Quasi-equilibrium during aging of the 2D Edwards-Anderson model

S. Franz, V. Lecomte, and R. Mulet

1 International Centre for Theoretical Physics, Strada Costiera 11, P.O. Box 586, I-34100 Trieste, Italy
2 École normale supérieure de Cachan, 94235 Cachan, France
3 "Henri Poincare" Chair of Complex Systems and Superconductivity Laboratory, Physics Faculty-IMRE, University of Havana, La Habana, Cuba

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We test the quasi-equilibrium picture of the aging dynamics -strictly valid in the asymptotic dynamical regime of aging systems- in the pre-asymptotic aging regime of the two dimensional Edwards-Anderson spin glass model. We compare the fluctuation-dissipation characteristic for spin autocorrelation function and response with a corresponding one obtained for a suitably defined new correlation function and its conjugated response. In agreement with the quasi-equilibrium picture we find that after a short transient the two corresponding fluctuation-dissipation ratios (FDR) coincide at equal times. Moreover we show that, as it happens for the usual FDR, the new dynamic FDR at finite time coincides with the static one at finite size.

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INTRODUCTION

In recent times, following developments in spin glass mean field theory \textsuperscript{[1,2]}, much emphasis has been put on the study of off-equilibrium fluctuation-dissipation relations during aging dynamics in glassy systems. These relations quantify the deviation of the ratio between correlation functions and conjugated responses from the one implied by the fluctuation dissipation theorem valid at equilibrium, and have been posed at the basis of a detailed thermodynamical and statistical description of the dynamics of glasses \textsuperscript{[3,4,5,6,7]}. Linear response theory allows to relate possible asymptotic violation of the fluctuation dissipation theorem to the failure of ergodicity at the level of the equilibrium measure \textsuperscript{[8]}. Given the correlation function \(C(t,t_w)\) of a certain observable \(A\), and its conjugated response function \(\chi(t,t_w)\) describing the effect at time \(t\) of a field conjugated to \(A\) acting from time \(0\) to time \(t_w\), one can define the fluctuation-dissipation ratio (FDR) \(X(t,t_w)\) from the relation:

\[
X(t,t_w) = T \frac{\partial C(t,t_w)}{\partial t_w} \frac{\partial t_w}{\partial \chi(t,t_w)}. \quad (1)
\]

This is just unity in equilibrium conditions while deviates from it off-equilibrium and in general depends on the observable quantity \(A\) at hand. In mean field spin glasses the FDR admits a non trivial limit in the aging regime, where the correlations assume a scaling invariant behaviour. Moreover, in the long time limit, taken after the thermodynamic limit, one can define the function

\[
x(q) = \lim_{t,t_w \to \infty} X(t,t_w) |_{C(t,t_w) = q} \quad (2)
\]

which can have a non trivial behavior. When this happens, \(x(q)\) turns out to have an important covariance property under exchange of the given observable \(A\) chosen in the measure of correlation and response. If we have a correlation function \(C_A(t,t_w)\) corresponding to an observable \(A\) and a correlation function \(C_B(t,t_w)\) corresponding to an observable \(B\), and we define an auxiliary limiting function \(q_B(q_A) = \lim_{t,t_w \to \infty} C_B(t,t_w) |_{C_A(t,t_w) = q_A}\), the following relation holds

\[
x_B(q_B(q)) = x_A(q_A), \quad (3)
\]

the meaning of which is that the functions \(X_A(t,t_w)\) and \(X_B(t,t_w)\) coincide asymptotically for equal times. Moreover, in ref. \textsuperscript{[8]} it has been shown that in a large class of finite dimensional systems with short range interaction \(x(q)\) defined in an out of equilibrium context is deeply related to the nature of the equilibrium free-energy landscape. In fact, considering the overlap probability function (OPF) \(P(q)\) \textsuperscript{[7]} describing the statistics at equilibrium of the correlations of the observable \(A\) in two configurations chosen with Boltzmann weight, the linear response theory implies:

\[
x(q) = \int_0^q dq' P(q'). \quad (4)
\]

This equality implies that either \(x(q)\) and \(P(q)\) are both non trivial or they are both trivial and could be taken as the starting point for an experimental measure of the equilibrium OPF from off-equilibrium dynamics. Of course it does not imply the existence of some short range system where it is verified non-trivially. Going through the derivation one realizes that \textsuperscript{[9]} expresses the commutation of the thermodynamic limit and the long time limit as far as certain susceptibilities are concerned. Notice also that, thanks to \textsuperscript{[8]}, equation \textsuperscript{[8]} expresses the fact that for two observables \(A\) and \(B\), couples of states with identical \(q_A\) also have identical \(q_B\), i.e. the function \(q_A(q_B)\) defined in the dynamics describes the relation between different overlaps in equilibrium ergodic
components. This property has been shown to be deeply related to ultrametricity in \( q \) where it was found that the combination of relations \( \delta \) and \( \mu \) implies ultrametricity.

The meaning of eq. \( \xi \) has been clarified in \( \xi \) where it has been discussed how \( x(q) \) can be related to the density of metastable states -or quasi-states- with free-energy density slightly above the minimum, implying that quasi-states of equal free-energy are selected with equal probability during the dynamical process. The identity \( \delta \) and the covariance property \( \mu \), allow to rationalize the interpretation of the ratios \( T/x(q) \) for different values of \( q \) as effective temperatures governing the exchanges of heat among slow modes evolving on waiting time dependent time scales \( \xi \).

Effective temperatures dependent on \( q \) mean that while modes evolving on the same scale are in equilibrium with each other, heat exchanges between modes evolving on widely separated scales do not occur. It has been recently shown \( \xi \) that in trap models where \( x(q) \) has a non trivial \( q \) dependence, but ultrametricity does not hold, different quantities define different FDR. A situation where it would be difficult to identify the FDR’s with effective temperatures. Conversely, J.-L. Barrat and L. Berthier \( \xi \) studied Lennard-Jones models of glass-forming liquids where an FDR constant in \( q \) seems to describe the off-equilibrium dynamics, and found that density fluctuations at different wave vectors define the same FDR.

Numerical simulations of 3 and 4 dimensional spin glass Edwards-Anderson models, comparing extrapolations of the OPF from finite size systems and extrapolations of the FDR from finite time indicate the non-triviality -and consistently the identity- of both functions \( \xi \). This has been taken as an evidence in favor of a “replica symmetry breaking scenario” (RSB) for finite dimensional spin glasses.

These extrapolations however have been questioned in a series of papers showing that the OPF in systems without RSB, i.e where the OPF is trivial in the thermodynamic limit, can be plagued by severe finite size effects such that for relatively small systems it appears similar to what one expect for systems with RSB \( \xi \). In such conditions RSB could be wrongly inferred from extrapolations of the finite size OPF \( P(q, L) \) of systems of too small sizes \( L \), while the true \( P(q) \) is a trivial single \( \delta \)-function. In the same way one could doubt that off-equilibrium dynamic simulation times are too short to reliably extrapolate the asymptotic FDR from the finite \( t_w \), and that the true asymptotic one is just a single flat step as in domain growth problems \( \xi \).

On the experimental side it is clear that many systems with slow aging dynamics are found in pre-asymptotic regimes. A common phenomenon is the one of interrupted aging, found e.g. in \( \xi \), where a slow dynamical regime similar to usual aging eventually crosses over to equilibrium behavior. In addition, even in three dimensional spin glasses, the paradigmatic systems where aging could persist indefinitely, one sees that many quantities are far from their final values. In particular the experiments of Ocio and Herisson \( \xi \) where the first experimental determination of the FDR in spin glasses was achieved, show FD curves that strongly depend on the waiting time, signifying that the dynamics is still in some pre-asymptotic regime. In such conditions it is of great interest to inquire if the concepts valid for aging in the asymptotic regime can be adapted to get an adequate picture of the dynamics on much shorter time regimes.

In this context, one can hypothesize that the identity between static and dynamic FDR found in 3 and 4 dimension is due to the fact that at a given time \( t_w \) there is a slowly growing length \( \xi(t_w) \) over which the system has effectively equilibrated, and \( X(q, t_w) \) would approximately respect the relation \( \xi \) with \( P(q, L = \xi(t_w)) \). Such an extension would suggest the approximate validity at finite time of a quasi-equilibrium picture of the aging dynamics in which quasi-states with equal free-energy are selected with equal probability, and the static-dynamic equivalence would just reflect the properties of the equilibrium landscape of finite size system. The hypothesis is rather suggestive as it would provide a framework to interpret aging properties in an appropriate time scale even for systems which display interrupted aging. Here, while in a certain time window slow evolution and approximated scaling laws for correlations and/or susceptibilities are observed, the final asymptotic state is ergodic.

To test this extension L. Berthier and A. Barrat \( \xi \) studied the 2D Edwards-Anderson (2DEA) model, which, on one hand displays strong aging effects at finite times, and a non trivial OPF for finite size, on the other it is known to finally reach a paramagnetic state at all finite temperatures. In that work it was found that indeed it exists a correspondence \( L \rightarrow t_w \) such that the relation \( \xi \) holds. More recently, Berthier also studied the three and four dimensional case in a pre-asymptotic regime obtaining similar results \( \xi \).

In the light of the previous considerations about the link among effective temperatures and time scale separation, these finding appear rather surprising. Here, no time scale separation is possible, slow modes have to exchange heat in order to eventually equilibrate. In order to save the picture, one can of course hypothesize that this exchange occur “adiabatically”, in such a way modes evolving at the same rate appear able to equilibrate at their effective temperature with faster or slower modes before exchange heat. If this consideration applies FDR corresponding to different quantities should appear approximately equal one to another. In order to test this hypothesis we consider as in \( \xi \), the 2D Edwards-Anderson (2DEA) model where as mentioned aging is interrupted after a finite relaxation time. In our analysis we define some suitable correlation and response func-
tion not obviously related to the usual spin autocorrelation and its associated response, and compare the FDR for both couples of functions. In addition, in two dimensions we test the equivalence between the static and the dynamic FDR for the new quantities.

Our results are then compared with analogous measures in the Viana-Bray diluted spin glass, where is known to hold non-trivially.

The remaining of the paper is organized as follows. In the next section, we introduce the relevant quantities, then we present and discuss the results of the simulations and finally the conclusions are outlined.

**DEFINITION OF THE OBSERVABLES.**

The model we will consider consists in a pair of spin glass systems with independent random coupling and identical number of spins coupled through random interactions. Before explicitly introduce the model let’s say a few words to motivate this choice, keeping in mind that our task will be to compare FDR’s corresponding to different correlation-response couples. In spin models, defined in terms of an exchange Hamiltonian \( H = \sum_{i<j} J_{ij} S_i S_j \) the natural and most commonly used choice to probe dynamical correlations is the spin autocorrelation function at different times: \( C(t, t_w) = N^{-1} \sum_i \langle S_i(t) S_i(t_w) \rangle \) the corresponding “zero field cooled” susceptibility with respect to small local i.i.d. Gaussian fields \( h_i \) with variance \( h^2 \), introduced in the systems at time \( t_w \) and kept on at later times reads, \( \chi(t, t_w) = \frac{1}{N h^2} \sum_i \langle h_i S_i(0) \rangle \) where the over-line denotes the average over the field. A second common choice is the “energy correlation function” also known as “link overlap” \( C_E(t, t_w) = N^{-1} \sum_i \langle S_i(t) S_i(t_w) \rangle \), and the associated response: \( \chi_E(t, t_w) = \frac{1}{N h^2} \sum_i \langle J_{ij} h_j S_i(t) \rangle \). In mean field, for Gaussian long range \( J_{ij} \)’s one can show that in the thermodynamic limit, choosing the variance of the \( J_{ij} \)’s to be equal to \( 1/N \) one has for all times and with no assumption about the dynamics:

\[
C_E(t, t_w) = C(t, t_w)^2 \quad \frac{\partial \chi_E(t, t_w)}{\partial t_w} = C(t, t_w) \frac{\partial \chi(t, t_w)}{\partial t_w}
\]

so that, automatically, for all times, the FDR defined with these quantities coincide with the one defined with the usual correlations and response. Analogously at equilibrium, one finds that the relation \( g_E(q) = q^2 \) holds and \( 2qP_E(q_E(q)) = P(q) \) independently of the ultrametric nature of the organization of the states.

Then, in order to test the quasi-equilibrium picture one needs to compare overlaps non-trivially related one to the other. Consider, therefore, two copies of spin glass systems, with identical number of spins, and identically distributed, but independent quenched disorder and coupled by a random field \( R_i \). The Hamiltonian of this compound system is defined by:

\[
H = \sum_{i,j} J^1_{ij} S_i^1 S_j^1 + \sum_{i,j} J^2_{ij} S_i^2 S_j^2 + \sum_i R_i S_i^1 S_i^2
\]

where \( J^1_{ij} \) and \( J^2_{ij} \) represent the quenched disorder in copies 1 and 2 respectively and are quenched variables respecting the lattice topology and otherwise taken as i.i.d. from a Gaussian distribution with mean 0 and variance 1. The variables \( R_i \) which couple spins with identical label in the two copies have been chosen randomly with values \( R_i = \pm K \).

The dynamical spin autocorrelation function now reads:

\[
C(t, t_w) = (2N)^{-1} \sum_i \langle S_i^1(t) S_i^1(t_w) + S_i^2(t) S_i^2(t_w) \rangle ,
\]

and the corresponding response

\[
\chi(t, t_w) = \frac{1}{2N h^2} \sum_i \langle h_i^1 S_i^1(t) + h_i^2 S_i^2(t) \rangle
\]

As second couple of correlation response pair we consider the spin cross-correlation function \( \chi_{cross} \):

\[
C_{cross}(t, t_w) = (2N)^{-1} \sum_i \langle S_i^1(t) S_i^2(t_w) + S_i^2(t) S_i^1(t_w) \rangle R_i
\]

and

\[
\chi_{cross}(t, t_w) = \frac{1}{2N h^2 K} \sum_i \langle (h_i^1 S_i^1(t) + h_i^2 S_i^2(t)) R_i \rangle
\]

Where the \( \langle \ldots \rangle \) indicates an average over the initial conditions and \( \cdots \) over the disorder. We will speak about direct correlation and response respectively for \( \chi \) and \( \chi_E \) and cross correlation and response for \( \chi_{cross} \) and \( \chi_{cross} \).

An explicit formula for \( C_{cross}(t, t_w) \) and \( R_{cross}(t, t_w) \) as functionals of \( C(t, t_w) \) and \( R(t, t_w) \) can be given for small \( K \) using linear response theory:

\[
C_{cross}(t, t_w) = K^2 \beta \int_0^{t_w} ds C(t, s) R(t_w, s) + \int_0^t ds C(t_w, s) R(t, s)
\]

\[
R_{cross}(t, t_w) = K^2 \beta \int_0^{t_w} ds R(t, s) R(t_w, s)
\]

which shows that if the cross FDR coincide with the direct one, it is for non trivial reasons.
RESULTS AND DISCUSSION

We studied the cross-quantities in two different systems of Ising spins with random quenched disorder, the Edward Anderson model, a bi-dimensional square lattice of spins of size \( N = L \times L \) and the fixed connectivity version \([20]\) of the Viana-Bray model \([21]\) where the spins are on a random lattice with fixed connectivity \( c = 10 \) and size \( N \). For both models, we considered two copies with identical number of spins and independent quenched disorder coupled by a random field \( R_i = \pm K \) as in the previous section with \( K = 1/2 \). For this large value of \( K \) we are out of the linear response regime that allowed us to derive the explicit form of the cross-quantities as functions of the usual ones, but even if the relations \([12]\) does not hold, there is no reason to believe that the relation between \( X_{\text{cross}} \) and \( X \) becomes trivial.

In order to have as a reference results for a system where the picture sketched in the introduction certainly holds we present first the data of quick simulations of the Viana-Bray model.

In a first test, we compared the FD plots in dynamic simulations of aging experiments with the static ones obtained through the parallel tempering technique. Our results are summarized in figure \( \text{FIG. 1} \). We can observe that, on one hand, the static characteristics has small finite size dependence, on the other, the dynamical curves little dependence on the waiting times. As expected the dynamic curves coincide with the static ones for the direct functions. For the cross functions they also coincide provide the static curves are shifted vertically, this is normal as it should be noted that, the maximum value of \( q_{\text{cross}} \) in the equilibrium OPF of finite systems is unity, while dynamically \( C_{\text{cross}}(t, t_w) \) is monotonically decreasing from the value \( C_{\text{cross}}(t, t_w) < 1 \) for \( t > t_w \). Therefore, one should subtract a constant to the second integral of \( \tilde{P}(q_{\text{cross}}) \):

\[
S(q_{\text{cross}}) = \int_{q_{\text{cross}}}^{1} x_{\text{cross}}(q') dq' \to \text{compare it with the the dynamic function.}
\]

We then tested to what extent equation \([3]\) is valid when finite systems in statics are compared to systems evolved for finite aging times in dynamics. From the statics we get the functions \( P(q) \) and \( \tilde{P}(q_{\text{cross}}) \) where \( q \) is defined as the usual (direct) overlap between two independent replicas \( S = (S^1, S^2) \) and \( S' = (S'^1, S'^2) \):

\[
q(S, S') = \frac{1}{2N} \sum_i S^1_i S'^1_i + S^2_i S'^2_i , \quad \text{while} \quad q_{\text{cross}}(S, S') = \frac{1}{2N} \sum_i R_i(S^1_i S'^2_i + S^2_i S'^1_i). \quad \text{Then using} \quad [4] \quad \text{we derive the equilibrium quantities} \quad x(q) \quad \text{and} \quad x(q_{\text{cross}}) \quad \text{and compare them with the results obtained from the dynamic simulations.}
\]

Although we did not try to measure the joined probability \( P(q, q_{\text{cross}}) \), we could extract a function \( q_{\text{cross}}(q) \) as implied by the relation \([3]\) and compare with the one directly obtained from the dynamics. The results can be seen in figure \( \text{FIG. 2} \) where one can see that the static and the dynamic curves approach each other for values of \( q_{\text{cross}} \) smaller than \( C_{\text{cross}}(t_w, t_w) \). This is what one should expect because, as discussed above, in dynamics this is the largest value of \( C_{\text{cross}}(t, t_w) \), and tends to its limit from below for \( t_w \to \infty \). Conversely in statics, for finite systems, the probability distribution always extends to values of \( q_{\text{cross}} \) larger than the maximum value for an infinite system.

We then pass to the study of the two dimensional system. We studied the aging dynamics of the 2DEA model with unitary Gaussian couplings at \( T = 0.43 \), where no sign of thermalization can be observed in the correlation function up to waiting times as high as \( t_w = 10^5 \). In our simulations we used \( h^2 = 0.02 \) and checked to be in the linear response regime using the value \( h^2 = 0.01 \). On the
equilibrium side, using the parallel tempering technique we were able to calculate with good precision, the spin glass order parameter $P(q)$, as well as the function $P(q)\text{cross}$.

In figure 4 we present a fluctuation-dissipation plot for the model. As observed by L. Berthier and A. Barrat, one can superimpose the finite time curves of the direct functions with the second integral of the equilibrium OPF of suitable size systems at the same temperature. The points represent the data obtained by the dynamic simulation, while the lines those obtained studying the static of the model using the parallel tempering technique. We present for clarity only plots at two different waiting times, $t_w = 10^2$ and $t_w = 10^3$, for the dynamic simulations and two lattice sizes, $L = 8$ and $L = 10$ for the static ones. The upper curves correspond to the usual functions (similar curves were already presented in ref. 13), while the lower ones, reflects the cross functions. Unfortunately, it turns out that in order to superimpose the static and dynamic curves, a vertical shift in $S(q)$ is not enough and an horizontal shift, should also be performed.

In order to understand this point we notice that differently to what happens for the direct function for which by construction $C(t, t) = 1$, the value of $C\text{cross}(t, t)$ evolves in time. In such conditions the definition of the FDR in terms of the simple correlation is not necessarily the most appropriate. In fact, the study of running away systems (e.g. brownian motion or particles in non confining random potentials 12, 24) shows that a better definition is obtained considering the following combination of the correlation function $B\text{cross}(t, t_w) = \frac{1}{2}[C\text{cross}(t, t) + C\text{cross}(t_w, t_w) - 2C\text{cross}(t, t_w)]24$. This obviously is not the only combination which could be used; e.g. in 11 it was suggested the use of $F\text{cross}(t, t_w) = C\text{cross}(t, t) - C\text{cross}(t, t_w)$, however, we preferred to present the data using $B\text{cross}$, which is symmetric in the configurations at the two times and admits the interpretation of a distance between the configurations at times $t_w$ and $t$. We checked all the results below using $F\text{cross}$ instead of $B\text{cross}$ which turn out to be equivalent within our numerical accuracy.

The static analogous of the function $B\text{cross}(t, t_w)$ is, given two configurations $S$ and $S'$, the quantity $b\text{cross}(S, S') = \frac{1}{2}[q\text{cross}(S, S) + q\text{cross}(S', S') - 2q\text{cross}(S, S')]$. In order to compare the dynamical FDR with the static one we should be cautious of the symmetry of the Hamiltonian under contemporary reversal of all the spins. As discussed in 24 the proper static probability distribution to compare with the dynamics is not the full.
distribution but the distribution modulo the symmetry of the Hamiltonian. For the function $P(q)$, symmetric under $q \rightarrow -q$ one just needs to consider the positive $q$ part of the function multiplied by 2 (for normalization).

In order to eliminate this symmetry in the distribution $P(b_{\text{cross}})$ in an analogous way, we can just consider the histogram of the $b_{\text{cross}}$ corresponding to configurations $S$ and $S'$ such that $q_{\text{cross}}(S, S')$ is positive. The results are presented in figure 8 which shows that the agreement between the static and dynamic curves for the cross quantities is comparable to the direct ones, for the same lattice sizes.

Next we compare the relation between $B_{\text{cross}}(t, t_w)$ and $B(t, t_w)$ obtained directly in dynamics and relating the values with equal $x$ in statics as explained above. This is shown in figure 5 where we show that for the times and lengths considered there is a good correspondence between statics and dynamics.

Finally, given the good quality of our susceptibility data, we could take the derivatives of the $\chi$ versus $B$ characteristics so to compare directly at equal times the cross FDR $X_{\text{cross}}(t, t_w)$ with the direct one $X(t, t_w)$. The comparison is shown in figure 6 which shows that even for waiting times as short as $t_w = 10^2$ the two quantities are very close to each other. Preliminary results indicate that this is also the case in three and four dimension.

FIG. 6: Direct comparison of the FDR for the cross and direct quantities in the 2D EA model. The temperature is $T = 0.43$ and the waiting times are, from bottom to top $t_w = 10^2, 10^3, 10^4$. After a short transient both quantities do coincide. The glass width is $L=512$ and averages are made upon 190 samples.

CONCLUSIONS

In this paper we have proposed the use of cross correlation functions and response in disordered systems to probe the existence of effective temperatures during aging of disordered systems. We have compared the behaviour of a mean-field model with the one of a paramagnet, where aging is a transient behavior. We find that the at equal time the FDR for direct and cross quantities coincide within numerical error after a short transient. The correspondence among dynamical FDR at finite time and static one for finite size is confirmed as far as the cross quantities are concerned. These two findings support on one hand the idea that aging dynamics can be described in terms of effective temperatures, on the other that these temperatures are related to the density of states of finite systems on a scale $L(t_w)$. Preliminary results in three and four dimension indicate that the same kind of behaviour is found in these systems for time scales much shorter than the ones needed to reach an asymptotic state.

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