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Measuring the fluctuation-dissipation ratio in glassy systems with no perturbing field

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A method is presented for measuring the integrated linear response in Ising spin system without applying any perturbing field. Large-scale simulations are performed in order to show how the method works. Very precise measurements of the fluctuation-dissipation ratio are presented for three different Ising models: the two-dimensional ferromagnetic model, the mean-field diluted three-spin model, and the three-dimensional Edwards-Anderson model.

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Disordered and frustrated models are a fascinating but still poorly understood subject in contemporary statistical mechanics. The interest in these systems also comes from their many interdisciplinary applications: from the physics of glass-former liquids to that of polymers and biomolecules, from the description of error correcting codes to the study of the computational complexity and phase transitions in theoretical computer science.

Here we will use the term *glassy system* for a generic model showing very slow relaxation to equilibrium [1]. Because of the huge equilibration time, a glassy system may be in the out of equilibrium regime for all the experimental times. Then a complete understanding of this regime is what one needs in order to correctly describe a real slow-evolving material. Moreover, numerical studies of the off-equilibrium regime do not suffer from finite-size effect since very large sizes can be used. They present finite time corrections which can be usually kept under control, thus allowing for better numerical estimations.

Among the numerical methods that can be used in the out of equilibrium regime, the study of the so-called *fluctuation-dissipation ratio* (FDR) [2] has been shown to be a very successful one [3,4]. This method is based on the comparison of how spontaneous and induced fluctuations relax. Actually one measures an autocorrelation function $C(t,s)$ [5] and the associated response function $R(t,s)$ and defines the FDR $X(t,s)$ through the formula

$$TR(t,s)=X(t,s)\partial_s C(t,s), \tag{1}$$

where T is the temperature. At equilibrium the fluctuation-dissipation theorem (FDT) holds, implying $X=1$.

In the large times limit—$s,t\to\infty$ with $C(t,s)\to q$—the FDR $X(t,s)$ converges to the limiting function $X(q)$. The physical meaning of the function $X(q)$ has been explained in Refs. [6], where it has been shown that under some hypothesis (stochastic stability) the equation

$$X(q)=x(q)\equiv\int_0^q P(q')dq' \tag{2}$$

holds. In Eq. (2) $P(q)$ represents the overlap probability distributioin function in the threshold states, that is, the states reached by the out-of-equilibrium dynamics on very large times, which could be different from the thermodynamical state [1]. It has been conjectured that the effective temperature $T_{\text{eff}}=T/X$ plays a central role in off-equilibrium glassy systems [7].

In numerical simulations the punctual response function $R(t,s)$ is very noisy, while a much better signal can be obtained for the integrated response function

$$\chi(t,t_w)=T\int_{t_w}^t R(t,s)ds. \tag{3}$$

With respect to the usual definition, the temperature T has been added in the above equation in order to simplify the notation in the following formulas and to have a well defined $\chi(t,t_w)$ in the $T\to 0$ limit. In the large time limit, Eq. (3) can be rewritten as

$$\chi(C)=\int_C^1 X(q)\,dq. \tag{4}$$

So the FDR can be simply written as $X(C)=-\partial_C\chi(C)$.

The aim of this Rapid Communication is to propose and to show the efficacy of a very precise method for measuring the integrated response $\chi(C)$ and the FDR $X(C)$ in spin models.

Up to now the best protocol for measuring $\chi(C)$ in spin systems has been the following [3,8]:

(1) Initialize the system in a random configuration.

(2) Quench the system at a temperature $T<T_c$ and evolve it for t_w Monte Carlo sweeps (MCS).

(3) Switch on a random magnetic field of very small intensity h and continue evolving the system while measuring $C_h(t,t_w)$ and $\chi_h(t,t_w)$.

The parametric plot of $\chi_h(t,t_w)$ versus $C_h(t,t_w)$ converges to the function $\chi(C)$ in the limit $t_w\to\infty$ and $h\to 0$. Even when extrapolations can be safely done, they always require a large numerical effort: for example, in order to correctly take the $h\to 0$ limit, the whole simulation must be repeated for many h values in the linear response regime. Moreover, in frustrated systems such as spin glasses the response may have strong nonlinearities even for very small probing fields and it is usually very hard to predict *a priori* which is the linear response regime. Furthermore in out-of-equilibrium simulations the size of the linear response regime may change with the age of the system: A fair conjecture is that it decreases for larger times. If this would be true, extrapolations to the interesting limit would become still more difficult.

For all these reasons we consider of primary importance the development of a method which allows one to calculate the linear response in a spin system without applying any probing field. After having taken *analytically* the $h \to 0$ limit, one is left only with the $t_w \to \infty$ limit. This limit will be somehow unavoidable as long as the only way for aging a glassy system will be to simulate it for a long time [9].

Inspired by a recent work by Chatelain [10], we write down an analytical expression giving the integrated response $\chi(t,t_w)$ in a simulation with no probing field [11].

Let us specialize on systems with N Ising spins and Hamiltonian $\mathcal{H}_0$ (generalization to Potts variables is straightforward [12]). The Hamiltonian $\mathcal{H}_0$ may contain some quenched disorder, but we do not need to specify it, since our calculations hold for a generic $\mathcal{H}_0$, either disorderd or not disordered. In the former case the final result can be eventually averaged over the quenched disorder distribution, but following formulas are valid for any given disorder realization.

When the probing field is switched on the Hamiltonian becomes $\mathcal{H} = \mathcal{H}_0 - \sum_{i=1}^N h_i \sigma_i$, where h_i are independent identically distributed random variables with $\overline{h_i} = 0$ and $\overline{h_i h_j} = h^2 \delta_{i,j}$. For simplicity we define $h_i = h \varepsilon_i$ with $\overline{\varepsilon_i} = 0$ and $\overline{\varepsilon_i \varepsilon_j} = \delta_{i,j}$.

The FDR for the observable $A(t) = \sum_i \varepsilon_i \sigma_i(t)$ is given in terms of the correlation and response functions

$$NC(t,s) = \overline{\langle A(t) A(s) \rangle} = \sum_i \langle \sigma_i(t) \sigma_i(s) \rangle, \tag{5}$$

$$NR(t,s) = \overline{\frac{\partial \langle A(t) \rangle}{\partial h(s)}} = \sum_i \overline{\varepsilon_i \sum_j \frac{\partial \langle \sigma_i(t) \rangle}{\partial h_j(s)} \frac{\partial h_j}{\partial h}}$$
$$= \sum_{i,j} \overline{\varepsilon_i \varepsilon_j} \frac{\partial \langle \sigma_i(t) \rangle}{\partial h_j(s)} = \sum_i \frac{\partial \langle \sigma_i(t) \rangle}{\partial h_i(s)}, \tag{6}$$

where $\langle \cdot \rangle$ represents the average over thermal histories. It is understood that in Eq. (6) all the derivatives are calculated in $h = 0$.

We use a discrete-time dynamics as the one taking place in a Monte Carlo simulation. The time t counts the number of single spin updates and not the number of Monte Carlo sweeps (which is then t/N). The function $I(t)$ gives the index of the spin to be updated at time t, and so it depends on the updating rule (e.g., random or sequential). At the tth time step the spin σ_i with $i = I(t)$ is updated according to heat-bath probabilities

$$\text{prob}(\sigma_i = \sigma) = \frac{\exp[\beta \sigma (h_i^{\mathrm{W}} + h_i)]}{2 \cosh[\beta (h_i^{\mathrm{W}} + h_i)]}, \tag{7}$$

where β is the inverse temperature and the Weiss field h_i^{W} takes into account the effect of Hamiltonian $\mathcal{H}_0$ on the spin to be updated. For example, in the case of two-spin interacting Hamiltonians the Weiss field is given by $h_i^{\mathrm{W}} = \sum_{j \neq i} J_{ij} \sigma_j$.

Under this dynamics the expectation value of the jth spin at a time t is given by

$$\langle \sigma_j(t) \rangle = \mathrm{Tr}_{\vec{\sigma}(t')} \left[\sigma_j(t) \prod_{t'=1}^{t} W_{I(t')}(\vec{\sigma}(t') | \vec{\sigma}(t'-1)) \right], \tag{8}$$

where $\vec{\sigma}$ is a shorthand notation for the N spin configuration, the trace is over all the trajectories $\vec{\sigma}(t')$ with $1 \leq t' \leq t$, and the transition probability is given by

$$W_i(\vec{\sigma} | \vec{\tau}) = \frac{\exp[\beta \sigma_i (h_i^{\mathrm{W}} + h_i)]}{2 \cosh[\beta (h_i^{\mathrm{W}} + h_i)]} \prod_{j \neq i} \delta_{\sigma_j, \tau_j}. \tag{9}$$

Note that $h_i^{\mathrm{W}}(\vec{\sigma}) = h_i^{\mathrm{W}}(\vec{\tau})$ since it does not depend on the spin in i. The transition probability W_i only depends on the perturbing field on site i, such that

$$\left. \frac{\partial W_i(\vec{\sigma} | \vec{\tau})}{\partial h_j} \right|_{h=0} = \delta_{i,j} W_i(\vec{\sigma} | \vec{\tau}) \beta (\sigma_i - \sigma_i^{\mathrm{W}}), \tag{10}$$

where we have defined $\sigma_i^{\mathrm{W}} \equiv \tanh(\beta h_i^{\mathrm{W}})$.

Now we suppose that an infinitesimal probing field h_k on site k is switched on at time t_w: $h_k(t) = h\, \theta(t - t_w)$. This means that the transition probability W_k (and only this one) will depend on the perturbing field for all times larger than t_w. Differentiation of Eq. (8) with respect to this field yields the integrated response

$$\chi_{jk}(t,t_w) = T \left. \frac{\partial \langle \sigma_j(t) \rangle}{\partial h} \right|_{h=0}$$
$$= \mathrm{Tr}_{\vec{\sigma}(t')} \left[\sigma_j(t) \prod_{t'=1}^{t} W_{I(t')}(\vec{\sigma}(t') | \vec{\sigma}(t'-1)) \times \sum_{s=t_w+1}^{t} \delta_{I(s),k} (\sigma_k(s) - \sigma_k^{\mathrm{W}}(s)) \right]$$
$$= \langle \sigma_j(t) \Delta \sigma_k(t,t_w) \rangle$$

$$\text{with} \quad \Delta \sigma_k(t,t_w) = \sum_{s=t_w+1}^{t} \delta_{I(s),k} (\sigma_k(s) - \sigma_k^{\mathrm{W}}(s)). \tag{11}$$

The correlation in Eq. (11) is what one has to measure in a numerical simulation with no perturbing field in order to get the integrated linear response.

Few comments are in order. The time-integrated quantity $\Delta \sigma_k$ only gets contributions when the spin σ_k is updated, so most of the times it is unchanged. The contributions summed up in $\Delta \sigma_k$ are the differences among the actual value of the spin σ_k and the expected one σ_k^{W}. So $\Delta \sigma_k$ is a random variable with zero mean, $\langle \sigma_k \rangle = \sigma_k^{\mathrm{W}} \Rightarrow \langle \Delta \sigma_k \rangle = 0$, and variance $\langle \Delta \sigma_k^2 \rangle \propto (t - t_w)/N$.

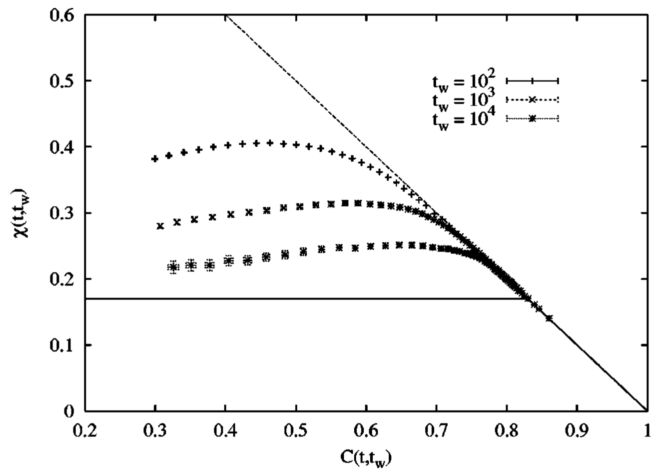

FIG. 1. FD plot for the 2D Ising ferromagnet at $T=2$. The horizontal line is the analytic long time limit.

In the $T=0$ limit Eq. (11) has a nice and simple physical interpretation. Since for $T=0$ we have that $\sigma_k-\sigma_k^{\mathrm{W}}=\sigma_k\delta_{h_k^{\mathrm{W}},0}$, then $\Delta\sigma_k$ takes a contribution only when the spin σ_k has a zero Weiss field on it, i.e., it is free to respond to an infinitesimal field. If the Weiss field is different from zero the spin is completely frozen and it cannot respond to an infinitesimal perturbing field. So the integrated response in Eq. (11) can be rewritten as a simple sum of correlation functions $\chi_{jk}(t,t_w)=\Sigma_s'\langle\sigma_j(t)\sigma_k(s)\rangle$, where the primed sum is over all the times larger then t_w when σ_k is updated under a zero Weiss field, i.e., being a free spin.

We now present numerical results for three-spin models which are believed to belong to three different classes: ferromagnetic model in two dimensions (2D) (coarsening system), diluted long-range three-spin model with fixed connectivity 4 (discontinuous spin glass), and Edwards-Anderson model in 3D (continuous spin glass). For each model we have checked that the $\chi_h(C_h)$ curve measured with the perturbing field converges for $h\to 0$ to the one measured with the present method. Hereafter times will be counted in MCS.

The first model is the ferromagnetic Ising model on the two-dimensional square lattice. We have simulated at $T=2\simeq 0.88T_c$ systems of sizes 1000^2 and 7000^2 in order to check the absence of any finite-size effect (the data we show are from the 1000^2 samples). For each waiting time, $t_w=10^2,10^3,10^4$, averages have been taken over 100 different thermal histories, and the corresponding $\chi(C)$ curves are shown in Fig. 1. The horizontal line is the analytical prediction for the large times limit, $\chi=1-m_{\mathrm{eq}}^2=0.17$. Numerical curves are clearly compatible with the analytical asymptote in the large times limit.

The second model we studied is the three-spin model defined on a random hypergraph with fixed connectivity 4. This model has been solved analytically with a one-step replica symmetry breaking ansatz in Ref. [13]. The dynamical critical temperature is $T_d=0.755\pm 0.01$. We have run simulations for a size $N=999\,999$ at temperature $T=0.5\simeq 0.66T_d$ and the resulting $\chi(C)$ curve is shown in Fig. 2. The number of samples used is 10 for $t_w=10,10^2$, 50 for $t_w=10^3$, and 20 for $t_w=10^4$. The straight line in Fig. 2 is a linear fit to $t_w=10^3$ data in the region $C(t,t_w)<0.9$, which perfectly interpolates the data (χ^2 per degrees of freedom $=0.82$). It gives a Parisi breaking parameter on threshold states equal to $m_{\mathrm{th}}(T=0.5)=0.5\pm 0.02$. The error is an estimate of systematic effects, mainly given by the slight increase of m with t_w. Comparison of this value for m_{th} with corresponding static predictions will be done in Ref. [13].

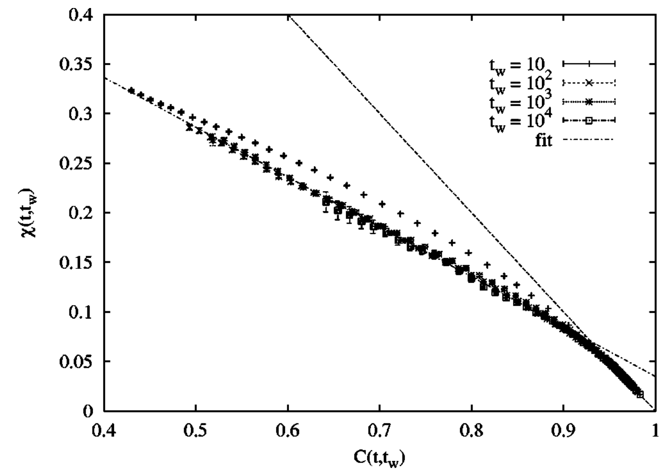

FIG. 2. FD plot for the long-range three-spin model with fixed connectivity 4 at $T=0.5$. The line $0.537\,45-0.502\,56\,C$ is the best linear fit to $t_w=10^3$ data with $C<0.9$.

The third model we studied is the three-dimensional Edwards-Anderson model with $J=\pm 1$ couplings, which undergoes a phase transition to a spin glass phase at $T_c=1.14\pm 0.01$ [14]. We have simulated samples of size $L=20$ at temperatures $T=0.75\simeq 0.66\,T_c$ and $T=0.5\simeq 0.44\,T_c$, for three different waiting times $t_w=10^2,10^3,10^4$. The results are shown in Fig. 3.

For a given temperature the $\chi(C)$ curves look very similar in shape, the main difference being the t_w-dependent Edwards-Anderson order parameter $q_{\mathrm{EA}}(t_w)$, here defined as the point where the $\chi(C)$ curve leaves the FDT line $1-C$. In order to exploit all the data we tried to collapse the curves before fitting. The collapse can be achieved either by shifting

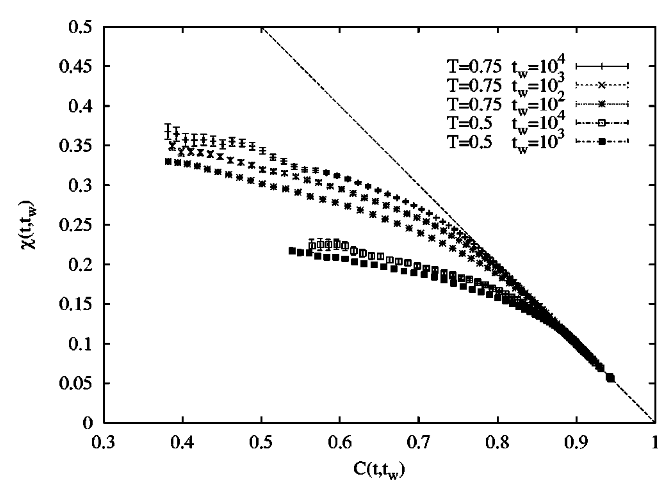

FIG. 3. FD plot for the 3D Edwards-Anderson model.

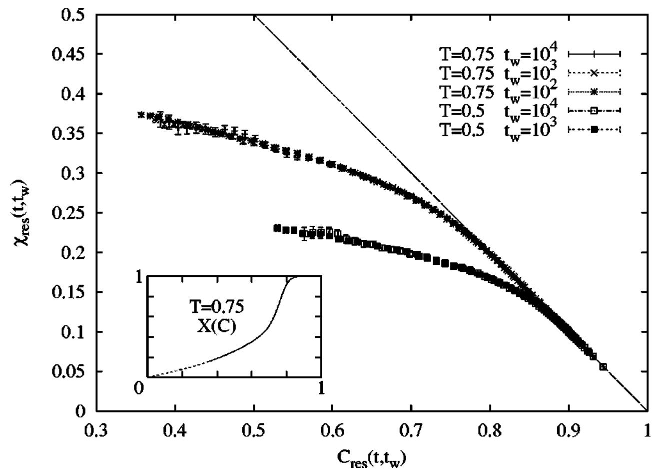

FIG. 4. Same as Fig. 3 with rescaled variables. Inset: FDR for $T=0.75$ obtained from the derivative of the rescaled data.

the curves such that the $q_{EA}(t_w)$ coincide, either by the following rescaling: $C_{res}(t,t_w)=\lambda\, C(t,t_w)/q_{EA}(t_w)$, $\chi_{res}(t,t_w)=1-\lambda[1-\chi(t,t_w)]/q_{EA}(t_w)$, with an arbitrary λ. Both scalings are statistically acceptable. In Fig. 4 we show the second one which is slightly better, with $\lambda=q_{EA}(10^4)$.

If the measured data are already in the asymptotic regime, i.e., the scaling is valid for larger times, and since $\lim_{t_w\to\infty} q_{EA}(t_w)=q_{EA}>0$, we can conclude that the FDR is nontrivial in the three-dimensional Edwards-Anderson model, with an $X(C)$ like the one depicted in the inset of Fig. 4 for $T=0.75$.

The Edwards-Anderson model is the one which took the great part of the simulation time. Indeed, in order to have reasonable error bars, we ran at each of the two temperatures 10^4 samples for $t_w\leqslant 10^3$ and almost 3×10^4 samples for $t_w=10^4$. Solely the $t_w=10^4$ runs took the equivalent of more than 1 y of CPU time on a latest generation 2.0 GHz computer. This is a consequence of the fact that errors on the linear response $\chi(t,t_w)$ increase like $\sqrt{t-t_w}$ and so the number of samples for keeping the error on $\chi(C)$ constant increases more or less linearly with the waiting time t_w. We believe that this is the main drawback of the present method for measuring the linear response: Although it is very successful for small times, it becomes very noisy at larger times and so it requires a huge statistics.

From this observation one could conclude that the usual old method of measuring the response with a small perturbing field would eventually remain the only valid one, but this is not true. Very probably the linear regime in the perturbing field h decreases with the age of the system. In order to remain in the linear response regime one should decrease the intensity of the perturbing field during the simulation, thus increasing the error on the χ for late times. Consequently, a fair comparison between the old method and the present one is very hard to do, since the way the linear response regime decreases with the age of the system is unknown.

Let us conclude with two remarks. First, having understood that the integrated response can be written as a correlation function, it should be clear that all the functions $C(t,t_w)$ and $\chi(t,t_w)$ can be calculated in the *same simulation* for any value of t and t_w. Moreover, correlation functions being self-averaging quantities, it should be possible in principle to calculate them in a *single simulation* of a sufficiently large sample. Second, the method presented here can also be used for any other Monte Carlo simulation (e.g., glass-former particle systems). The only condition for using present analytical expressions is the discreteness of time.

Numerical simulations have been run on our Linux cluster IDRA. I thank ICTP for kind hospitality during the completion of this paper. This work was supported in part by the European Community's Human Potential Program under Contract No. HPRN-CT-2002-00307, Dyglagemem.

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