^4 - \mu r^2\right) dr . \tag{7}$$

The last condition corresponds to the closure condition

$$\sum_{p=1}^{N/2} \left\langle |B_p|^2 \right\rangle = 1 \tag{8}$$

the internal energy is given by

$$e = \frac{\partial \beta f}{\partial \beta} = \sum_{p=1}^{N/2} \left\langle |B_p|^4 \right\rangle - 1 \tag{9}$$

and the mean values $\langle \cdots \rangle$ are evaluated using the effective Hamiltonian

$$\mathcal{H}(\{B_p\}) = -\beta \sum_p |B_p|^4 - \mu \sum_p |B_p|^2 . \tag{10}$$

The integration variables B_p are complex variables and the mean values $\langle \cdots \rangle$ are obtained by integrating over the real and imaginary parts of the B_p.

These expressions are valid for the periodic model down to the temperature at which the entropy vanishes, which is $T_{\mathrm{RSB}}^{\mathrm{C}} \sim 0.1$ (the superscript C denotes the periodic model and O the open case). This result is surprisingly close to that given by the GB approximation. In that approximation one obtains the energy and the entropy

$$e = \frac{1}{1+4\beta} \qquad s = \log(2) - \tfrac{1}{4} \log(1+4\beta) + \frac{\beta}{1+4\beta} . \tag{11}$$

The entropy vanishes at $T_{RSB} \sim 0.096\,43$ and the energy at that temperature is close to 0.0235. We indicate this temperature by the subindex RSB because at this temperature replica symmetry is broken. Below T_{RSB}^{C} the entropy is nearly zero and the energy is constant, a situation very similar to that of spin glasses with one step of replica-symmetry breaking [8, 17]. Obviously the previous expression (6) is not valid for the open model, for which a high-temperature resummation is still lacking. Using the Golay approximation we can estimate this transition to be close to $T_{RSB}^{O} \sim 0.047$.

As we will see in the following sections, the transition T_{RSB} for the periodic and for the open model are not the true *glass transition.* As discussed in the introduction, the true glass transition corresponds to the transition where dynamical stability is lost (i.e. the temperature given by the marginality condition) and it can be several times larger than the corresponding transition given by the statics. This result was already known in spin glasses but it was not known that this result also applies in the case of deterministic models. The following sections are devoted to the numerical determination of this transition in the open and periodic cases. We will also see how off-equilibrium phenomena, and particularly the property of aging, yield a very nice and precise way to determine this glass transition temperature. Regarding the dynamical behaviour of both models we can advance the case that the main conclusions will be the same for the open and the periodic case. Because the open model has historically received more attention than the periodic version we will present more dynamical results in the former case.

3. A first determination of the glass transition

The main property of the glass transition in low autocorrelation models regards the first-order nature of this dynamical transition. From the thermodynamic point of view this transition is second order. So, for instance, the energy and the entropy are continuous while the specific heat experiences a jump. Because the transition is purely dynamical, this implies a transition for the correlation and response functions. In this section we will explore the behaviour of thermodynamic quantities leaving the discontinuous feature of the order parameter to the next section. For the periodic and open models we have made the same kinds of studies. In fact, we have discovered that they are strongly similar except for the fact that the periodic model is solved analytically in the high-T phase and displays an explicit ground state for chain lengths N such that N is prime and of the type $4k + 3$, k being an integer.

Starting from a random initial configuration in the high-temperature region, we have progressively decreased the temperature using a Monte Carlo annealing. We have simulated several sizes up to $N = 1000$ (because it is a long-range problem the number of bit operations in a Monte Carlo updating procedure grows very quickly with the size of the system). We have also tested that finite-size corrections are negligible and different initial conditions give the same result. As was pointed out in the introduction, we now have only one realization of disorder on which we have to do simulations. We have computed the main thermodynamical observables such as the energy, magnetization and their associated dissipative quantities like specific heat and magnetic susceptibility. The behaviour of the energy is shown in figures 1 and 2 for the periodic and open model, respectively. The energy decreases down to a certain temperature where it remains constant. This is very similar to what happens in the random energy model (REM) [8]. The broken curve in figures 1 and 2 corresponds to the GB approximation and the full curve (only for the periodic model) corresponds to the correct high-temperature prediction (6) which is in agreement with the data. As has already been mentioned, the glass transition is higher than the static transition (close to 0.1 in the periodic model). Figure 1 shows where the entropy of the

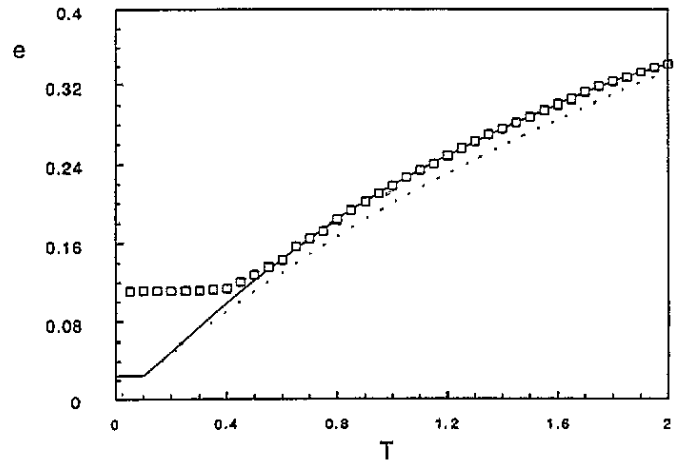

Figure 1. Energy of the periodic model versus temperature. The full curve is the high-temperature result (6). The broken curve is the GB approximation. Simulation results are for $N = 100$

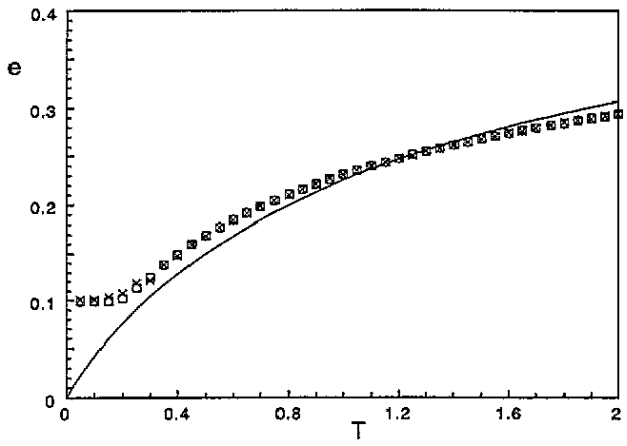

Figure 2. Energy of the open model versus temperature. The full curve is the GB approximation. Simulation results are for $N = 500$ (□) and $N = 1000$ (×)

high-temperature expression of (6) vanishes (this is where the energy (9) becomes constant as a function of the temperature). Curiously it does so at a temperature very close to that at which the entropy vanishes in the GB approximation. We have no explanation for this result, but it could be a pure accident. If this were also true in the opened case one would be tempted to state that the GB approximation is enough to predict the static transition. Figures 3 and 4 show the behaviour of the specific heat for the periodic and open model, respectively. The specific heat has been computed by measuring the fluctuations of the energy

$$c = \beta^2 N\left(\langle H^2\rangle - \langle H\rangle^2\right) \tag{12}$$

where the factor N in the expression arises from the appropiate normalization of the temperature. Also in these cases we plot the results for the GB approximation and, for the case of the periodic model, we also plot the high-temperature prediction (6). In both cases we

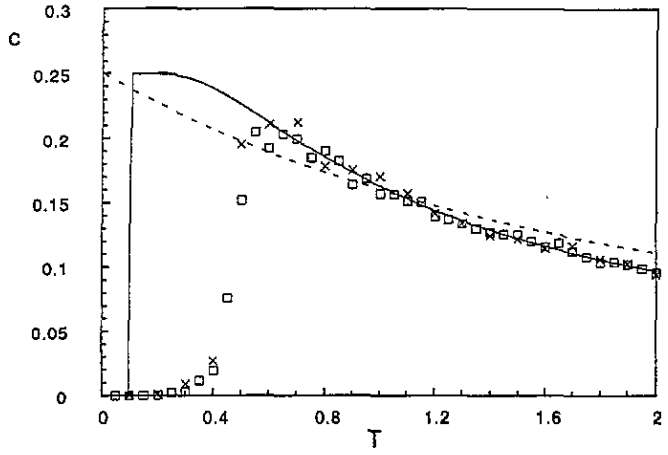

Figure 3. Specific heat of the periodic model versus temperature. The full curve is the high-temperature result (6). The broken curve is the GB approximation. Simulation results are for $N = 100$ (□) and $N = 500$ (×).

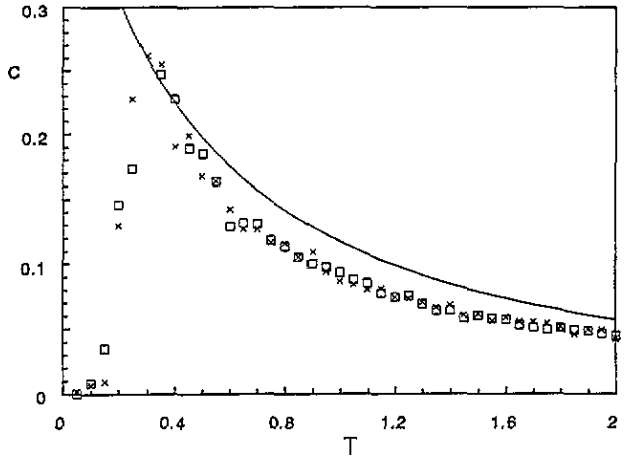

Figure 4. Specific heat of the open model versus temperature. The full curve is the GB approximation. Simulation results are for $N = 100$ (□) and $N = 500$ (×).

observe a discontinuous jump of the specific heat. It appears at a temperature $T_G^C \sim 0.45$ for the periodic model and $T_G^O \sim 0.2$ for the open case. We have to note that this energy and specific heat in the low-T phase are purely dynamical. Anyway, they satisfy fluctuation–dissipation theorems like the relation $C = \partial e/\partial T$, where C is the specific heat and e is the internal energy.

We have also measured the magnetization and its associated dissipative quantity (the magnetic susceptibility) fluctuations. The global magnetization is zero above T_G and below this temperature remains stacked to a certain small non-zero value (of the order of the standard mean deviation $1/\sqrt{N}$). Valuable information can be obtained from its fluctuations like the linear susceptibility and the Binder parameter. If $P(M)$ is the probability distribution of the magnetization, we expect it will be a Gaussian at very large temperatures and become more and more flattened as the glass transition is approached. We are going to show that this

really is the case and that fluctuations are very large even if we stay at high temperatures. In other words, the linear susceptibility and the Binder parameter are the variance and the curtosis of the probability distribution $P(M)$. The linear susceptibility is given by

$$\chi = \beta\left(\langle M^2\rangle - \langle M\rangle^2\right) \tag{13}$$

where M is the global magnetization and we recall the fact that one factor N has been absorbed in the temperature in order to have an appropriate thermodynamic limit. The Binder parameter [20] is given by

$$g = \tfrac{1}{2}\left(3 - \frac{\langle M^4\rangle}{\langle M^2\rangle^2}\right). \tag{14}$$

Now we would like to approximately compute this quantity in the high-T phase above the glass transition. From (5) we observe that the Hamiltonian is the sum of $\frac{1}{2}N$ Fourier components $B(p)$. We can suppose that these Fourier components are, at least, independent in the high-T phase (in some sense this is the original idea of Golay for resumming the high-T series). One can soon realize that this approximation has to fail because the total number of Fourier components is too large (it diverges with N). But this is the easiest approximation one can do. In order to reach the correct expression it should be necessary to solve the low autocorrelation models in a magnetic field. Within this approximation and using the Hamiltonian (5) we observe that the zero-momentum term $|B(0)|^4$ corresponds to the fourth power of the magnetization. The only difference between the magnetization and B_p is that these last Fourier components are complex while the magnetization is real. According to (10) the effective probability distribution of the magnetization is given by

$$P(M) \sim \exp\left(-\beta M^4 - \mu M^2\right). \tag{15}$$

We immediately observe that only at infinite temperature will the probability distribution be a Gaussian, and at finite β non-Gaussian corrections can be very strong (the same discussion is valid for any Fourier component B_p). This result was observed numerically by Migliorini studying the local-field distribution [21] in the open model. Using this approximation and (8) for the periodic model one gets

$$\chi = \beta \tag{16}$$

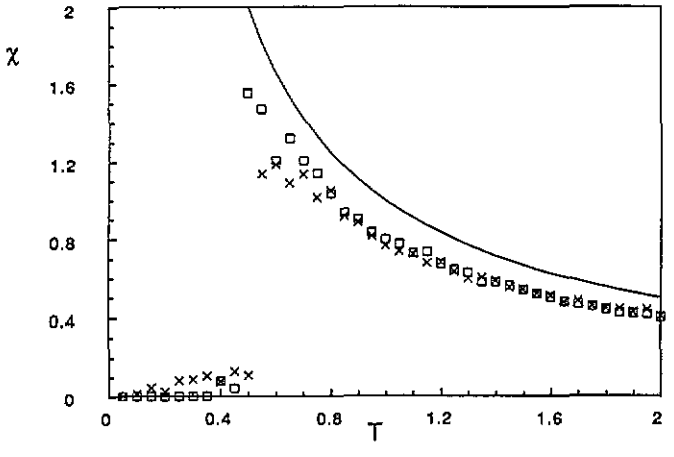

Figure 5. Magnetic susceptibility of the periodic model versus temperature. The full curve is the approximation (16). Simulation results are for $N = 100$ (□) and $N = 500$ (×).

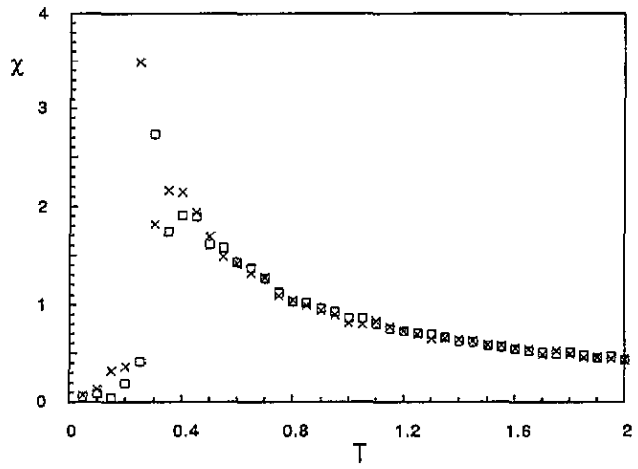

Figure 6. Magnetic susceptibility of the open model versus temperature. Simulation results are for $N = 500$ (□) and $N = 1000$ (×).

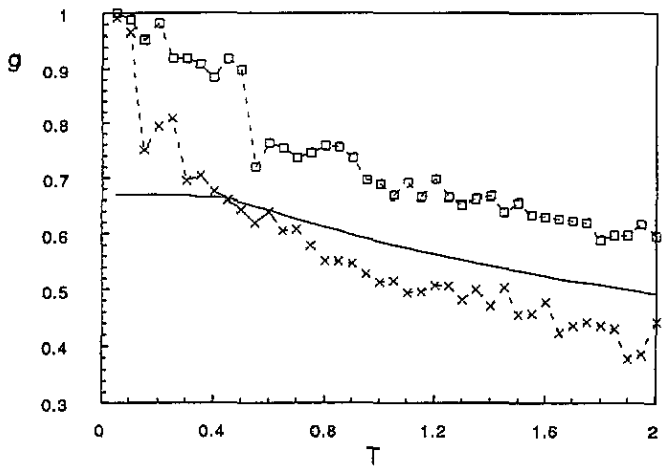

Figure 7. Binder parameter of the periodic and open models versus temperature. The full curve is the approximate high-temperature result to the periodic case (17). Data is shown for $N = 100$ in the periodic model (□) and $N = 500$ in the open case (×).

for the linear susceptibility of the periodic model. Figures 5 and 6 show the linear susceptibility obtained during an annealing process. Figure 5 also shows the prediction (16) for the periodic model. The values obtained for the glass transition from the discontinuity of the linear susceptibility agree with those obtained measuring the specific heat (figures 3 and 4).

In the case of the Binder parameter we use (9) which we can obtain in terms of the internal energy (now one has to be a little bit careful and realize that the integral of the fourth power of the magnetization, which is a real variable, over the probability distribution (15) is $\frac{3}{2}$ times the integral of the fourth power of any complex Fourier component B_p over the effective Hamiltonian (10)). One gets the result

$$g = \tfrac{3}{4}(1 - e)\,. \tag{17}$$

We show in figure 7 the behaviour of the Binder parameter associated with the magnetization for the periodic model (Monte Carlo results are also shown for the open case). It is shown up to $T = 2$ (five times the predicted glass temperature of the periodic model). For very large temperatures the Binder parameter should vanish because the magnetization distribution becomes a Gaussian. In our case it decays very slowly to zero, which indicates that well above the glass temperature fluctuations in the magnetization are large. Also from figure 7 we can observe a jump for the Binder parameter at the glass transition to a value close to 1. One comment about the high value of g above T_G is now appropriate. This large value of the curtosis parameter means that the probability distribution of the magnetization is far from being a Gaussian. It is a symmetric distribution very flat close to $M = 0$ and with possibly two peaks distributed symmetrically. As we will see in the next section, this result has strong implications for the dynamics. We expect that well above T_G the spin–spin correlation function $\langle \sigma(t_0)\sigma(t) \rangle$ decays to zero very quickly but the system can preserve a certain memory of the configuration at time t_0. In fact, if the $P(M)$ is so much flattened around $M = 0$, the system can need a very large time to reach configurations completely uncorrelated from the memorized configuration at t_0.

Let us summarize the results of this section. Performing annealings, starting from large temperatures down to the low-T region, we observe a glass transition where the energy freezes and fluctuations vanish. This temperature is several times larger than that predicted by the statics and this is related to the peculiar structure of the high-energy metastable states which the systems explore during the relaxation. More concretely, we have learned that the glassy temperature occurs at $T_G^C \simeq 0.45$ for the periodic model and $T_G^O \simeq 0.2$ for the open case. In the next section we will confirm these results by studying the off-equilibrium dynamics of these models. In particular, aging phenomena will appear as a good method for determining the glass transition.

4. Aging and the first-order nature of the dynamical transition

As we said in the last section this transition is of first-order nature in the dynamical order parameter. In principle, the dynamics are described by the two-time correlation functions $C(t_1, t_2)$ and the response functions $G(t_1, t_2)$. They are defined as usual by

$$C(t_1, t_2) = \langle \sigma_i(t_1)\sigma_i(t_2) \rangle \tag{18}$$

$$G(t_1, t_2) = \frac{\delta \langle \sigma_i(t_1) \rangle}{\delta h(t_2)} \quad t_2 < t_1 \tag{19}$$

where $\langle \cdots \rangle$ is the usual time average over different noise realizations in the dynamics and $h(t_2)$ is the magnetic field applied to the system at the time t_2. We have performed discrete Monte Carlo dynamics which we expect to give similar results as well as a usual Langevin dynamical process.

In the high-temperature regime, above the glass transition, we expect that the correlation and the response functions are related to each other by the fluctuation–dissipation theorem. Also in this high-T region the correlation and the response functions satisfy the time-homogeneity hypothesis, i.e. the functions $C(t_1, t_2)$ and $G(t_1, t_2)$ only depend on the time difference $t_1 - t_2$. Both functions decay very quickly in time.

Below the glass transition the time behaviour of the correlation and response function change drastically and, for instance, time correlations decay very slowly in time. In this low-T regime the time-homogeneity hypothesis is lost and strong aging effects start to appear. Then the decay of the correlation functions depends on the previous history of the system. More concretely, it depends on the time t_1 at which the spin configuration is

memorized (in the case of the correlation functions) or on the time t_2 at which the magnetic field is switched off (in the case of the response function).

For reasons of simplicity we have focused our research on the two-time correlation function (one could also perform aging experiments measuring the remanent magnetization). In this case we have measured the time–time correlation function between the spins configuration at the waiting time t_w and the configuration at the next time $t_w + t$,

$$C(t_w, t_w + t) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i(t_w)\, \sigma_i(t_w + t)\,. \tag{20}$$

Above the glass transition temperature we expect time homogeneity to apply (this means that $C(t_w, t_w+t)$ only depends on t) and time correlation functions should decay very quickly to zero. The following condition holds:

$$\lim_{t_w \to \infty} C(t_w, 2t_w) = 0\,. \tag{21}$$

Just below T_G the correlation function decays very slowly in time to a finite value q_1. This finite value q_1 is positive and smaller than the static Edwards–Anderson order parameter at the static transition point. This value q_1 is zero above T_G and is very close to 1 just below T_G and increases as the temperature decreases (linearly with T at low temperatures). We have to call readers attention to the fact that this value is physically related to the local order parameter associated with the metastable states and this is smaller than the local overlap associated with the true equilibrium configurations (the static Edwards–Anderson order parameter). The procedure for determining the value of q_1 has been applied recently to a particular deterministic model (see [11]) and corresponds to the replica order parameter within the same block as the one-step replica of replica-symmetry breaking. This is evaluated at the dynamical transition point where the free energy is maximized according to the marginality condition. More precisely, we can write (for an infinite system)

$$\lim_{t_w \to \infty} C(t_w, 2t_w) = q_1 \tag{22}$$

where q_1 depends on the temperature. For low autocorrelation models we know that the value of q_1 is very close to 1 (for instance, this is the greatest difference between p-spin glasses [26] or Potts glasses [27] and low autocorrelation models; the last ones show a very large discontinuity in the value of q_1). Because the value of q_1 jumps from zero above T_G to a finite value below T_G the transition is of a discontinuous type. Before showing our dynamical results in the case of low autocorrelation binary sequences we would like to note that, as regards dynamical experiments, deterministic models are much more suited than disordered models. Because our model is ordered, we do not need to save the realization of the random couplings. The number of random couplings, in the case of a long-range model, can be very large and this sets a limit on the maximum size one is able to memorize in the computer. The major part of the numerical results we will show correspond to $N = 5000$ in both models (open as well as in the periodic case).

The existence of aging is one of the most outstanding features of spin glasses [28]. Now we are going to show that low autocorrelation models also exhibit these phenomena just below the glass transition. Because the results we have obtained for the periodic and the open case are very similar, in some cases we will present the results for just the open case. Figure 8 shows the correlation function (20) for the open model, for different values of the waiting time above the glass transition T_G (as estimated in the previous section). The data in this case corresponds to a temperature $T = 0.45$. This figure shows that above the glass transition the aging effects are absent (i.e. the correlation functions do not depend on the

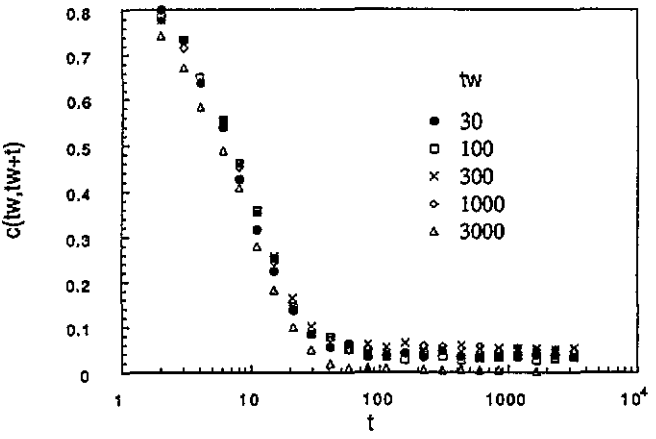

Figure 8. $C(t_w, t + t_w)$ for the open model for different values of t_w above the glass transition at $T = 0.45$. The size is $N = 5000$.

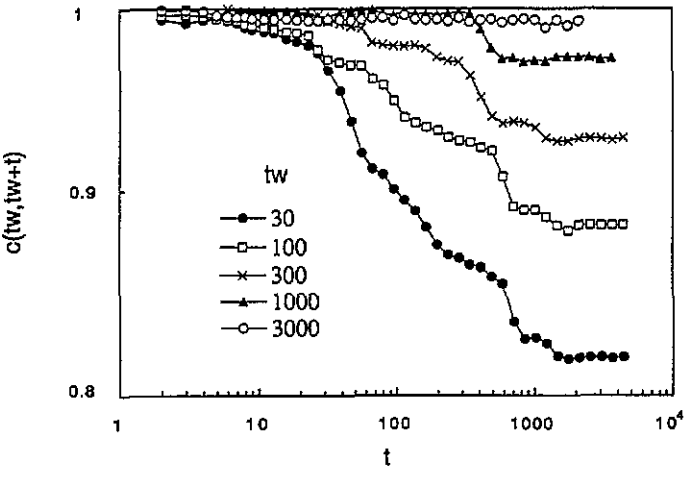

Figure 9. $C(t_w, t + t_w)$ for the open model for different values of t_w below the glass transition at $T = 0.1$. The size is $N = 5000$.

value of t_w). Also, all correlation functions decay very quickly with the time. Surprisingly (as shown in figure 8) they do not always decay to zero. In some cases, they decay to a small finite value (for the suspicious reader we will note that this value is larger than the standard deviation $1/\sqrt{N}$). This means that, well above the glass transition, the system preserves a small temporal correlation with previous configurations. As discussed in the previous section, this is strongly related to the non-Gaussian nature of the fluctuations (for instance, this was shown in the case of the magnetization). This behaviour is far from being paramagnetic. It is not clear to us what is the real dynamical nature of this high-T region..

As soon as we go below T_G the dynamics slow down dramatically. The system remains trapped in metastable states and it takes a very long time for the system to overcome the barriers and explore new configurations. This is seen clearly in the results of figure 9 where we show the correlation function below the glass transition at $T = 0.1$ for one realization of the noise for the open model. Aging effects are present and we expect correlation functions

to depend mainly on the ratio t/t_w, for large enough values of t_w. Some comments are now in order. As shown in figure 9, the correlation function stays very close to 1 during a time of the order of 10^4 Monte Carlo steps for all different waiting times. This is because for enough low temperatures the system is able to surmount only a few numbers of states and the shape of the correlation function is strongly dependent on the noise realization. To get smooth correlation functions one should average over a very large number of trajectories and this demands a lot of computer time. From these considerations it emerges that a scaling law of the type

$$C(t_w, t + t_w) \sim f(t/t_w) \tag{23}$$

is very difficult to observe in a small number of decades of time. This scaling law has been obtained by Bouchaud in his phenomenological approach to the off-equilibrium dynamics [29]. Cugliandolo and Kurchan [15] have shown explicitly that this is indeed a solution of the off-equilibrium equations in case of the p-spin spherical spin-glass model and the Potts model [30]. These models do have a spin-glass phase with one step of replica-symmetry breaking. It is reasonable to suppose that the scaling law (23) also applies in the case of low autocorrelation models for which a REM-like transition describes the low-T behaviour well. We should also note that the dynamical behaviour we are observing in these models is strongly different from the dynamical relaxation of the SK model [31] or short-range Ising spin glasses [32]. In this case, one does not have a first-order dynamical transition and the free-energy landscape is not so rough. The system is not trapped in the metastable states and correlation functions decay to zero smoothly without apparent jumps [19]. When a strong metastability is present (as in low autocorrelation models) new numerical techniques like those recently developed by Krauth and Pluchery [23] and Krauth and Mezard [22] are very useful. If one wants to observe smooth aging over a reasonable time scale, it is mandatory to go to higher temperatures. Precisely at the glass temperature we expect that the system will display nice aging and the scaling law (23) will be satisfied for enough large sizes. This is shown in figure 10, where we have measured the aging at a temperature

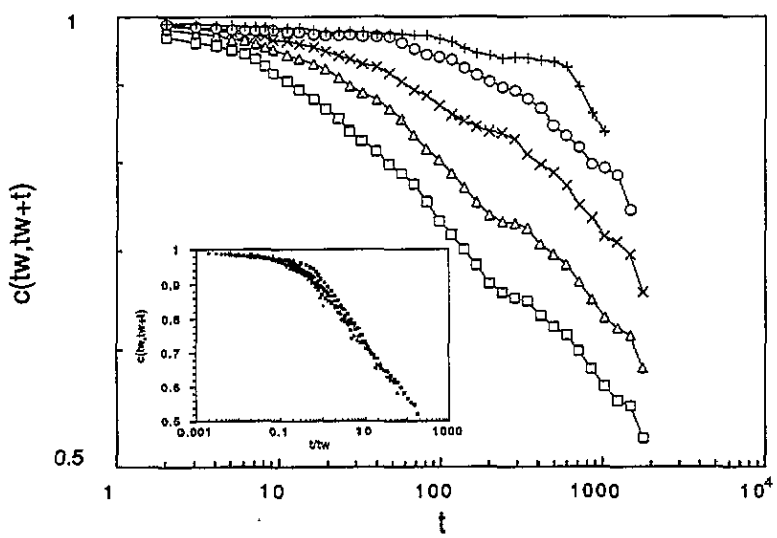

Figure 10. $C(t_w, t+t_w)$ for the open model for different values of t_w close to the glass transition ($T_G \sim 0.19$). The inset shows the scaling law (23). The size is $N = 10000$. The symbols correspond to different values of t_w: 30 (+), 100 (○), 300 (×), 1000 (△) and 3000 (□).

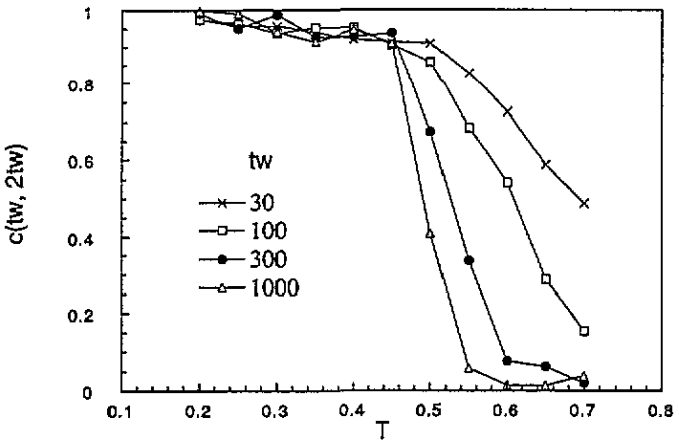

Figure 11. $C(t_w, 2t_w)$ for the periodic model for different values of $t_w = 30, 100, 300$ and 1000 as a function of the temperature.

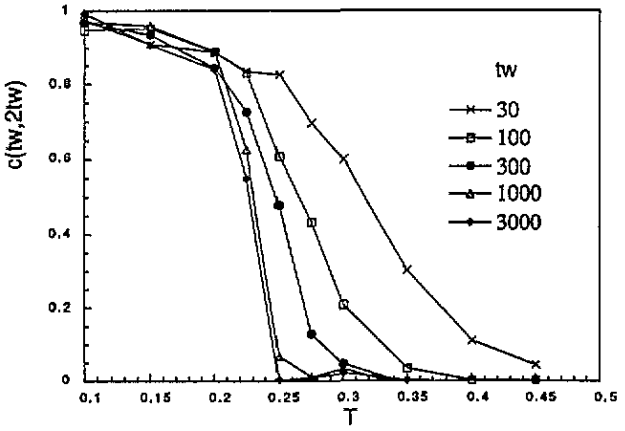

Figure 12. $C(t_w, 2t_w)$ for the open model for different values of $t_w = 30, 100, 300, 1000$ and 3000 as a function of the temperature.

$T_G \sim 0.19$ for the open model and a very large size $N = 10000$. The inset of figure 10 shows the scaling law (23).

Now we want to show how aging allows for a nice confirmation of the first-order nature of the glass transition. This is one of the main results of this work. Because the nature of this glass transition is purely dynamical we can use the relations (21) and (22) in order to find the temperature at which the discontinuity of the order parameter appears. A similar technique could be used by coupling two replicas, as has been done in case of the p-spherical spin-glass model [33]. Nevertheless, we think that our dynamical technique is more direct because we do not need the introduction of an extra coupling parameter in the model.

We have computed the correlation function for different waiting times t_w and also different temperatures. Then, for each temperature, we computed $C(t_w, 2t_w)$, averaging the correlation function in a logarithmic scale. We proceeded in this way in order to get smooth values of the correlation $C(t_w, 2t_w)$ as a function of the temperature and the waiting time.

We have done this numerical analysis for different values of $t_w = 100, 300$ and 1000 in the periodic model and $t_w = 100, 300, 1000$ and 3000 for the open model. Figures 11 and 12 show the results for the periodic and open model, respectively. From this data we can clearly see the discontinuity because the predicted value of q_1 is very close to 1 just below T_G.

In order to obtain T_G we have performed a usual finite-time scaling analysis. To this end we have measured the relaxation curves above the glass transition and also above the temperature at which finite-size effects are negligible (approximately $T = 0.25$ for the open model and $T = 0.55$ in the periodic case). Correlation functions decay exponentially and one can estimate the relaxation time τ as a function of T. In this range of temperatures we expect the correlation time will diverge as a power-law singularity of the type

$$\tau \sim (T - T_G)^{-\gamma} \tag{24}$$

where γ is a dynamical exponent. We note that this kind of divergence is also typical of disordered systems with long- or short-range interactions. In the case of frustrated models without disorder the situation can be different depending on the range of the interaction. Low autocorrelation models are of the long-range type. It is possible that for more realistic models of glasses the dynamics will be much more complex and very different relaxation behaviours, like the Arrhenius or the Vogel–Fulcher law, could take place. Now we want to observe that usual critical dynamics works well in the case of low autocorrelation models. This is not surprising if (as we have seen in this work) glasses and spin glasses do have so much in common [34]. We have fitted the correlation functions in the high-T regime with a scaling law of the type

$$c(t) \sim f(t/\tau) \tag{25}$$

where τ is given in (24). The scaling behaviour is shown in figures 13 and 14 for the open model and the periodic model, respectively. Good fits are obtained with $T_G \sim 0.21 \pm 0.02$ and $\gamma \sim 2 \pm 0.5$ for the open model and $T_G \sim 0.43 \pm 0.2$ and $\gamma \sim 2 \pm 0.5$ for the periodic model. The scaling function $f(t/\tau)$ is nearly an exponential in both cases. The exponent γ is the equivalent of the product of exponents $z\nu$ for the usual critical dynamics and it is certainly much lower than known values in realistic glasses (typically these are of the order of 10, see [34]). As we have already indicated, low autocorrelation models are

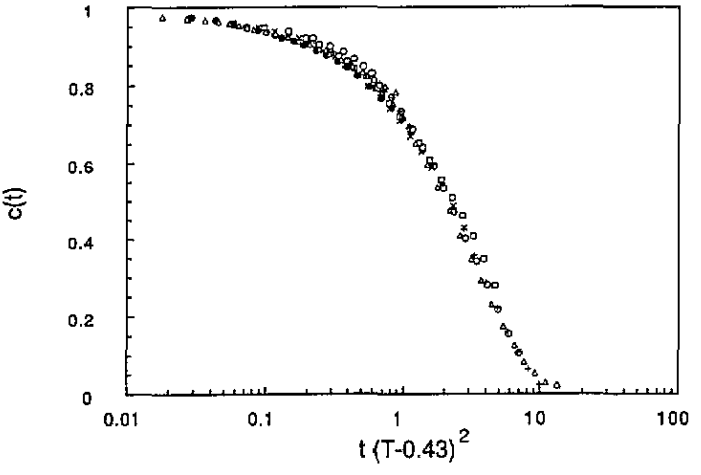

Figure 13. Finite-time scaling (25) for the periodic case. Good scaling is obtained with $T_G \sim 0.43 \pm 0.02$ and $\gamma \sim 2$.

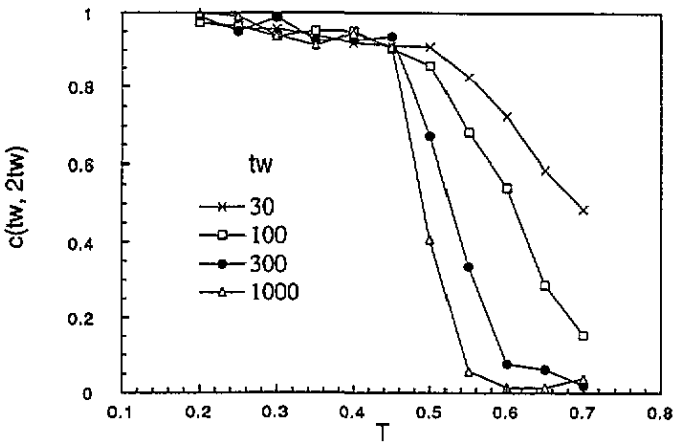

Figure 14. Finite-time scaling (25) for the open case. Good scaling is obtained with $T_G \sim 0.21 \pm 0.02$ and $\gamma \sim 2$.

long-range models. Realistic glasses are not of the long-range type and it could well be that the exponent γ increases as the dimensionality decreases. This happens in the case of Ising spin glasses where the product $z\nu$ ranges from 2 in mean-field theory to 6 in three dimensions [35] (in the case there is a true phase transition [36]).

5. Conclusions

Low autocorrelation models display a dynamical behaviour very similar to disordered spin glasses. The reason for this similarity is that these models (and more generally, glasses) do have a broad distribution of higher free-energy metastable states, as happens in the case of spin glasses [7].

The feeling which emerges from recent studies by several groups is that deterministic models display a glassy behaviour of a purely dynamical nature. This glassy behaviour seems to be associated with spin-glass models with one step of replica-symmetry breaking [17]. In the case of models with an infinite number of breakings like the SK model [18] the situation is different [19].

We have also seen that the open case and the periodic case behave very similarly. We have studied the relaxation of magnitudes like the internal energy, specific heat and magnetic susceptibility. More interestingly, the Binder parameter associated with the magnetization has a non-Gaussian shape even for very large temperatures above the glass transition. This result should very probably also apply for any other Fourier component B_p of the configuration of the spins.

According to this result we have seen that well above the glass transition the dynamical correlation functions decay exponentially fast to a small non-zero value. The system is not fully ergodic because it has some memory about the previous configurations it has visited. We have given an explanation of this fact but it remains unsolved as to what the real nature of this high-T phase is. We want to stress that the high-T phase, not being fully ergodic, makes the real nature of this dynamical phase transition unclear. It seems purely first-order but we think it is more complex than the glass transition found in the case of other deterministic models [2,5] or spin glasses (i.e. models with an exact solution at one

step of replica-symmetry breaking).

Above the glass transition temperature finite-time scaling analysis has revealed a good technique in order to locate the transition and the dynamical exponents. For the open and periodic models we obtain the equivalent of the product exponents $z\nu$ of the critical dynamical theory. Values close to 2 are obtained. Compared with experimental values obtained in the case of real glasses, these are small, but this could be an artifact of the long-range interactions of the low autocorrelation models.

We have also investigated the dynamics below the glass transition, where aging phenomena are present. This is one of the main features in spin glasses. At the glass transition, where the effect of the traps is not very strong, we have found that the scaling law (23) is well reproduced.

We conclude by saying that the techniques developed in this work are very general and should be applicable to a large variety of systems where disorder is not present. In particular, we think that the behaviour of $c(t_w, 2t_w)$ as a function of temperature is well suited in order to characterize the transition. It remains to be understood to what extent the results obtained in this work are generic for real glasses and to what extent short-range interactions can modify the main conclusions of this work.

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