Unifying Concepts in Granular Media and Glasses
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On pre-asymptotic aging in finite dimensional spin glasses.

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We study the off-equilibrium dynamics in the pre-asymptotic aging regime of the two, three and four dimensional Edwards-Anderson spin glass model. We define an exotic correlation function and the corresponding response, and we compare the resulting fluctuation-dissipation ratio (FDR) with the usual one obtained by the ordinary spin-spin correlation function and relative response. In all systems we find that that after a short transient the two corresponding fluctuation-dissipation ratios coincide at equal times. Our findings support the idea that the FDR defines a unique set of effective temperatures for degrees of freedom evolving on the same time scale. In addition we show that in 2D, as it happens for the usual FDR, the new dynamic FDR at finite time can be relates to the static overlap probability function (OPF) of systems of suitable finite size.

1. Introduction

Glasses are trapped for long times in off-equilibrium states. Their relaxation assumes the character of aging, becoming slower and slower as the system evolves towards more and more optimized regions of the configuration space. A fundamental open question is to give a statistical description of aging, understanding how the configuration space is sampled during this process[1–3,6].

In connection with this problem, in recent time a lot of attention has been devoted to the study of the violations of the fluctuation dissipation theorem. 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 defines the fluctuation-dissipation ratio (FDR) $X(t,t_w)$ from the relation:

$$X(t,t_w) = T\frac{\partial C(t,t_w)/\partial t_w}{\partial \chi(t,t_w)/\partial t_w}. \tag{1}$$

Deviation of the FDR from unity indicate off-equilibrium behaviour. In generic off-equilibrium situations one can expect the FDR to depend on the observable quantity A at hand.

The theory of mean field spin glasses, has shown the existence of systems where the FDR admits a non-trivial long time limit, depending on the path by which t and t_w are sent to infinity. If t and t_w are sent to infinity fixing the values of the correlation $C(t, t_w)$ one gets a function

$$x(q) = \lim_{t,t_w \to \infty} X(t, t_w)|_{C(t,t_w)=q}. \tag{2}$$

Importantly, for these systems the FDR for different couples of conjugated correlations and responses admit the same limit along the same path. If we consider 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, asymptotically the FDRs $X_A(t, t_w)$ and $X_B(t, t_w)$ tend to coincide. More precisely, if 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

$$x_B(q_B(q_A)) = x_A(q_A). \tag{3}$$

At present it is not clear if in some finite dimensional system, with non singular interactions, the FDR admits a non-trivial limit. If this happens however, this has to be related to static ergodicity breaking. In ref. [4] it has been shown that $x(q)$ can be related to the overlap probability function (OPF) $P(q)$ [5] describing the statistics of the pure states at equilibrium not related by a symmetry of the Hamiltonian:

$$\frac{dx(q)}{dq} = P(q). \tag{4}$$

This relation, which holds trivially in ergodic systems where both $x(q)$ and $P(q)$ are equal to δ-functions are both either non-trivial or trivial could assume a non trivial content in systems with aging persisting for all times.

The identity (4) and eq. (3), support the interpretation of the ratios $T/x(q)$ for different values of q as effective temperatures governing the heat exchanges between slowly evolving modes[7].

Despite the attractiveness of this description, its strict validity is confined to the asymptotic regime where the energy and all other single time observables are close to their equilibrium values. However, both in simulations and in experiments one is often very far from such an ideal long time regime.

Extrapolations of numerical simulations of 3 and 4 dimensional spin glasses comparing the OPF of small systems and the FDR for finite times indicate the non-triviality -and consistently the identity- of both functions [8]. However these extrapolations have been criticized in a series of papers explicitly displaying systems where the OPF is trivial in the thermodynamic limit, but resembles the one of mean field for small enough volumes [9]. Moreover, in the experimental side it is manifest that many aging systems are found in pre-asymptotic regimes. For example the experiments of Ocio and Herisson [10] show FD curves that strongly depend on the waiting time and very far from a reasonably guessed asymptote. In structural glasses where the observed values of one time quantities are cooling rate dependent, the situation is even worse.

It is therefore of great interest to inquire if the concepts valid for the asymptotic regime can be adapted to get an adequate picture of the dynamics on much shorter time scales.

It is possible to hypothesize that the identity between static and dynamic FDR found in 3 and 4 dimension could be the effect of a slowly growing length $\xi(t_w)$ over which the system has effectively equilibrated. $X(q,t_w)$ would then approximately respect the relation (4) with the OPF $P(q, L=\xi(t_w))$ of a system of size $L=\xi(t_w)$. This extension put forward by A. Barrat and L. Berthier in [11] 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. In [11] and [12] it was found that indeed the conjectured relation among finite time FDR and finite size OPF quite remarkably exists.

At a first sight these findings appear in contrast with the relation among effective temperatures and time scale separation. For finite times, strict time scale separation is not possible and slow modes have to exchange heat in order to eventually equilibrate. However the picture can be saved hypothesizing an "adiabatic cascade", in which modes evolving at the same rate appear able to equilibrate at their effective temperature before exchanging heat with neighbouring modes. In such conditions FDR corresponding to different quantities should approximately coincide. In a recent paper [13] we have tested this hypothesis in the the 2D Edwards-Anderson (2DEA) model where as mentioned aging is interrupted after a finite relaxation time. Here we summarize this work, and we present additional data on the early time pre-asymptotic regime of the Edwards-Anderson model in three and four dimension.

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.

2. Definition of the observables.

In spin systems, in usual FD plots, one compare the spin-spin autocorrelation function $C(t,t_w) = N^{-1}\sum_i \langle S_i(t)S_i(t_w)\rangle$ to the response to an external field: the "zero field cooled" susceptibility to small local Gaussian fields h_i with variance h_o^2, introduced in the systems at time t_w $\chi(t,t_w) = \frac{1}{Nh_o^2}\sum_i \langle h_i S_i(t)\rangle$.

The task of this section is to define a different couple of correlation/response, non trivially related to the former. Consider two copies of Edwards-Anderson 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 is then

$$H = \sum_{i,j} J^1_{<ij>} S^1_i S^1_j + \sum_{<i,j>} J^2_{ij} S^2_i S^2_j + \sum_i R_i S^1_i S^2_i \tag{5}$$

where the spins are Ising variables, the quenched disorder J^1_{ij} and J^2_{ij} in copies 1 and 2 are i.i.d. centered Gaussian variables with unit variance, and the variables R_i which couple spins with identical label in the two copies are chosen randomly with values $R_i = \pm K$.

We now define the cross-correlation function,

$$C_{cross}(t,t_w) = (2N)^{-1} \sum_i \overline{\langle (S^1_i(t)S^2_i(t_w) + S^2_i(t)S^1_i(t_w))R_i\rangle} \tag{6}$$

and its conjugated cross-response

$$\chi_{cross}(t,t_w) = \frac{1}{2Nh_o^2K^2}\sum_i \overline{\langle (h_i^2 S_i^1(t) + h_i^1 S_i^2(t))R_i \rangle} \qquad (7)$$

Where the $\langle \ldots \rangle$ indicates an average over the initial conditions and $\overline{\cdots}$ over the disorder. As opposed to the cross-correlation and response, the usual correlation and response will be called "direct".

The justification for using the cross functions can be found in their linear response valid for small values of K:

$$\begin{aligned} C_{cross}(t,t_w) &= K^2\beta[\int_0^{t_w} dsC(t,s)R(t_w,s) \\ &\quad + \int_0^t ds\, C(t_w,s)R(t,s)\ ] \\ R_{cross}(t,t_w) &= K^2\beta\int_{t_w}^t ds\, R(t,s)R(s,t_w), \end{aligned} \qquad (8)$$

showing that there is not a trivial relation between these quantities and the direct ones valid independently of the dynamical process.

In comparing static OPF and dynamic FDR for the cross-functions, an additional grain of salt is needed. One can notice that while for all times $C(t,t) = 1$, the value of $C_{cross}(t,t)$ will depend on time. In such conditions a better suited quantity to use in FD plots instead of the correlation is the "difference"-function $B_{cross}(t,t_w) = \frac{1}{2}[C_{cross}(t,t) + C_{cross}(t_w,t_w) - 2C_{cross}(t,t_w)]$. The static analogous of $B(t,t_w)$ to be used as variable in the OPF can be defined, given two configurations $\mathbf{S}$ and $\mathbf{S}'$, by the quantity $b_{cross}(\mathbf{S},\mathbf{S}') = \frac{1}{2}[q_{cross}(\mathbf{S},\mathbf{S}) + q_{cross}(\mathbf{S}',\mathbf{S}') - 2q_{cross}(\mathbf{S},\mathbf{S}')]$.

3. Results and Discussion

We compared the behaviour of the cross and direct quantities in the Edward Anderson model, in 2, 3 and four dimensions choosing the value $K = 1/2$ as the strength of the coupling term. 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 function of the usual ones, but even if the relations (8) does not hold, there is no reason to believe that the relation between X_{cross} and X becomes trivial.

We first considered the 2D model, and compared the dynamic FD plot obtained at different times with the static one for small volumes obtained integrating twice the OPF. The dynamic results were obtained through regular metropolis simulations of a 512×512 systems where finite size effects where not seen on the time scales we probed. The static data where obtained using parallel tempering on small samples. The results for $T = 0.43$ are summarized in figure 1, where we trace the FD characteristics both for the direct and the cross functions. The direct characteristics is completely analogous to the one found by Berthier and Barrat showing that tuning appropriately the waiting times one can approximately superimpose the aging characteristic with the equilibrium ones for finite volume. The cross characteristics, remarkably, shows that the agreement of the cross functions is perfectly comparable with the one of the direct one. In our view this fact supports the idea of a characteristic length $\xi(t_w)$, growing with the waiting time, over which the system is equilibrated, and that the equilibrium is similar to that of an isolated system of that size. If that correspond to the truth both direct and cross functions should define the same effective temperature. We then tested the idea that $X(t, t_w)$ and $X_{cross}(t, t_w)$ could have the same behaviour for finite times. In order to do that we needed very good data for correlations and especially responses, in order to extract derivatives from the FD plots. This has been achieved averaging each curve over 190 different samples. The results in 2D can bee seen in figure 2. For very short waiting times $t_w = 10$ one sees that the curves are different, while, starting fro waiting times as short as $t_w = 100$ both FDR coincide within numerical error.

We tested the same property in three and four dimension for short times t_w, and large systems so that finite size effects were negligible. In figures 3 and 4 we plot the FD characteristic for both models. It can be seen that the curves are strongly dependent of t_w. Despite this fact, we can see in fig. 5 and 5 that the slopes of the curves coincide at equal times. This indicates that in this regime while both FDR are time dependent, degrees of freedom that evolve on the same time scales are in mutual equilibrium.

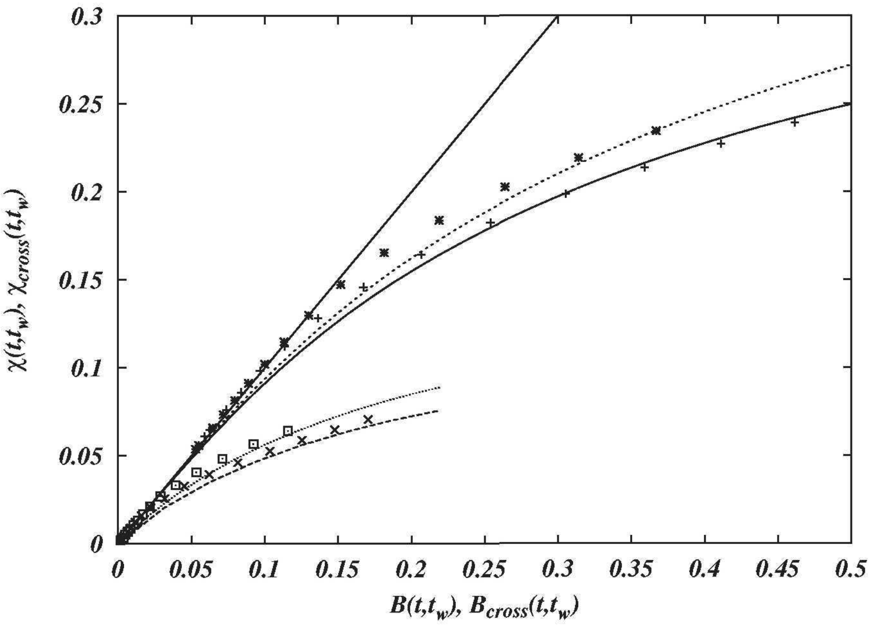

Figure 1. Fluctuation dissipation plot for the 2DEA model using B and B_{cross} as abscissas. The agreement of the dynamical and the static data for the cross quantity is comparable to the direct ones.

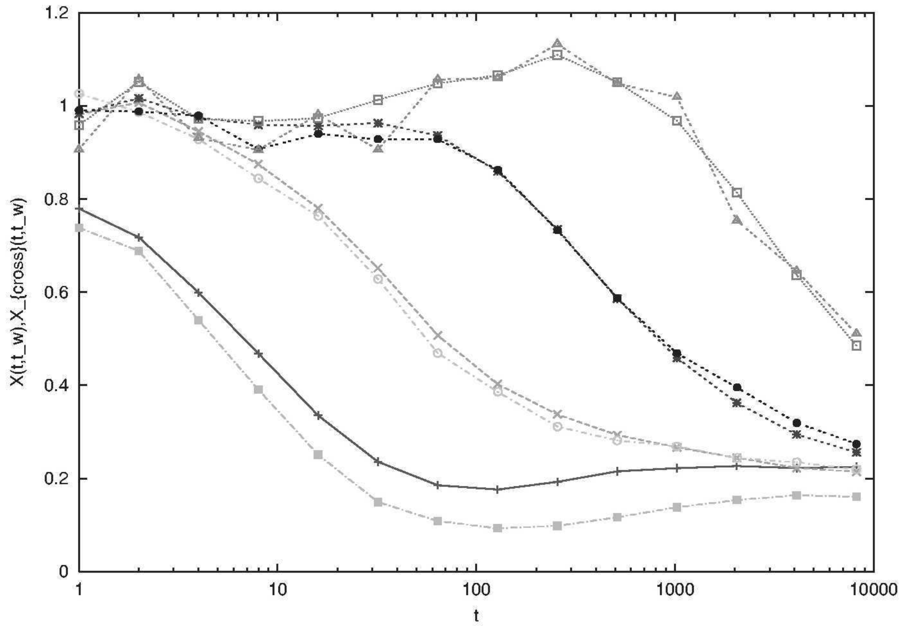

Figure 2. Comparison between the FDR for the cross and direct quantities in the 2D EA model. The temperature is $T = 0.43$ and the waiting times are, from bottom to top $t_w = 10, 100, 1000, 10000$. Notice that while the two FDRs at $t_w = 10$ are markedly different, both quantity coincide for $t_w \geq 100$.

4. Conclusions

In this paper we review our results on the analysus of cross-correlation and response functions in the pre-asymptotic aging regime of the 2D Edwards-Anderson spin glass model. We show how the behaviour of these function supports the idea that even at finite waiting times there is a set of uniquely defined effective temperatures, and the idea of a growing length over which the system has reached local equilibrium. In addition we presented new data in 3D and 4D on pre-asymptotic aging, finding that also in that case direct and cross quantity are in mutual equilibrium with each other. These findings suggest that the ideas coming from the asymptotic analysis of mean field systems, performed in the thermodynamic limit for infinite times, could be useful to understand the behaviour of the glassy dynamics of finite dimensional systems at finite times.

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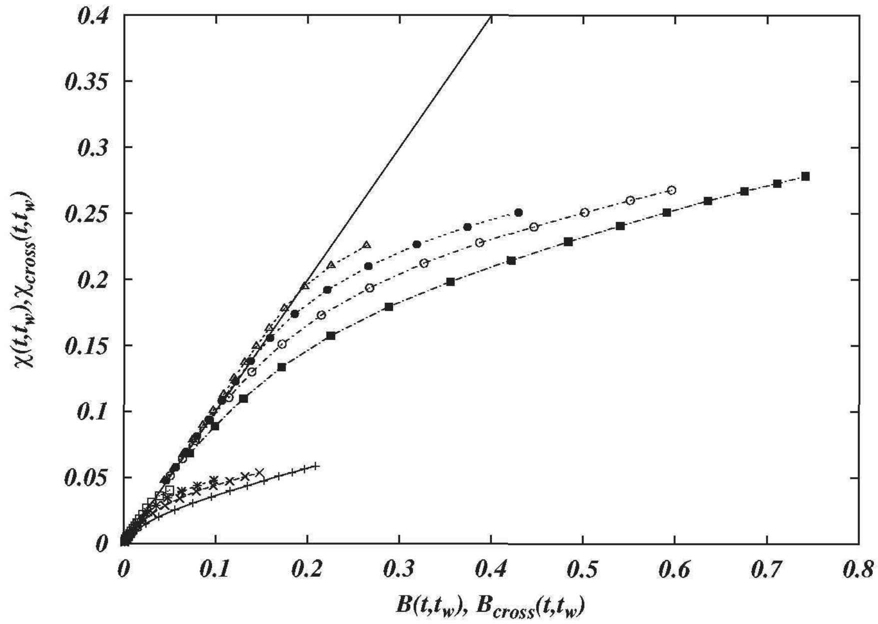

Figure 3. Fluctuation dissipation plot for the 3D EA model using B and B_{cross} as abscissas. The temperature is $T = .43$ and the waiting times are $t_w = 10, 100, 1000, 10000$. We see that on that time scales the curves are strongly t_w-dependent.

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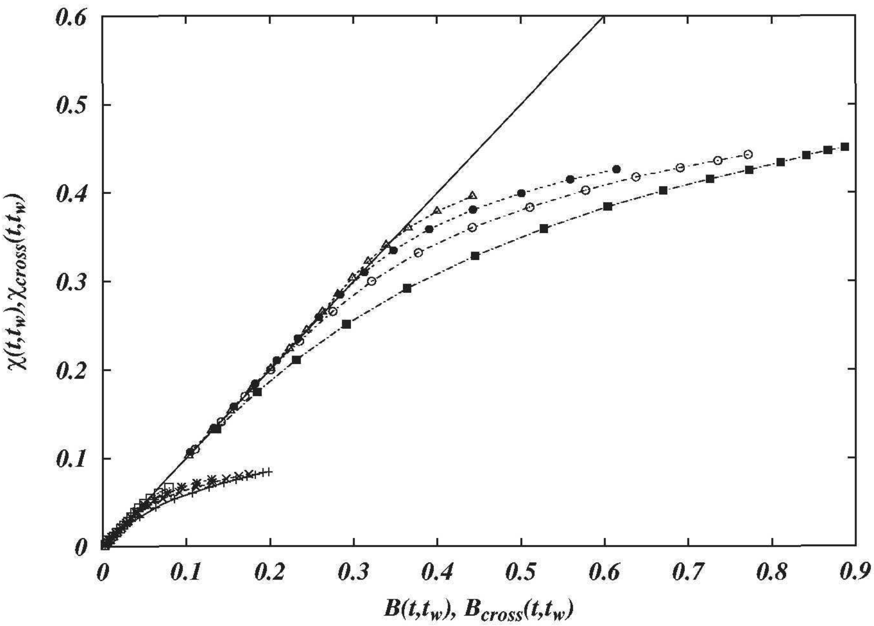

Figure 4. Fluctuation dissipation plot for the 4D EA as in fig. 3 . The temperature is $T = .43$ and the waiting times are $t_w = 10, 100, 1000, 10000$. Also in this case we see a strong dependence of the curves on t_w.

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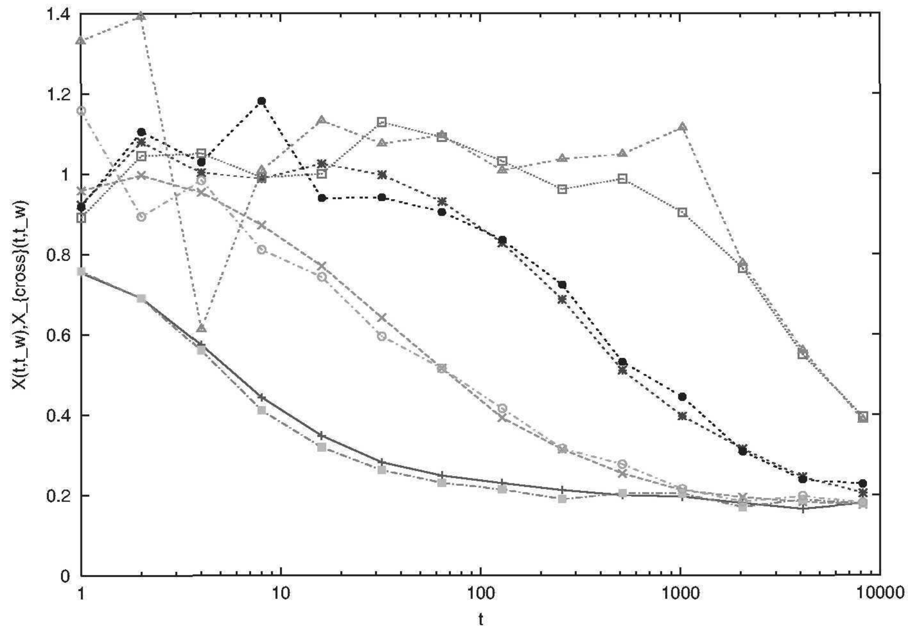

Figure 5. Same as fig. 2 in three dimension. The temperature is $T = 0.43$ and the waiting times are, from bottom to top $t_w = 10, 100, 1000, 10000$. In this case the curves coincide even for the shortest t_w. The quality of the data at longer waiting times is poorer due to less statistics.

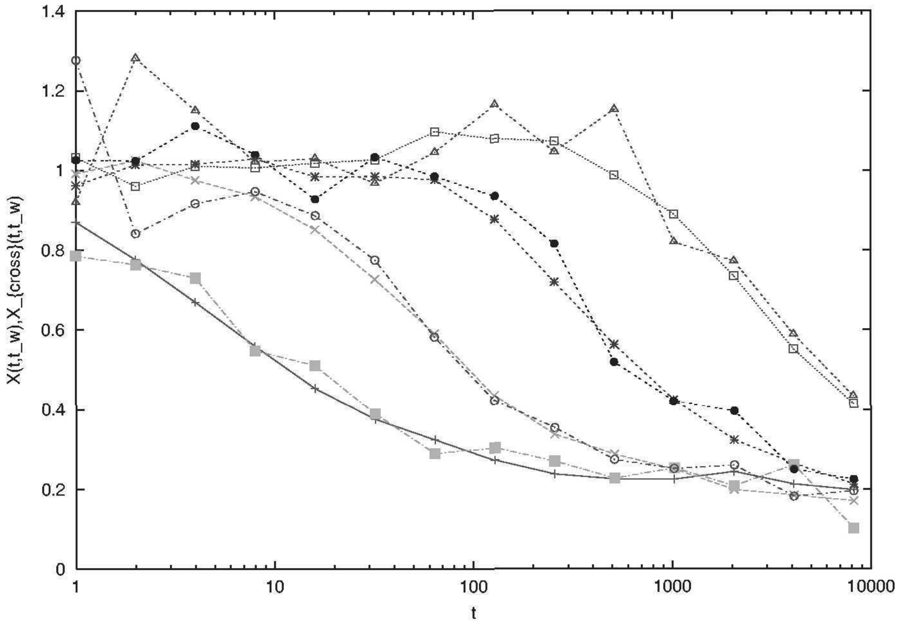

Figure 6. Direct comparison of the FDR for the cross and direct quantities in the 4D EA model. The temperature is $T = 0.43$ and the waiting times are, from bottom to top $t_w = 100, 1000, 10000$. After a shor transient both quantities do coincide.