Off equilibrium glassy dynamics: a simple case

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Abstract We consider the relaxational dynamics of a particle in a random potential, taking into account the effects of a finite waiting time t_w . In the limit of an embedding space of infinite dimension, we solve numerically the closed set of causal equations relating the correlation and response functions in the glass phase. The results at large waiting times agree with the static replica symmetry breaking approach and with previous studies of the equilibrium dynamics. For finite t_w there may exist a hierarchical structure of crossover regimes between the measurement time and some functions of t_w .

LPTENS preprint 03/39

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A lot of efforts have been devoted to the study of equilibrium static and dynamic properties of spin glasses. Yet it is clear that some of the most interesting experimental findings in these systems, like the slow relaxation of the thermoremanent magnetization, aging, and memory effects during temperature cycling experiments, are inherently out of equilibrium phenomena (for a recent phenomenological discussion, and references to experiments, see [1]).

The first attempts to a microscopic description of these effects have concentrated on the mean field theory of spin glasses close to the critical temperature, taking into account explicitly the changes in external parameters like temperature or magnetic field [2, 3]. Recent studies, analytical and numerical, have emphasized the role of the existence of an initial time for the dynamics, and that of a finite waiting time [4, 5, 6, 7, 8].

In this paper we shall follow this line of thought. We consider a very simple model of a glassy system [9], the "toy model" of a single particle in N dimensions, submitted to a potential which is the sum of a quadratic well and a Brownian process. This is an extreme -zero dimensional- case of the very general and important problem of directed manifolds in random media, the statics of which has received a lot of attention in recent years (see [11] and references therein). In spite of this simplification one may hope that many interesting aspects of the dynamics are kept by this toy model, as is true for the statics [11, 10].

We shall work in the limit of an infinite dimensional embedding space ($N \rightarrow \infty$). This limit allows for the derivation of exact integrodifferential equations for the correlation and response functions. The static properties can also be studied in details in this limit using the replica method, which shows the existence of a glassy low temperature phase with a full hierarchical replica symmetry breaking (rsb) [11].

The equilibrium Langevin dynamics of these manifolds in the large N limit has been worked out by Kinzelbach and Horner in two interesting recent papers [12, 13], following the general strategy used by Sompolinsky and Zippelius [14, 15] in spin glasses. We shall basically reconsider their approach, using the nonequilibrium dynamics corresponding to a finite waiting time [5]. Technically the difference is that in our system the dynamical evolution starts at a time $t_0 = 0$. Therefore the correlation function $C(t, t')$ and the response function $r(t, t')$ depend explicitly on both t and t' . In the equilibrium dynamics the time t_0 is sent to $-\infty$, and the correlation and response become functions of the differences between t and t' : $C_{eq}(t - t')$ and $r_{eq}(t - t')$.

In spite of some formal similarities, one should keep in mind that these two approaches are actually quite different. In equilibrium dynamics, C_{eq} and r_{eq} satisfy coupled equations which depend explicitly on an anomaly of the response occurring on infinite time scales. One must assume the existence of a regularization of these diverging times by considering for instance a system with a finite number of degrees of freedom. The "dynamical" solution on diverging time scales, which turn out to be identical to the static (r.s.b.)

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equations of the replica method, is not really dynamical (for instance it is invariant under arbitrary reparametrizations of time). In our opinion it rather gives an "intuitive" and appealing description of the strange algebra of the replica method [17]. In non equilibrium dynamics, $C(t, t')$ and $r(t, t')$ obey causal equations which have a unique solution [5]. One can work directly with an infinite system, and there is no need to introduce diverging time scales. An important point is that the introduction of a finite waiting time provides a regularization which is a natural substitute to the use of a finite volume system.

Our work is based on a numerical solution of the off equilibrium dynamical equations of the toy model. We shall present numerical evidence that at low temperature: 1) There exists a limiting response function $r_{\text{as}}(\tau) = \lim_{t_w \rightarrow \infty} r(t_w + \tau, t_w)$; 2) This function is the same as that derived in equilibrium dynamics [12], with a certain condition of criticality of the anomalous response coming from diverging time scales; 3) Similar results hold for the correlation. In particular, the values of $C_{\text{as}}(0)$ and $C_{\text{as}}(\tau \rightarrow \infty)$ agree with the results for the statics from the full r.s.b. solution; 4) The energy $E(\tau)$ also converges to its static r.s.b. value at large τ .

In order to understand the origin of these results, one needs to study the correlation and response for finite waiting times. A full analysis goes beyond the scope of this work. Here we shall point out a few effects: 1) On the time scales we study, we see strong aging effects showing that dynamics can not be interpreted as a relaxation to equilibrium. 2) It is possible to find a family of approximate solutions of dynamical equations at large times. These solutions are technically related to the solutions of the dynamics on diverging time scales found in [13], but the role of the "diverging time scales" is now played by some functions of the waiting times (like for instance t_w^x). 3) The off-equilibrium dynamics has a single solution, which might belong to the above family. This choice of the solution by the dynamics at relatively short times, where the simulations show an interesting aging regime, is an important unsolved problem.

We now turn to a brief presentation of the computations. In the toy model, the particle at a position ϕ_α , $\alpha \in 1, \dots, N$, feels a potential energy $H = (\mu/2)\dot{\phi}^2 + V(\phi)$, where V is a gaussian random potential with correlations:

$$\overline{V(\phi)V(\phi')} = -Nf\left(\frac{(\phi - \phi')^2}{N}\right); \quad f(b) \equiv \frac{(\theta + b)^{1-\gamma}}{2(1-\gamma)}. \quad (1)$$

We use the Langevin dynamics at temperature T , with an independent gaussian noise $\eta_\alpha(t)$ on each component α , of variance $2T$. This dynamics can be studied by usual field theoretical techniques [15], which are reviewed in the present context in [12]. For the off equilibrium dynamics, we find that the correlation $C(t, t') = \langle \phi(t)\phi(t') \rangle / N$ and the response: $r(t, t') = \frac{1}{N} \sum_\alpha < \partial \phi_\alpha(t) / \partial \eta_\alpha(t') >$ satisfy the following equations for $t > t'$:

$$\frac{\partial r(t, t')}{\partial t} = -\mu r(t, t') + \int_0^t ds \, m(t, s)(r(t, t') - r(s, t')), \quad (2)$$

$$\frac{\partial C(t, t')}{\partial t} = -\mu C(t, t') + 2 \int_0^{t'} ds \, w(t, s) r(t', s) + \int_0^t ds \, m(t, s) (C(t, t') - C(s, t')), \quad (3)$$

$$\frac{1}{2} \frac{dC(t, t)}{dt} = -\mu C(t, t) + 2 \int_0^t ds \, w(t, s) r(t, s) + \int_0^t ds \, m(t, s) (C(t, t) - C(s, t)) + T. \quad (4)$$

In these equations, we have used the following notations:

$$m(t, t') = f'(b(t, t')), \quad w(t, t') = 4f''(b(t, t'))r(t, t') \\ b(t, t') = C(t, t) + C(t', t') - 2C(t, t'). \quad (5)$$

This set of equation is causal. The boundary conditions on r are $r(t, t^-) = 1$. Given an initial condition $C(0, 0)$, it has a unique solution.

We have computed this solution using the discretization which is induced by the discretization of the Langevin dynamics (with Ito convention). We solve the discrete equations with time steps $4h$, $2h$, and h , and we extrapolate the solution to $h = 0$ by a second degree polynomial. We choose h such that this extrapolation does not differ too much from the linear extrapolation of the data at $2h$ and h .

We first present the results for the asymptotic behaviour at large times, and the comparison to the statics. The simulations we present have been done with values of the parameters $\gamma = 1/2$, $\theta = 5$, $\mu = 1/8$ and $C(0, 0) = 21.5$; the results do not depend on this choice of $C(0, 0)$. The static results for these values of the parameters can be obtained using the method of [11]. One finds a critical temperature $T_c = .6875$. Below T_c , there is a full r.s.b. and the static correlations are: $\bar{q} = \langle \phi^2 \rangle / N > 21.5$. The r.s.b. implies the existence of a non trivial distribution $P(q)$ of the overlaps q between two identical copies of the system. Unless otherwise stated, the simulations we shall present were done at temperature $T = .5$. The function $q(u)$, which is the inverse of $u(q) = \int_0^q dq' P(q')$, is of the form $q(u) = 24 - (81/512)u^{-4}$ between two plateaux at $q_0 = 16$ and $q_1 = 18.46$. A detailed study of the physical interpretation of r.s.b. presented in [11] suggests that there is ergodicity breaking in the large N limit. Therefore one can expect that the asymptotic correlation $C_{\text{as}}(\tau) = \lim_{t_w \rightarrow \infty} C(t_w + \tau, t_w)$ will be equal to q_1 at large τ .

In fig.1 we plot the equal time correlations $C(t, t)$ versus time. The inset shows that $dC(t, t)/dt$ is well approximated by a power law (with an exponent equal to $-1.73 \pm .05$). We have used this power law fit of $dC(t, t)/dt$ in order to extrapolate $C(t, t)$ to infinite t . The result is $21.42 \pm .1$ which is in agreement with the r.s.b. prediction 21.5. For lower temperatures the agreement is not quite as good. For instance at $T = .2$ the same procedure gives $\lim_{t \rightarrow \infty} C(t, t) = 21.2 \pm .1$. We suspect that there may exist extra small

powers of $\log(t)$ which are responsible for this small discrepancy. We have checked similarly that the energy goes to its static r.s.b. value -1.366 at large times (a convergence to its replica symmetric value -1.380 provides a much poorer fit to the data).

In fig. 2a we plot the response $r(t_w + \tau, t_w)$ versus τ for various values of the waiting time t_w . We also give the result $r_{as}(\tau)$ of a three parameter power law extrapolation of these data at $t_w = \infty$. The same is done in fig. 2b for the correlation $b(t_w + \tau, t_w)$. According to the statics, the correlation should go to $2(\bar{q} - q_1) = 6.068$ at large τ . The data is compatible with this asymptota, with a power law approach. However, in view of the relatively short times τ accessible here (keeping $\tau < t_w$), we prefer to use a direct comparison to an analytic solution of the asymptotic equations, which we now explain.

Using (2, 3, 4), one can derive the equations for $r_{as}(\tau)$ and $b_{as}(\tau)$:

$$\begin{aligned} \frac{db_{as}}{d\tau} &= (-\mu + M_{as} + \bar{M})b_{as}(\tau) - \int_0^\tau dt' m_{as}(\tau - t') b_{as}(t') + 2T \\ &\quad - \int_0^\infty dt' ((m_{as}(\tau + t') - m_{as}(t'))b_{as}(t') + 4(w_{as}(\tau + t') - w_{as}(t'))r_{as}(t')), \\ \frac{dr_{as}}{d\tau} &= (-\mu + M_{as} + \bar{M})r_{as}(\tau) - \int_0^\tau dt' m_{as}(\tau - t') r_{as}(t'), \end{aligned} \quad (6)$$

where m_{as} and w_{as} are defined in a way similar to (5), but using the asymptotic correlation and response, and $M_{as} \equiv \int_0^\infty m_{as}(\tau)d\tau$. The constant $\bar{M}$ cannot be expressed in terms of the asymptotic functions. To understand its origin, let us look at the equation (2) for r , at times $t = t_w + \tau$, $t' = t_w$. The second term in this equation becomes $r_{as}(\tau) \int_0^{t_w+\tau} ds m(t_w + \tau, s)$. The integral contains a contribution M_{as} from times s in the asymptotic regime (finite difference with t_w), and also in some cases a contribution $\bar{M}$ from the other regions of s . Therefore we define $M_{as} + \bar{M} \equiv \lim_{t_w \rightarrow \infty} \int_0^{t_w+\tau} ds m(t_w + \tau, s)$. $\bar{M}$ is the analog of the "anomalies generated by diverging time scales" encountered in the equilibrium dynamics. Here, this "anomaly" corresponds to contributions where the times are not in the asymptotic regime, i.e. times such that aging effects are important. Having noticed this correspondence with the equilibrium dynamics approach, we can use the solution of (6) found by Kinzelbach and Horner [12]. For a whole range of values of $\bar{M}$, there exist solutions of these equations obeying the fluctuation dissipation theorem (f.d.t.): $db_{as}/d\tau = 2Tr_{as}(\tau)$. We choose $\bar{M}$ such that $b_{as}(\infty) = 2(\bar{q} - q_1)$ (in equilibrium dynamics this choice can be justified by considerations on the diverging time scale dynamics), and computed the corresponding functions $r_{as}^*(\tau)$ and $b_{as}^*(\tau)$. These functions are also plotted in fig. 2 a, b. The agreement with the extrapolations at large t_w of the solutions of the off equilibrium dynamics is very good. This confirms that the asymptotic dynamics coincides with the equilibrium dynamics on finite time scales, and agrees with the static r.s.b. results. Note that this does not happen e.g. in the spherical p-spin model considered by Cugliandolo and Kurchan ([5]). In our opinion the coincidence between asymptotic dynamics and r.s.b. statics is to be expected whenever the r.s.b. is of the full continuous kind ([17, 13]).

We now turn to the non asymptotic times. A relevant question is how one can generate an anomaly such as $\bar{M}$. We shall first present a rather general scenario for this, and then discuss briefly how it compares to our numerical results.

The scenario relies on a division of the octant ($0 \leq t' \leq t$) into "crossover domains". A crossover domain $\mathcal{D}_u$ is defined using an increasing function $h_u(t)$ as the set of times t, t' which are both large, but keeping the ratio $h_u(t')/h_u(t) = \exp(-\tau)$ fixed, with $\tau \in [0, \infty]$. Suppose that in the crossover domain $\mathcal{D}_u$ one has:

$$b(t, t') = \hat{b}_u(\tau) ; \quad r(t, t') = \frac{d \ln(h_u(t'))}{dt'} \hat{r}_u(\tau). \quad (7)$$

Then the contribution to $\int_0^t ds m(t, s)$ from all the times s such that s and t are in $\mathcal{D}_u$ is finite. In a simple problem like for instance the high temperature phase, there should be a single crossover domain, the asymptotic one defined by $h(t) = e^t$. In a glass phase, we can have a relatively simple scenario in which there exists, beside the asymptotic domain, another one defined by some other function $h(t)$. Such an example (with $h(t) = t$) has been found recently by Cugliandolo and Kurchan [5] in a simple spin glass system. But one can also have some systems with many crossover domains. The condition we impose is that they do not overlap. We can index them by a parameter u such that, if $w < u < v$ and the points (t, t') belong to $\mathcal{D}_u$, then $h_u(t')/h_u(t) = 0$ and $h_w(t')/h_w(t) = \infty$. A possible choice leading to such a behaviour would be for instance $h_u(t) = \exp(t^u)$. With this choice the points (t, t') belong to $\mathcal{D}_u$ when $t' = t - t^{(1-u)}\tau/u$.

We would like to outline two aspects of this scenario. The hierarchical structure is reminiscent of the ultrametricity assumption underlying both the statics and the equilibrium dynamics [18]. Here, we have a hierarchy of time crossovers. Considering three times $t'' < t' < t$, one sees that, if (t, t') belongs to the crossover domain $\mathcal{D}_u$ and (t', t'') belongs to $\mathcal{D}_{u'}$, then (t, t'') belongs to $\mathcal{D}_{\min(u, u')}$, which is an ultrametric inequality. Furthermore, whenever the crossover domain is not the asymptotic one (i.e. $h_u(t)$ grows slower than an exponential), one can neglect the time derivatives in the dynamic equations. Then the equations for b_u and $\hat{r}_u$ are independent of the choice of all the functions $h_u(t)$. In fact these equations are identical to those derived in equilibrium dynamics on diverging time scales. They have been shown [13] to possess solutions satisfying the quasi f.d.t. relation: $u db_u/d\tau = 2T \hat{r}_u(\tau)$, which reproduce the algebra of the static replica solution. In particular in any such hierarchical scenario, the large time limit of the k th "dynamical susceptibility" introduced by Cugliandolo and Kurchan [5]:

$$C_k(t) \equiv k \int_0^t ds \tau(t, s) C(t, s)^{k-1} \quad (8)$$

is related to the k th moment of the $P(q)$ function by: $\lim_{t \rightarrow \infty} C_k(t) = \int_0^1 dq P(q) q^k$. The main difference between this hierarchical scenario and

the equilibrium dynamics is that the diverging time scales are replaced by some functions of the waiting time (for instance $t_w^{-\alpha}$, if $h_a(t) = \exp(t^\alpha)$). Unfortunately this scenario does not get rid of the second problem of the equilibrium dynamics. As in equilibrium dynamics ([16]), at large times the equations of motion become invariant under arbitrary reparametrizations of time. A whole family of solutions exists, obtained from a particular one by arbitrary changes of the functions $h_a(t)$ (preserving the non overlapping of domains and ultrametricity). This reparametrization invariance, some aspects of which have been already noticed [3, 16], is actually a very general phenomenon [17] which appears because the dynamic equations (2.3) do not depend explicitly on time, if one drops the time derivatives.

As we said before, the off equilibrium dynamics has a single solution which may belong, at large times, to this scenario. But the arbitrariness induced by the reparametrization invariance make this statement difficult to test numerically. Here we shall just make a few remarks. In fig.3 we plot the level curves of $b(t, t')$ for $T = .5$. On all the time scales we have reached, we see some clear evidence for aging. We also notice that if we had a continuous set of functions $h_a(t)$, then the whole region $t, t' \rightarrow \infty, (t'/t) = a$ fixed, $a \in]0, 1[$, should belong to a single crossover domain, and thus (for a continuous $q(u)$ function as we have here) $\lim_{t \rightarrow \infty} b(t, at)$ should be independent of a . An analysis of fig.3 shows that the data is consistent, on the observed time scales, with a power law approach $b(t, at) \sim 8 - f(a)t^{-.25}$. Thus on this point the data is consistent with the above hierarchical scenario setting in on much longer time scales. However we claim that many interesting quantities have already stabilized at the time scale we can reach. We have computed for instance the first five dynamical moments (8), and compared them to the moments of the $P(q)$ function found in the statics: $M_1 = 2T/\mu = 8$, $M_2 = 3.09 \times 10^2$, $M_3 = 9.01 \times 10^3$, $M_4 = 2.35 \times 10^5$, $M_5 = 5.76 \times 10^6$. At time $t \sim 800$, the relative differences range from .01 ($k = 1$) to .15 ($k = 5$). If the whole dynamics could be interpreted as the equilibration relaxation inside a single valley, the asymptotic value for C_k should be equal to $\bar{q}^k - q_1^k$. We find a clear departure from this form which indicates that equilibrium is never reached. To conclude these remarks on the aging domain, we cannot make conclusive claims at this stage about the compatibility of our data with the hierarchical scenario, which requires to go to very large times. But our data, obtained on relatively short time scales, is in rather good agreement with the predictions of this scenario for the moments C_k . A better understanding of this aging regime on relatively short times is needed in order to make really dynamical predictions.

The dynamical equations (2.3,4) are easily generalized to the case where one takes a D dimensional manifold with $\mu = 0$ pulled by an external force. This very interesting problem, which is relevant for instance to the computation of critical currents in dirty type II superconductors, should thus be amenable to a treatment similar to the one presented here.

We would like to thank J.P. Bouchaud, L. Cugliandolo, H. Kinzelbach, J. Kurchan, H. Horner and G.Parisi for many interesting discussions.

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Figure Captions

Fig. 1: The autocorrelation $C(t, t)$ as a function of time. From top to bottom, the curves result from a solution of the discrete equations with $h = 1, 2$, $h = .6$, $h = .3$, and the extrapolation at $h = 0$. The parameters of the simulation are those quoted in the text. The asymptota predicted by the static rsb solution is 21.5. In the inset, the derivative of $C(t, t)$ versus time shows that the approach to the asymptota is nearly a power law.

Fig. 2: In a), the response $r(t_w + \tau, t_w)$ versus τ . From top to bottom, $t_w = 432, 504, 576, 648$. Also shown (bottom curve) is the power law extrapolation of these curves to $t_w \rightarrow \infty$, together with the prediction for $r_{as}(\tau)$ from the asymptotic dynamics (these last two curves are nearly undistinguishable). In b), similar curves for the correlation $b(t_w + \tau, t_w)$. From top to bottom, $t_w = 432, 504, 576, 648$, the extrapolation and the expected result from the asymptotic dynamics.

Fig. 3: The level curves of the correlation $b(t, t')$ in the sector $0 < t' < t$. From top to bottom are the curves $b(t, t') = 0, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 16$.

Fig. 2a

Fig. 2b

Fig. 3