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LETTER TO THE EDITOR

Relaxation processes and entropic traps in the Backgammon modelSilvio Franz^{†§} and Felix Ritort^{‡||}[†] International Center for Theoretical Physics, Strada Costiera 11, PO Box 563, 34100 Trieste, Italy[‡] Institute of Theoretical Physics, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

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Abstract. We examine the density–density correlation function in a model recently proposed to study the effect of entropy barriers in glassy dynamics. We find that the relaxation proceeds in two steps with a fast beta process followed by alpha relaxation. The results are physically interpreted in the context of an adiabatic approximation which allows one to separate the two processes and define an effective temperature in the off-equilibrium dynamics of the model. We investigate the behaviour of the response function associated with the density and find violations of the fluctuation dissipation theorem.

The relaxation in supercooled liquids near the glass transition has a characteristic two-step form. Experiments on very different materials reveal the existence of a first fast relaxation process, called beta relaxation, followed by a much slower one, called alpha relaxation [1]. One of the most striking successes of mode coupling theory [2] is its ability to capture this phenomenon and to give a correct prediction for the relation among the exponents characterizing the two relaxations. However, we believe that comprehension of the basic mechanisms underlying the relaxation in glasses is missing. Experiments in glasses have been recently interpreted in terms of traps models [3, 4]. In these models, the system evolves among traps—or metastable states—which have a lifetime that grows with decreasing temperature, and finally diverges at the glass transition. The two-step relaxation follows naturally from the hypothesis that equilibration inside a trap occurs much faster than ‘jumps’ among different traps. How a trap may be defined and described for real systems or microscopic models is an interesting open problem. If the traps have to be interpreted as the result of energy barriers in a rough energy landscape, one finds the difficulty that the relaxation should appear as a random process even on a large scale. A ‘jump’ among two different traps should imply a discontinuity in various quantities as the energy or the correlation function. This problem was already noted in [4], where it was proposed, as a way out, that real systems could be composed of a large number of quasi-independent subsystems leading to the observed self-averaging properties for the different quantities. In this direction, it can be instructive to investigate a different mechanism for slow relaxation and, in particular, the role of entropy barriers.

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In this letter we study the nature of density fluctuations in the so-called ‘Backgammon model’, a microscopic model that has proved useful in studying some mechanisms underlying the glassy relaxation and, in particular, the role of entropy barriers. The model [5] is a Boltzmann gas with N particles in an N site space with Hamiltonian given by the total number of empty sites,

$$H = - \sum_{r=1}^N \delta_{n_r,0} \quad (1)$$

where $r = 1, \dots, N$ denotes the sites of the space and n_r the occupation number of the site r . The system evolves following a single-particle Metropolis dynamics: at each sweep a particle to move and an arrival site are chosen at random. The particle is moved with probability 1 if the energy does not increase and with probability $\exp(-\beta)$ if the move costs one unit of energy. The relaxation of the energy has been studied in detail in [5–9]; we briefly re-assume here the main results. At zero temperature the dynamics are slower and slower as time goes by: the average density of particles in the occupied states increases and as a consequence the dynamics slows down. This observation has allowed for the identification of fast and slow degrees of freedom: the relaxation within the occupied sites at a given time proceeds much faster than the variation of the energy and the diffusion of ‘towers of particles’. This allows a self-consistent treatment of the dynamics which is in very good agreement with the exact solution. At large times the occupation probability $P(n, t)$ mimics the equilibrium probability,

$$P(n, t) = e^{\beta(t)\delta_{n,0} - \zeta(t)} \frac{\zeta(t)^{n-1}}{n!} \quad (2)$$

with an effective time-dependent temperature $T(t) = 1/\beta(t)$ larger than the real one, and effective fugacity $\zeta(t)$ related to $\beta(t)$ by the condition of constant density $\langle n_r(t) \rangle = 1$, i.e. $e^{\beta(t)} + e^{\zeta(t)} - 1 = \zeta(t) e^{\zeta(t)}$. At zero temperature, the decay of the energy follows the law $E(t) \sim -1 + O(1/\log(t))$, whereas at small but finite temperatures this behaviour is cut off for times of the order of the relaxation time $\tau \sim \exp(\beta)/\beta^2$ when the relaxation becomes exponential. Probing the system on finite time scales, for example mimicking heating–cooling experiments, one finds a characteristic glassy behaviour as hysteresis loops for the energy [6]. Additional information on the off-equilibrium dynamics is gained by studying the energy–energy autocorrelation function [5]

$$C_E(t, s) = \frac{\langle \delta_{n_r(t),0} \delta_{n_r(s),0} \rangle - E(t)E(s)}{E(s)(1 - E(s))}.$$

This quantity shows aging at zero temperature with a scaling behaviour $C_E(t, s) \sim (s/t)^{\frac{1}{2}} (\log(s)/\log(t))$ [9]. Again, at finite temperature this scaling is observed up to times of the order of the relaxation time.

Here we concentrate our attention on the relaxation of the density–density correlation function, a quantity that is measured in experiments on real systems [1]. This is a better quantity to use when studying fast processes in systems since on short timescales local densities vary while the energy stays essentially constant.

The fluctuations of the local density around its average $\langle n_r(t) \rangle = 1$ are studied by introducing the density–density correlation function

$$C^{(r)}(t, s) = \langle n_r(t) n_r(s) \rangle = \sum_{n,m} nm P^{(r)}(n, t|m, s) P^{(r)}(m, s) \quad (3)$$

and its associated response

$$R^{(r)}(t, s) = \frac{\delta \langle n_r(t) \rangle}{\delta h_r(s)} \quad (4)$$

having denoted as $P^{(r)}(n, t)$ the probability that state r is occupied by n particles at time t , $P^{(r)}(n, t|m, s)$ the same probability conditioned to have m particles at time s and h_r as an infinitesimal inhomogeneous ‘pressure field’ coupled linearly with the local density in the Hamiltonian[†]. We will present data for the normalized correlation

$$C_{\text{norm}}(t, s) = \frac{\langle n_r(t)n_r(s) \rangle - 1}{\langle n_r(s)^2 \rangle - 1}.$$

Choosing a site-independent initial distribution, the correlation function remains site independent while the response at finite time depends on the distribution of $h_{r'}$ on the different sites in the form of a dependence on $\mu^{(r)} = \text{Prob}(h_{r'} > h_r)$ and $\nu^{(r)} = \text{Prob}(h_{r'} < h_r)$. Despite this, in the following we will drop the index r from the various quantities. At equilibrium, correlation and response are time translation invariant and related by the fluctuation–dissipation theorem relation $TR(t-s) = \partial C(t-s)/\partial s$. In off-equilibrium conditions it has been often proved useful to characterize the violation of equilibrium by the ‘fluctuation dissipation ratio’ [10, 11]

$$x(t, s) = \frac{TR(t, s)}{(\partial C(t, s)/\partial s)}. \quad (5)$$

The evolution of the previously defined functions can be studied starting from the hierarchy of equations for $P(n, t)$, $P(n, t|m, s)$ and related quantities following a procedure similar to the one used in [7]. One can then derive closed integral equations in terms of a few functions that can be integrated numerically [7] or analytically in the long time limit [9]. Details of this analysis, and in particular the full set of hierarchies for the density–density correlation (3) and the associated response function (4), will be presented elsewhere. In this paper we integrate directly, truncating the hierarchy to some large order. In practice we have found that for low enough temperature and not too large times the truncation at $n = 100$ yields excellent results.

Let us now discuss the form of the density correlation function in equilibrium. Starting from a random initial configuration, after times of the order of $\tau_\alpha \approx e^\beta/\beta^2$ the system eventually reaches equilibrium. The correlation function is then time translation invariant and can be studied exactly as a Laplace transform. It turns out that for temperatures small enough the dominant contribution to the equilibrium correlation function for all times is given by the superposition of two Debye processes,

$$C_{\text{norm}}^{\text{eq}}(t) = \frac{\zeta - 1 + e^{-t/\zeta}}{\zeta} e^{-t/\tau_\alpha} \quad (6)$$

with $\tau_\alpha = 2((\zeta - 1)e^\zeta + 1)/\zeta^2 \approx 2e^\beta/\beta^2 \gg \zeta$. The fast and slow processes at equilibrium are related to the relaxation within occupied states and to diffusion, respectively. We note that the value of the plateau at equilibrium is $(\zeta - 1)/\zeta$, which corresponds to complete decorrelation within occupied states but no diffusion. The equilibrium curve for $T = 0.05$ is the dashed curve in figure 1. In the time window shown in figure 1 the correlation function stays essentially constant and equal to the plateau value $(\zeta - 1)/\zeta \simeq 0.94$, decaying to zero afterwards. Here the alpha relaxation time is $\tau_\alpha \simeq 3 \times 10^6$.

Regarding the off-equilibrium correlation function, we show in figure 1 the data for the $C_{\text{norm}}(t, s)$ for $T = 0.05$ as a function of $t - s$ for various values of s . Over the time window we explore, the system is far from being thermalized. The integration at $T = 0$ on the same time window leads to almost identical results. The α and β processes are well

[†] A homogenous pressure would not have any effect in the system due to the constraint on the global density $\sum_{r=1}^N n_r = N$.

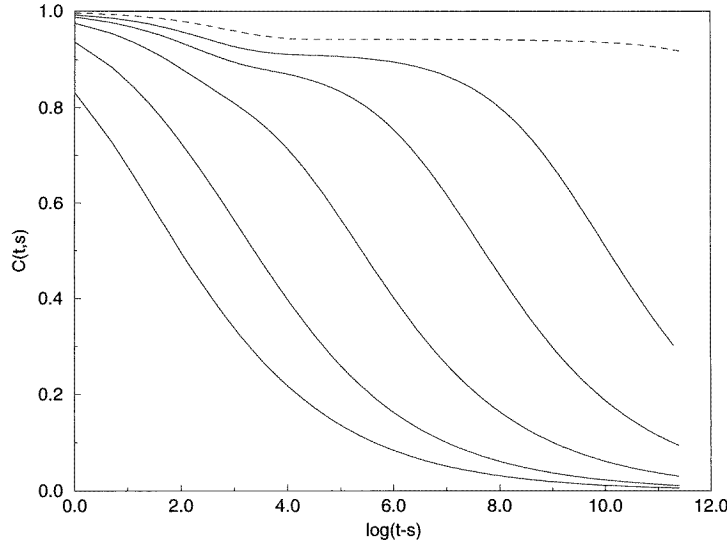


Figure 1. The density–density correlation function $C_{\text{norm}}(t, s)$ as a function of $t - s$ for different values of $s = 1, 10, 10^2, 10^3, 10^4$ (from left to right) at $T = 0.05$ (continuous curves). The existence of a plateau separates the beta and alpha regimes. The dashed curve corresponds to the equilibrium $C_{\text{norm}}^{\text{eq}}(t - s)$. The curves with $s = 10^3, 10^4$ are excellently fitted by the form (9) with $b(s) = 2.20, 3.85$, respectively. For the same times, $\zeta(s) = \log P(1, s) = 8.93, 11.51$.

separated for large enough s . In this case, the shape of the off-equilibrium relaxation curve can be understood qualitatively within the framework of the adiabatic approximation. The decorrelation time for the density among filled states is much smaller than the time needed to diffuse and/or change sensibly the energy; there must then be a timescale such that we can approximate

$$P(n, t|m, s) \approx \delta_{m,0}\delta_{n,0} + (1 - \delta_{m,0})(1 - \delta_{n,0}) \frac{P(n, s)}{1 - P_0(s)}. \quad (7)$$

This equation reflects the simple fact that empty states never become occupied. The second factor is determined by the closure condition $\sum_n P(n, t|m, s) = 1$. Consequently

$$C_{\text{norm}}(t, s) = \frac{\zeta(s) - 1}{\zeta(s)}. \quad (8)$$

For short times ($t - s \ll s$), $\zeta(s) = -\log(P_1(s))$ does not vary too much; it is then natural to describe the beta relaxation by form (6) just substituting ζ by $\zeta(s)$. In this way we have checked that we correctly describe even the beginning of the alpha relaxation. However, the best combined description of slow α relaxation together with β relaxation is obtained by functions of the aging form:

$$C_{\text{norm}}(t, s) \approx \frac{\zeta(s) - 1 + e^{-(t-s)/\zeta(s)}}{\zeta(s)} \frac{(1 + b(s))}{(1 + (b(s)\sqrt{t} \log(t)/\sqrt{s} \log(s)))} \quad (9)$$

a form inspired by that of the energy–energy correlation function found in [9]. At finite temperature, $b(s)$ is a crossover function to form (6).

In figure 2 we see that the two relaxation processes are also manifest in the response function. In order to characterize better the two processes in off-equilibrium conditions we study the relation between the response and correlation during the dynamics. The first

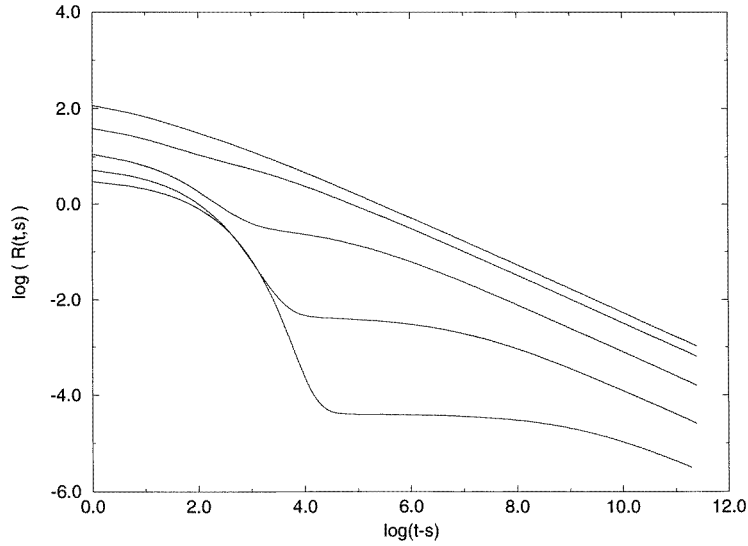


Figure 2. The response function for the values of $s = 1, 10, 10^2, 10^3, 10^4$ (from top to bottom) at $T = 0.05$.

quantity of interest is the value of the fluctuation–dissipation ratio at equal times. We see that $x(t, t)$ reaches values close to one long before total equilibrium sets in. This is a further indication that the system is in local equilibrium and yields in a natural way the notion of a trap in this system. Note that the traps in the Backgammon model are purely entropic. This means that the system escapes from the trap even at zero temperature when thermal excitations are absent. In other words, the dynamics are slowed down by entropic traps which can be considered as metastable states with a finite (energy-dependent) lifetime.

Most interestingly, we find that for large times (large values of s) $x(t, s)$ remains nearly constant in each of the two processes. This is shown in figure 3 where we plot $x(t, s)$ as a function of $1 - C_{\text{norm}}(t, s)$ for different values of s . We find that $x(t, s)$ is close to 1 in the beta relaxational process and jumps to a s -dependent smaller value $x_\alpha(s)$ at a value $C_{\text{norm}}(t, s) = q_{EA}$ which remains constant in the alpha process.

It is rather natural, with the adiabatic approximation in mind, to look for a possible interpretation of x as the ratio between the effective and actual temperature. Unfortunately we found negative evidence for such interpretation of the data. For low enough temperature and times smaller than τ_α the actual value of $x(t, s)$ is nearly temperature independent. The step behaviour of $x(t, s)$ is quite reminiscent of the dynamics in spin glasses with one step of replica symmetry breaking [10]. This in turn represents the suitable off-equilibrium generalization of mode coupling theory [12] in the case of a Whitney fold glass singularity, i.e. precisely the case where there are well separated α and β relaxations. We do not know at this stage if this corresponds to a deep analogy or is a mere coincidence. We stress that at equilibrium, the ending of the beta relaxation, as well as the onset of the α relaxation, are described by power laws in mode coupling theory. As is seen in (6), in our case the equilibrium relaxation is the superposition of two exponentials.

Summarizing, we have shown the existence of two step relaxational processes (alpha and beta relaxation) in the Backgammon model, which is a simple model where the slow dynamics is a consequence of pure entropic barriers. We have closed the dynamical

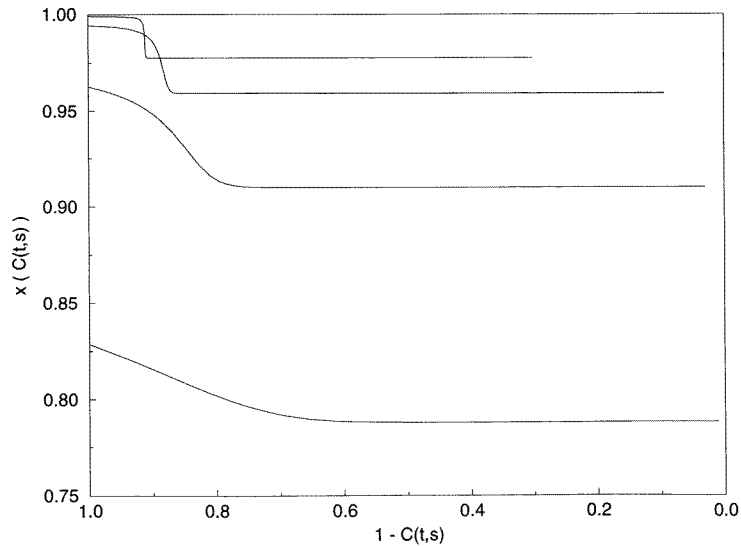


Figure 3. The fluctuation–dissipation ratio $x(t, s)$ for different values of $s = 10, 10^2, 10^3, 10^4$ (from bottom to top) as a function of $1 - C_{\text{norm}}(t, s)$ at $T = 0.05$. The two plateaux correspond to the alpha and beta relaxations.

equations for the density–density correlation function and the response of the system to a staggered field coupled to the density. Our results for those quantities and the fluctuation dissipation ratio allow for a clear identification of the fast (beta) and slow (alpha) relaxation processes in this system. The physical interpretation of these processes leads naturally to the concept of an entropic trap. In the case of entropic traps, the entropy barrier associated with the trap itself depends on the number of available configurations within the trap. Because the height of the entropic barriers varies in a continuous way, the dynamics proceeds slowly but without macroscopic jumps in the energy. The results presented here for the Backgammon model are expected to apply for slowly relaxing systems where the dynamics are mainly driven by entropy barriers (as for instance, Bose–Einstein condensation). A detailed account of our work will be given elsewhere.

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