Short time aging in binary glasses

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Abstract

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

Aging has been discovered long time ago and it is has been experimentally studied in great details in some materials [1]. It has been later realized that it is a quite common phenomenon in physics. It has been the subject of wide theoretical investigations only recently [2, 3, 4]. In the nutshell 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 to the waiting time t_w, i.e. the time at which the systems has been carried to conditions at which the experiment has been done.

Aging has being 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 ration 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 in numerical simulations [5, 6, 7], (although some small modification may be needed). Slightly different forms of aging have been proposed, e.g the scaling variable could be t/t_w^μ with μ near but not equal to 1. Here we stick to the t/t_w scaling and we will refer to it by the name of *simple aging.*

The aim of this note it to start a systematic study of aging using numerical simulations in real 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 to further more systematic investigations the study of the behaviour at larger times and in bigger systems.

The numerical experiment 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 make a photograph of the system at time t_w and we compare the later evolution of the system with this reference configuration.

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

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

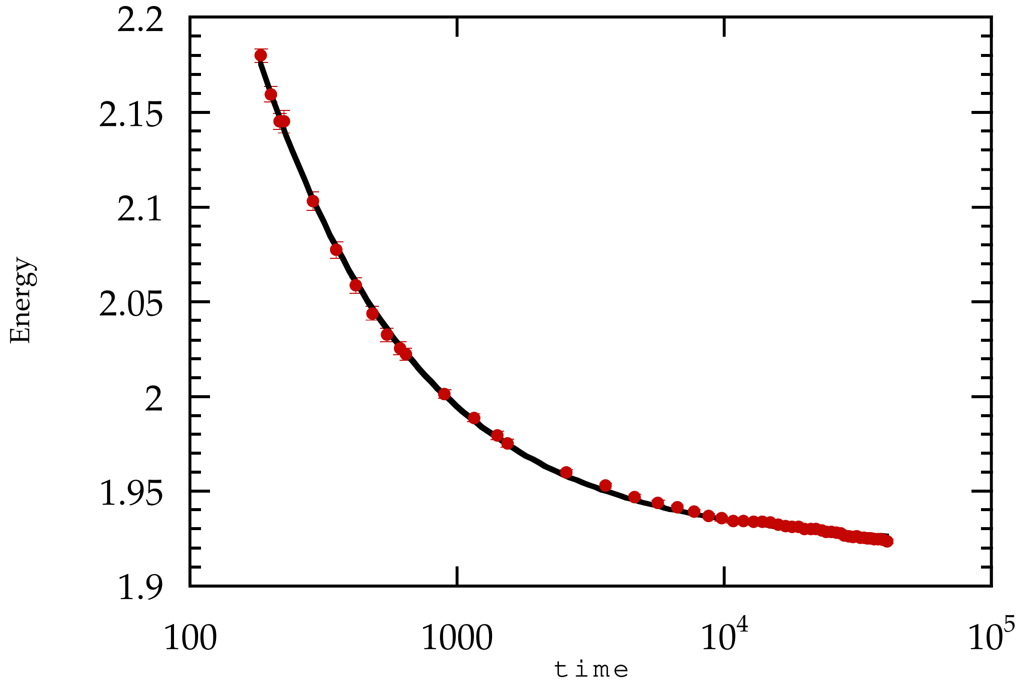

Figure 1: The energy density for 258 particles as function of time. The fit is $E = E_\infty + At^{-\lambda}$ with $E_\infty = 1.92$, $A = 12$ and $\lambda = .7$.

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 definitions where the sum is restricted to $i \neq k$).

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

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

We have tried to test this relation for binary fluids. The model we consider is the following. We have taken a mixture of soft particle 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 studied in the past [8, 9, 10]. It is known that a choice of the radius such that $\sigma_B/\sigma_A = 1.2$ strongly inhibits crystallisation and the systems 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/ρ, T and ρ being respectively the temperature and the density. For definiteness we have taken $\rho = 1$. The model as been widely studied especially for this choice of the parameters. It is usual to introduce the quantity $\Gamma \equiv \beta^4$. The glass transition is known to happen around $\Gamma = 1.45$ [9].

Our simulation are done using a Monte Carlo algorithm, which is more easy to deal with 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 .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 of the same vector in order to keep the center of mass fixed [11]. This last step in introduced in order to avoid drifting of the center of mass and it would be not 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 placing the particles at random 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 function of the Monte Carlo time (t) is shown in fig. 1. The data are the average over 25 different realization of the dynamics with different initial conditions. The energy seems to decay to an asymptotic value with some corrections which vanishes as a power of time.

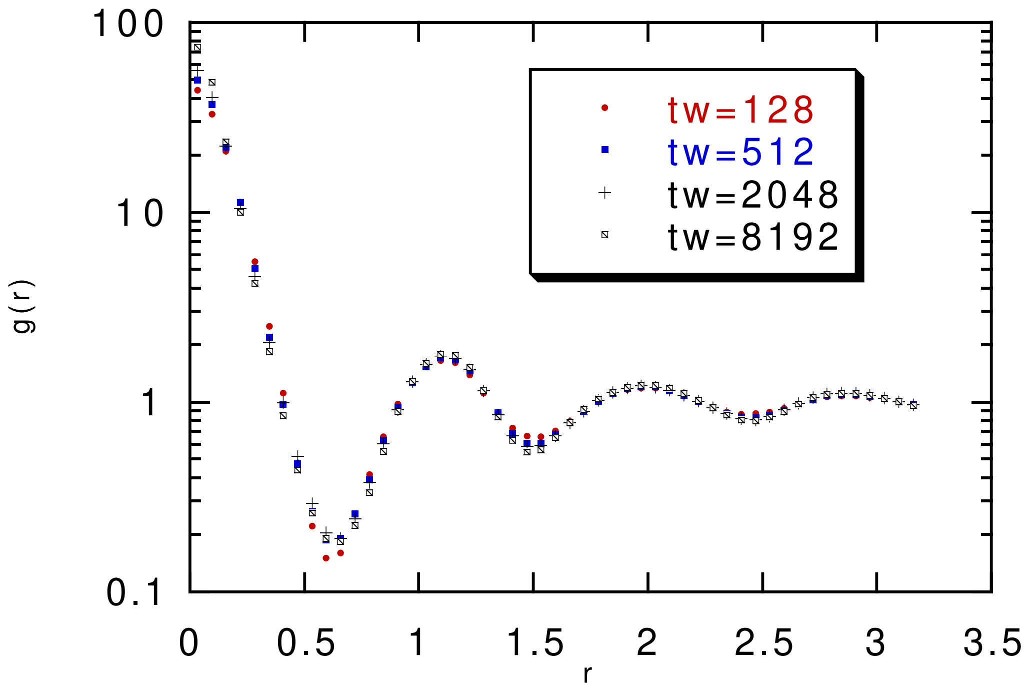

Figure 2: The correlation function $G(r, t_w, t)$ as function of r for $N = 258$ for different values of t_w (t_w=128, 512,2048 ,8192, at t/t_w equal to 3. The data have been averaged over 25 different initial conditions

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

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

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 $a = .3$ The function f is very small when $x >> .3$ and near to 1 for $x < .3$. The value of q will thus be a number very near to 1 for similar configurations (in which the particles have moved of less than a) and it will be much smaller value (less than .1) for unrelated configurations; using the same terminology as in spin glasses [12, 13, 14] q can be called the overlap of the two configurations.

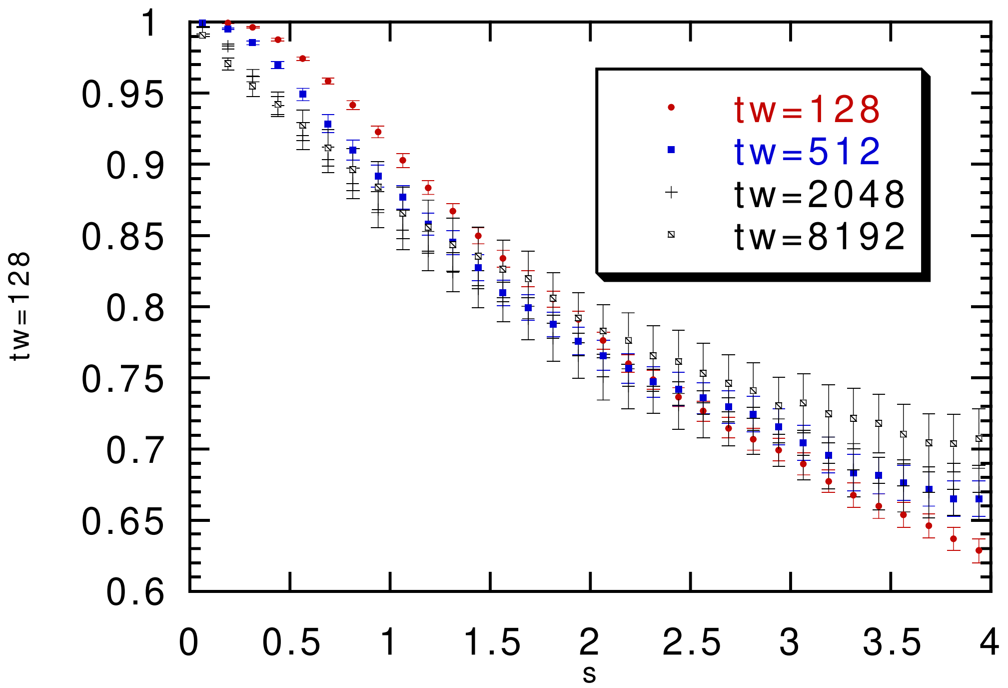

Figure 3: The overlap q as function of s for t_w=128, 512, 2048, 8192 and $N = 258$, averaged over 25 initial conditions.

In fig.3 we plot the overlap as function of s at different value of the waiting time. We notice that for s near to zero there is noticeable dependence on the waiting time, which can be related to the fact that t is not large. There is a small drift of the data at large s. In order to see evidenziate the effect we plot in fig.(4) the function q at $s = 4$ as function of t_w.

It is not clear if the increase at larger values of t_w is due to finite size correction or to small violations of the simple aging hypothesis. This point should be carefully investigated in the future and its clarification goes beyond the aim of this note. The data on smaller systems indicates that there are definitely strong volume effects at large times [15]. This may seem surprising; in order to find the physical origine of this effect it is instructive to look to the time dependance of the fluctuations of q from sample to sample, i.e. to

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

where the average is done over different realization of the initial conditions. This quantity seems to increase a a power of t_w with and exponent μ near to 1/2. In fig. 5 we show the data (at $s = 4$) for

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

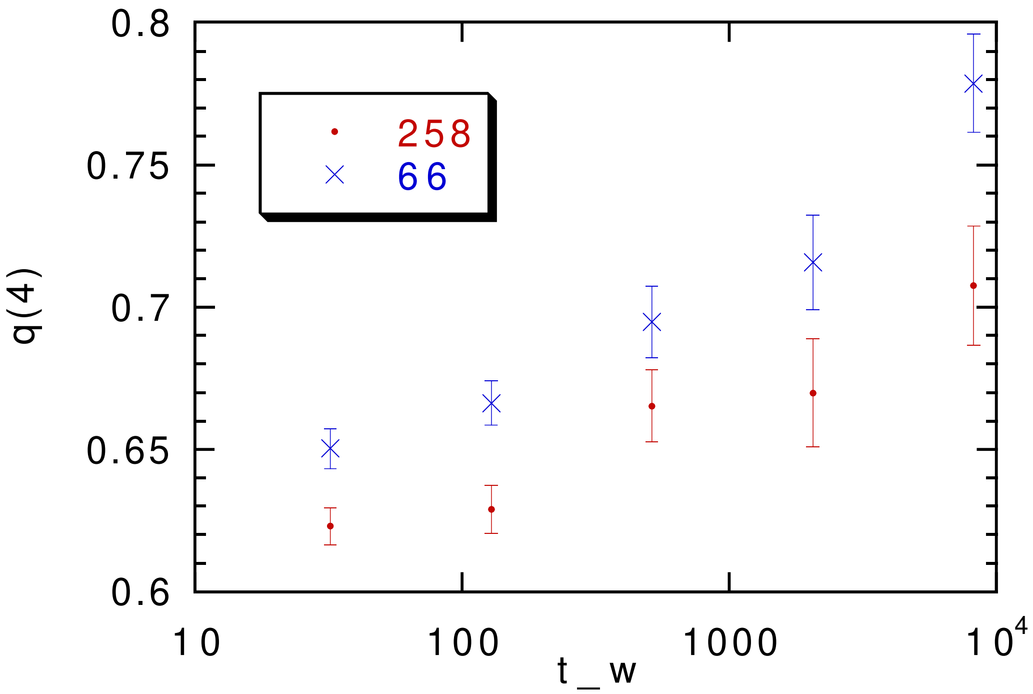

Figure 4: The value of the overlap q at $s=4$ as function of t_w for $N=66$ and $N=258$.

versus $t_w^{1/2}$. The quantity $M(t_w)$ seem to increase a a power of time and shows a weak dependance on the size (as expected, usually fluctuations goes to zero as $N^{-1/2}$).

In order to interprete this 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 time needed to arrive to it. In the most extreme picture we have a punctuated equilibrium of long period of stasis intermixed by fast, thermally activated, tunnelling events. Increasing the value of t_w the barrier that we have to cross become higher ad higher and such collective movements involves a large number of particles. Roughly speaking we expect that the variance Δ is inversely proportional to the number $(N/M(t_w))$ of regions which have been moved independently, i.e.

$$\Delta(t_w) \propto \frac{M(t_w)}{N}. \tag{9}$$

The previous result imply that the time variation of q is dominated by events which involve the rearrangements of regions of size which increase at least as $t^{\mu/3}$. This type of behaviour (i.e. a dynamical correlation length increasing as a power of time) has been seen in quenched disordered systems like spin glasses [16, 17]. It is quite evident that there is a change in the behaviour when the number particles involved in a typical rearrangement becomes of the same order of the sample size. Independently from any theoretical speculations it is clear than when the variance Δ becomes comparable to $(1-q)^2$ the distribution of q cannot be anymore Gaussian (the overlap cannot become greater than 1!) and we enter in a new regime. Strong finite size effects are thus expected for sufficient large time, i.e. for times which increase as $N^{1/\mu}$. It is also quite likely that for sufficient large times a finite system reaches a sufficient low state such that further jumps are inhibited or happen on a much lager time scale [18].

Summarizing the conclusion are this note are the following:

- Aging effects can be observed also at relatively short times in binary glasses.

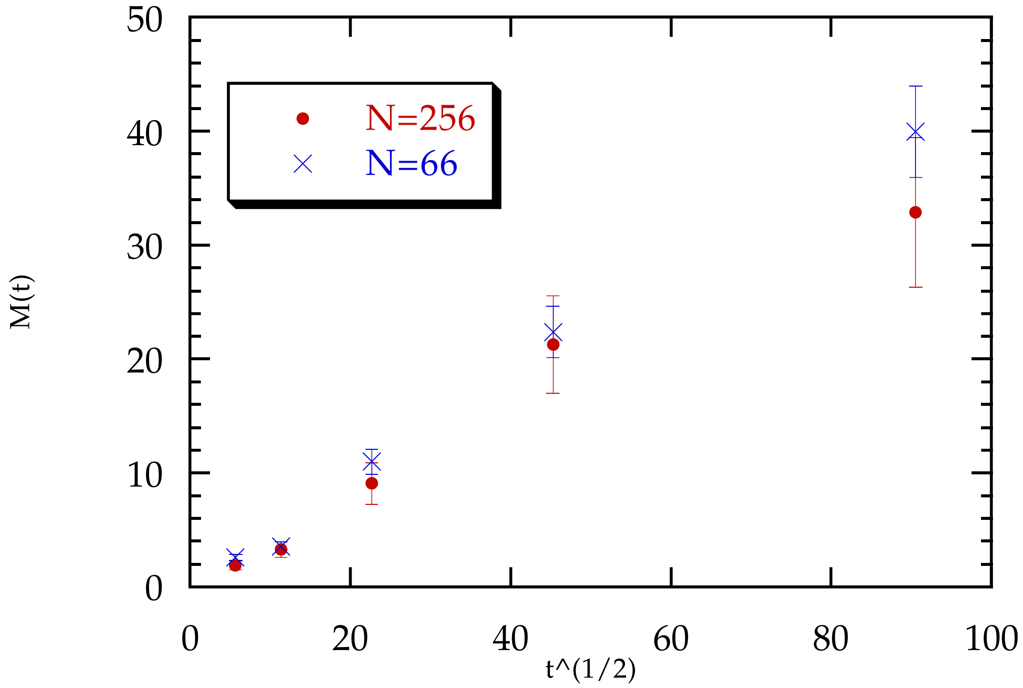

Figure 5: The value of $M(t_w)$ as function of $t_w^{1/2}$ at $s = 4$.

- Simple aging is observed for a variation of about two order of magnitude in the waiting time with deviations with 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 [11]).

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

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References

[1] L. C. E. Struik; *Physical aging in amorphous polymers and other materials* (Elsevier, Houston 1978).

[2] J.-P. Bouchaud; J. Phys. France **2** 1705, (1992).

[3] L. F. Cugliandolo and J.Kurchan, Phys. Rev. Lett. **71**, 1 (1993).

[4] S. Franz and M. Mézard *On mean-field glassy dynamics out of equilibrium*, cond-mat 9403004.

[5] L. F. Cugliandolo, J. Kurchan and F. Ritort; Phys. Rev. **B49**, 6331 (1994).

[6] S. Franz and H. Rieger Phys. J. Stat. Phys. **79** 749 (1995).

[7] E. Vincent, J. Hammann, .M. Ocio, J.-P. Bouchaud, L. F. Cugliandolo, cond-mat 9607224.

[8] B.Bernu, J.-P. Hansen, Y. Hitawari and G. Pastore, Phys. Rev. **A36** 4891 (1987).

[9] J.-L. Barrat, J-N. Roux and J.-P. Hansen, Chem. Phys. **149**, 197 (1990).

[10] J.-P. Hansen and S. Yip, Trans. Theory and Stat. Phys. **24**, 1149 (1995).

[11] D. Lancaster and G. Parisi, in preparation.

[12] S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

[13] M.Mézard, G.Parisi and M.A.Virasoro, *Spin glass theory and beyond*, World Scientific (Singapore 1987).

[14] G.Parisi, *Field Theory, Disorder and Simulations*, World Scientific, (Singapore 1992).

[15] J. Horbach, W. Kob, K. Binder, C. A. Angell *Some Finite Size Effects in Simulations of Glass Dynamics*, cond-mat 9610066.

[16] H. Rieger, J. Phys. I (France) **4**, 883 (1994).

[17] E. Marinari, G. Parisi, J. J. Ruiz-Lorenzo and F. Ritort, Phys. Rev. Lett. **76**, 843 (1996).

[18] J.-P. Bouchaud, E. Vincent and J. Hammann; '*Towards an experimental measure of the number of metastable states in spin-glasses?*', cond-mat 9303023.