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LETTER TO THE EDITOR

Short-time aging in binary glasses

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Abstract. We present some simple computer simulations that indicate that short-time aging is realized in a simple model of binary glasses. It is interesting to note that modest computer simulations are enough to prove this effect. We also find indications of a dynamically growing correlation length.

1. Introduction

Aging was discovered a long time ago and it has been experimentally studied in great detail in some materials [1]. Later it was realized that it is a quite common phenomenon in physics. It is only recently [2–4] that this has been the subject of wide theoretical investigations. Basically, aging predicts that the response of the system to a force that has been applied for a time t depends on t (also for very large times) when t is comparable with the waiting time t_w, i.e. the time the systems remained in the final conditions before starting the experiment.

Aging has been studied analytically in generalized spin glasses: in the simplest form it predicts that the correlation functions among a configuration at time t_w and at time $t_w + t$ depend only on the ratio t/t_w in the limit of large times [3]. This form of aging is approximately found to be correct in spin glasses, both in experiments and numerical simulations [5–7] (although some small modification may be needed). Slightly different forms of aging have been proposed, for example the scaling variable could be t/t_w^u with μ near but not equal to 1. Here we stick to the t/t_w scaling and refer to it as *simple aging*.

The aim of this letter is to start a systematic study of aging using numerical simulations in glasses. We will show that the aging regime starts at relatively short times and some of its properties can be investigated with a modest amount of computer time. We limit ourselves to the analysis in the initial-time region, leaving the study of the behaviour at larger times and in bigger systems to future, more systematic investigations.

The numerical experiment that we present here is rather simple: we run a numerical simulation where the system starts from a fully random configuration (i.e. at infinite temperature). The system is then carried (at time zero) at temperature T. We take a photograph of the system at time t_w and compare the latter evolution of the system with this reference configuration.

The main quantity on which we concentrate our attention is the two-times correlation function

$$g(r, t_w, t) = \sum_{i,k=N} \frac{\langle \delta(|x_i(t_w) - x_k(t_w + t)| - r) \rangle}{N} \tag{1}$$

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where N is the total number of particles and $x_i(t)$ denotes the position of the particle i at time t. In the limit of large times, $g(r, t, t)$ goes to the usual correlation function for liquids (apart from an extra delta function at the origin, which is absent in the usual definition where the sum is restricted to $i \neq k$).

For this function simple aging predicts that for *both* t and large t_w, we have the scaling relation

$$g(r, t_w, t) \approx G(r, s) \qquad \text{where } s \equiv \frac{t}{t_w}. \tag{2}$$

We have tested this relation for binary fluids. The model we consider is the following. We have taken a mixture of soft particles of different sizes. Half of the particles are of type A, half of type B and the interaction among the particle is given by

$$\sum_{i<k} \left(\frac{(\sigma(i) + \sigma(k)}{|x_i - x_k|} \right)^{12} \tag{3}$$

where the radius (σ) depends on the type of particles. This model has been carefully studied in the past [8–10]. It is known that a choice of the radius such that $\sigma_B/\sigma_A = 1.2$ strongly inhibits crystallization and the system goes into a glassy phase when it is cooled. Using the same conventions of the previous investigators we consider particles of average diameter 1, more precisely we set

$$\frac{\sigma_A^3 + 2(\sigma_A + \sigma_B)^3 + \sigma_B^3}{4} = 1. \tag{4}$$

Due to the simple scaling behaviour of the potential, the thermodynamic quantities depend only on the quantity $T^4/\rho, T$ and ρ being respectively the temperature and the density. For definiteness we have taken $\rho = 1$. The model has been widely studied, especially for this choice of parameters. It is usual to introduce the quantity $\Gamma \equiv \beta^4$. The glass transition is known to occur around $\Gamma = 1.45$ [9].

Our simulations are performed using a Monte Carlo algorithm, which is more easy to determine than molecular dynamics, if we change the temperature in an abrupt way. Each particle is shifted by a random amount at each step, and the size of the shift is fixed by the condition that the average acceptance rate of the proposal change is about 0.5. Particles are placed in a cubic box with periodic boundary conditions and at the end of each Monte Carlo sweep all the particles are shifted by the same vector in order to keep the centre of mass fixed [11]. This last step is introduced in order to avoid the centre of mass drifting and it would not be necessary in molecular dynamics if we start from a configuration at zero total momentum.

In our simulations we have considered a relatively small number of particles, $N = 34$, $N = 66$ and $N = 258$ (most of the data we show are for $N = 258$). We start by randomly placing the particles and we quench the system by putting it at $\Gamma = 1.8$, i.e. at a temperature well below the glass transition. The energy, as a function of the Monte Carlo time (t is the number of Monte Carlo sweeps), is shown in figure 1. The data are averaged over 25 different realizations of the dynamics with different initial conditions. The energy seems to decay to an asymptotic value with some corrections which vanish as a power of time.

We have measured the correlation function G for different choices of t_w (i.e. $t_w = 32$, 128, 512, 2048, 8192) at $s \equiv t/t_w$ equal to 3. If we exclude the points at $t_w = 32$ (which we have not plotted), the data for the correlation functions have a very similar shape independently of t_w at fixed s, as expected from simple aging. In order to check the aging

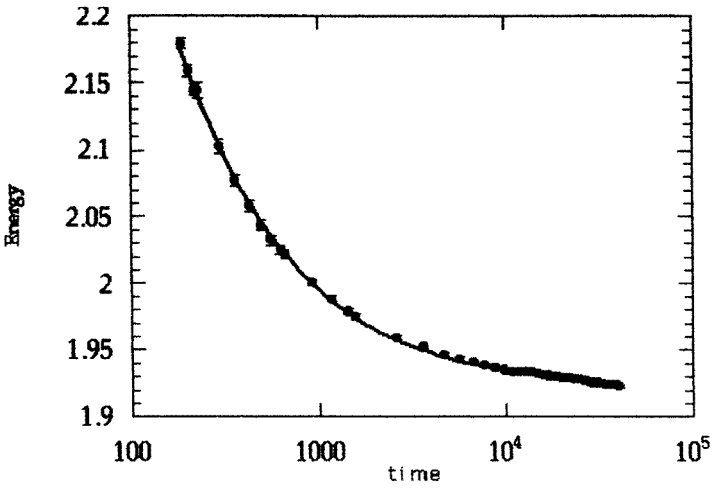

Figure 1. The energy density for 258 particles as a function of time. The fit is $E = E_\infty + At^{-\lambda}$ with $E_\infty = 1.92$, $A = 12$ and $\lambda = 0.7$.

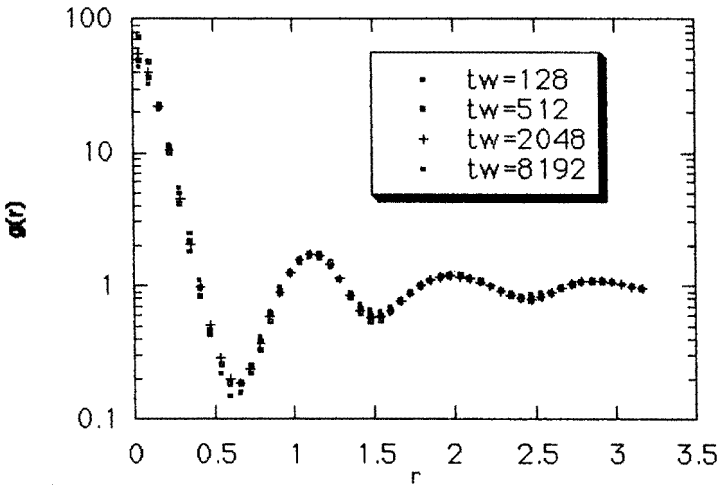

Figure 2. The correlation function $G(r, t_w, t)$ as function for r for $N = 258$ for different values of $t_w (t_w = 128, 512, 2048, 8192$, at t/t_w equal to 3. The data have been averaged over 25 different initial conditions.

in a more quantitative way and to prove possible violations of aging, we have introduced the quantity $q(t_w, t)$ defined as

$$q(t_w, t) = \int \mathrm{d}x\, g(x, t_w, t) f(x) \equiv \sum_{i,k=1,N} \frac{f(x_i(t + t_w) - x_k(t_w))}{N^2} \tag{5}$$

where we have chosen the function f in such a way that it is sensitive to the area of the central peak, i.e.

$$f(x) = \frac{a^{12}}{x^{12} + a^{12}} \tag{6}$$

with $a = 0.3$. The function f is very small when $x \gg 0.3$ and near to 1 for $x < 0.3$. The

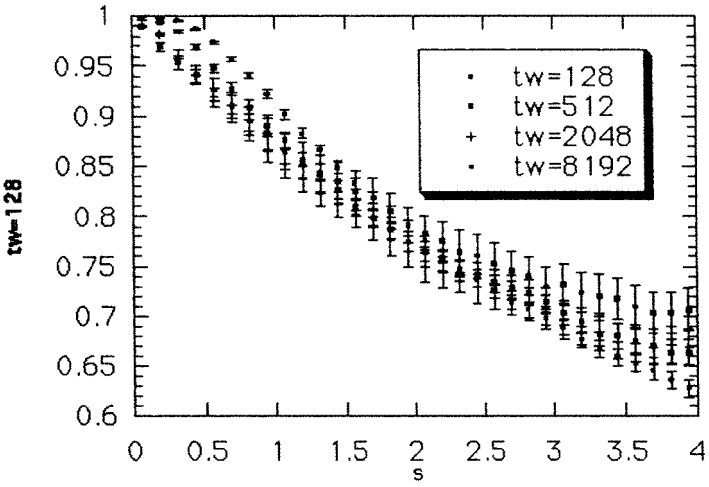

Figure 3. The overlap q as function of s for $t_w = 128, 512, 2048, 8192$ and $N = 258$, averaged over 25 initial conditions.

value of q is a number very near to 1 for similar configurations (in which the particles have moved less than a) and it is a much smaller value (less than 0.l) for unrelated configurations; using the same terminology as in spin glasses [12–14] q can be called the overlap of the two configurations.

In figure 3 we plot the overlap as a function of s at different waiting times. We note that for s near to zero there is a noticeable dependence on the waiting time, which can be related to the fact that t is not large. There is a small upward drift of the data at large s. In order to illustrate the proof of the effect, in figure 4 we plot the function q at $s = 4$ as a function of t_w. In this pattern of violations of simple aging, a downward drift at small s and an upward drift at large s is quite a common phenomenon. Here it is not clear whether these violations are the effects of transient pre-asymptotic terms or the effect of small violations of the simple aging hypothesis in the asymptotic limit. This point should be carefully investigated in the future and its clarification goes beyond the aim of this letter.

It would be interesting to study which is the most relevant scale of distances in the aging process. A possible indirect approach to this question is the following. The data on smaller systems indicates that there are strong volume effects at large times [15]. In order to find the physical origin of this effect it is instructive to look to the time dependence of the fluctuations of q from sample to sample, i.e. to

$$\Delta(t_w, t) \equiv \langle (q(t_w, t) - \langle q(t_w, t) \rangle)^2 \rangle \tag{7}$$

where the average is found over different realization of the initial conditions.

In figure 5 we show the data (at $s = 4$) for

$$M(t_w) \equiv N\Delta(t_w, 4t_w) \tag{8}$$

versus $t_w^{1/2}$. The quantity $M(t_w)$ seems to increase as a power of time with the exponent μ near $\frac{1}{2}$ and shows a weak dependence on the size (as expected, usually fluctuations are proportional to $N^{-1/2}$).

In order to interpret these results it is convenient to recall the physical picture at the base of simple aging: the system evolves by a sequence of quasi-equilibrium states and remains in a given state for a time proportional to the time needed to arrive at it. In the

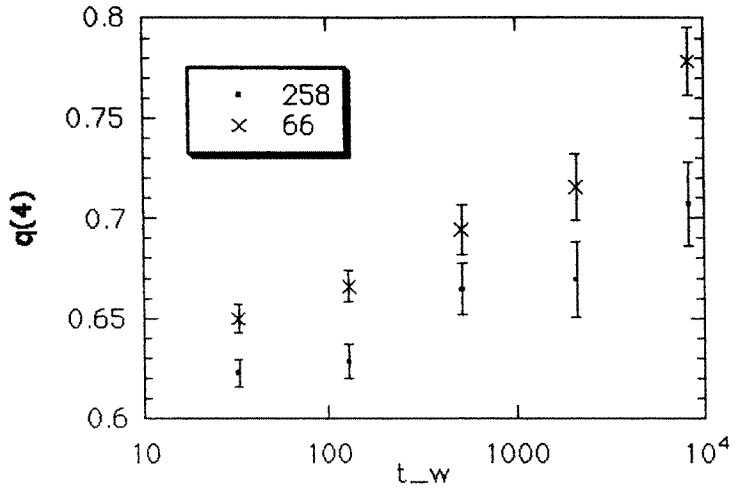

Figure 4. The value of the overlap q at $s = 4$ as a function of t_w for $N = 66$ and $N = 258$.

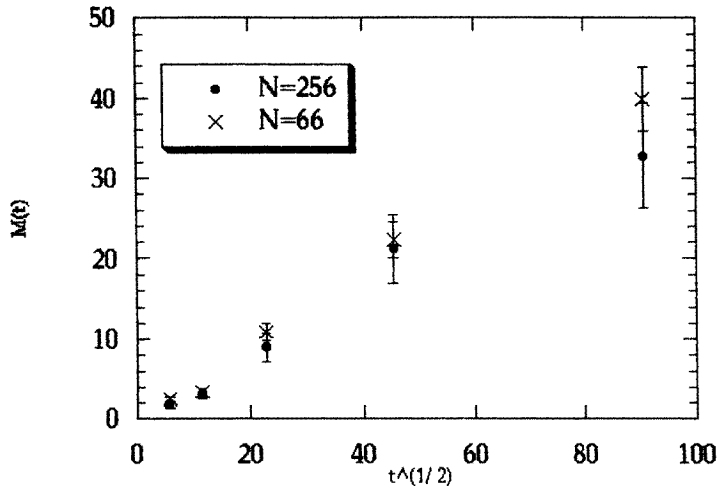

Figure 5. The value of $M(t_w)$ as a function of $t_w^{1/2}$ at $s = 4$.

most extreme picture we have a punctuated equilibrium of a long period of stasis intermixed by fast, thermally activated, tunnelling events. Increasing the value of t_w, the barrier that we have to cross becomes higher and higher, such that collective movements involve a large number of particles. Roughly speaking, we expect that the variance of q (i.e. Δ) is inversely proportional to the number ($\mathcal{N}(t_w)$) of regions which have been moved independently i.e.

$$\Delta(t_w) \propto \mathcal{N}(t_w)^{-1} = N^{-1}(\mathcal{N}(t_w)/N)^{-1}. \tag{9}$$

The quantity $\mathcal{N}(t_w/N)$ may be interpreted as the volume of the regions that move together in a simultaneous way. The previous result implies that the time variation of q is dominated by events which involve the rearrangements of regions of a size which increases at least as $t^{\mu/3}(\mu/3 \approx \frac{1}{6})$. This type of behaviour (i.e. a dynamical correlation length increasing as a power of time) has been seen in quenched-disordered systems such as spin glasses [16, 17].

These considerations imply a change in the behaviour of the system when the number

of particles involved in a typical rearrangement becomes of the same order as the sample size. It is evident that when the variance of $q(\Delta)$ becomes comparable with $(1-q)^2$ the distribution of q can no longer be Gaussian (the overlap cannot become greater than 1!) and we enter into a new regime. Strong finite-size effects are thus expected for sufficiently large times, i.e. for times which increase as $N^{1/\mu}$. It is also quite likely that for sufficiently large times a finite system reaches a low-energy state such that further jumps are inhibited or occur on a much larger timescale [18].

Therefore the conclusions of this letter are as follows.

- Aging effects can also be observed at relatively short times in binary glasses.
- Simple aging is observed for a variation of about two orders of magnitude in the waiting time with deviations which are at most 10%.
- It is suggested that there is a dynamical correlation length, that indicate the size of the regions which are collective rearranged, which diverges as a power of time. (A direct study of the size of the rearranged regions in the equilibrium dynamics can be found in [1].)

Further numerical simulations are needed to decide whether the small violations of simple scaling are finite-volume effects or they survive in larger samples. It would also be interesting to study the temperature dependence of the effect and compare the results with detailed theoretical predictions.

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References

[1] Struik L C E 1978 *Physical Aging in Amorphous Polymers and other Materials* (Houston: Elsevier)
[2] Bouchaud J-P 1992 *J. Physique* **2** 1705
[3] Cugliandolo L F and Kurchan J 1993 *Phys. Rev. Lett.* **71** 1
[4] Franz S and Mézard M 1994 *Europhys. Lett.* **26** 209
[5] Cugliandolo L F, Kurchan J and Ritort F 1994 *Phys. Rev.* B **49** 6331
[6] Franz S and Rieger H 1995 *Phys. J. Stat. Phys.* **79** 749
[7] Vincent E, Hammann J, Ocio M, Bouchaud J-P and Cugliandolo L F 1997 *Sitges Conference on Glassy Systems* ed M Rubi (Berlin: Springer)
[8] Bernu B, Hansen J-P, Hitawari Y and Pastore G 1987 *Phys. Rev.* A **36** 4891
[9] Barrat J-L, Roux J-N and Hansen J-P 1990 *Chem. Phys.* **149** 197
[10] Hansen J-P and Yip S 1995 *Trans. Theor. Stat. Phys.* **24** 1149
[11] Lancaster D and Parisi G 1997 *J. Phys. A: Math. Gen.* **30** 5911
[12] Edwards S F and Anderson P W 1975 *J. Phys. F: Met. Phys.* **5** 965
[13] Mézard M, Parisi G and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific)
[14] Parisi G 1992 *Field Theory, Disorder and Simulations* (Singapore: World Scientific)
[15] Horbach J, Kob W, Binder K, Angell C A 1996 *Some Finite Size Effects in Simulations of Glass Dynamics* preprint cond-mat 9610066
[16] Rieger H 1994 *J. Physique* **4** 883
[17] Marinari E, Parisi G, Ruiz-Lorenzo J J and Ritort F 1996 *Phys. Rev. Lett.* **76** 843
[18] Bouchaud J-P, Vincent E and Hammann J 1995 *Phys. Rev.* B **52** 1050