

Fluctuation-Dissipation Ratio in Three-Dimensional Spin Glasses

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We present an analysis of the data on aging in the three-dimensional Edwards-Anderson spin-glass model with nearest-neighbor interactions, which is well suited for the comparison with a recently developed dynamical mean-field theory. We measure the parameter $x(q)$ describing the violation of the relation among correlation and response functions implied by the fluctuation-dissipation theorem.

KEY WORDS: Spin glasses; nonequilibrium dynamics; Monte Carlo simulations.

On experimental time scales spin glasses are out of equilibrium. Experiments have pointed out that "aging effects," i.e., the dependence of some measurable quantities on the time spent in the low-temperature phase after a quench, persist at least for times of the order of years.⁽¹⁾ The same kind of phenomena have been recorded in numerical simulations of various spin glass models (see ref. 2 for a review).

A lot of activity has been devoted to understanding the origin of these phenomena with phenomenological approaches⁽³⁻⁶⁾ and from the analysis of mean-field models.⁽⁷⁻⁹⁾ This last approach is rapidly evolving, and major progress has been made toward a mean-field theory of the off-equilibrium dynamics of spin glasses. In this note we want to compare some features of the mean-field theory of spin glasses with the more realistic three-dimensional Edwards-Anderson model. In mean-field theory (MFT) aging is associated with a phase transition, there is a high-temperature phase in which the systems equilibrate, and a low-temperature phase where the systems settle in an asymptotic off-equilibrium state.

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On the time scales we can reach we cannot certainly claim that the system has reached an asymptotic behavior, neither we can exclude a cross-over from aging to equilibrium dynamics for very long times. The question whether aging in a 3D system is really asymptotic or gradually disappears, although fundamental in principle, may not be the most relevant one from an experimental point of view.

We compare the behavior of finite time in 3D systems with the predictions of the mean-field theory. Among these, we will focus on a systematic analysis of the violations of the fluctuation-dissipation theorem (FDT). The FDT cannot hold in a nonequilibrium situation, where the probability distribution for the spin configurations is time dependent (see the discussion in ref. 10). The fundamentally new idea developed in refs. 7–9 is that a quantitative analysis of this violation could reveal a deeper insight into long-time off-equilibrium properties of spin glasses.

In spin-glass dynamics crucial quantities of interest are the spin autocorrelation function $C(t, s)$ and its associated response function $G(t, s)$,

$$\begin{aligned} C(t, s) &= [\langle S_i(t) S_i(s) \rangle]_{\text{av}} \\ r(t, s) &= \partial \langle S_i(t) \rangle / \partial h_i(s) \quad (t > s) \end{aligned} \quad (1)$$

where $\langle \dots \rangle$ means an average over the stochastic process describing the dynamical evolution of the system at a temperature $T = \beta^{-1}$ (starting with a random initial configuration) and $[\dots]_{\text{av}}$ means an average over the quenched disorder. At thermal equilibrium these functions are homogeneous, and related by the fluctuation-dissipation theorem relation $r_{\text{eq}}(t-s) = \beta \partial C_{\text{eq}}(t-s) / \partial s$. In general, to characterize off-equilibrium situations it is possible to introduce the “fluctuation-dissipation ratio” as the function

$$x(t, s) = \frac{r(t, s)}{\beta \partial C(t, s) / \partial s} \quad (2)$$

It is convenient for the following analysis to change a bit the definition of this function. First we define a function $\tilde{s}(q, t)$ as the time s such that $C(t, s) = q$, which is unique due to the monotonicity of $C(t, s)$ with s . Then we consider the fluctuation-dissipation ratio at this time

$$\bar{x}(t, q) = x(t, \tilde{s}(q, t)) \quad (3)$$

The above-mentioned MFT makes a particular set of predictions for $x(t, s)$ [and *a fortiori* for $\bar{x}(t, q)$] in the limit $t, s \rightarrow \infty$. There are different ways in which one can take this limit, depending on the relation between

t and s . In ordinary equilibrating systems, the relevant procedure is to fix the difference $t - s = \tau$ to a finite value. This yields limiting functions $C_{as}(\tau)$, $r_{as}(\tau)$. The correlation function $C_{as}(\tau)$ decreases monotonically from the value 1 at $\tau = 0$ to a value that we call q_{EA} for $\tau \rightarrow \infty$, and the FD relation is respected ($x = 1$). In any different limiting procedure that would imply $t - s \rightarrow \infty$ one would find that the correlation function tends to q_{EA} . In other words, for $t, s \rightarrow \infty$ all the observable dynamical effects are concentrated in the finite- τ region. In aging systems this does not happen: dynamical effects persist in regions of the plane (t, s) where the limit is taken differently. This is apparent in experiments⁽¹¹⁾ where important dynamical effects are observed on time scales τ of the order of the “waiting time” (s).

In mean-field spin glasses, dynamics takes place both in a region of time homogeneity where the FDT relation is respected and in an aging region. This was first theorized in ref. 7 and then verified by a numerical solution of mean-field off-equilibrium dynamical equations for a particular model in ref. 8. An ansatz which allows for a precise definition of the infinite-time limit in the homogeneous and aging regimes has been put forward in refs. 7–9. Without entering into the details of this limiting procedure, we just summarize some consequences of the analysis. The time-homogeneous regime is qualitatively similar to an equilibrium regime where $\lim_{\tau \rightarrow \infty} C_{as}(\tau) = q_{EA}$, $x(q) = 1$ for $q_{EA} < q \leq 1$.

In the aging regime the function $C(t, s)$ decreases, for decreasing s , from q_{EA} to a value q_{min} ($q_{min} = 0$ for spin glasses in the absence of a magnetic field). The function $\bar{x}(t, q)$ tends, for any q in the interval $[q_{min}, q_{EA}]$, to a well-defined limit $x(q)$.

It turns out that the function $x(q)$ is formally related to the inverse of the static Parisi function $q_{stat}(x)$, $x_{stat}(q)$. A nontrivial $x(q)$ is found in these models which statically exhibit replica symmetry breaking.⁽¹¹⁾ In all cases in which the replica symmetry breaking is associated with a continuous $q_{stat}(x)$, we have $x_{stat}(q) = x(q)$. If the static $q_{stat}(x)$ is discontinuous, $x(q)$ turns out to be different from its static counterpart. This is the case, e.g., in the p -spin spherical model,⁽⁷⁾ where $x(q)$ is a step function. However, in both cases, $dx(q)/dq$ has all the properties defining a probability distribution, as happens for dx_{stat}/dq . At present there is not a complete physical comprehension of the relation between the static definition of $x(q)$ and the dynamic one and of the fact that the latter is associated with a probability distribution.

In this paper we extract the above-defined function $x(q)$ from numerical data obtained for the 3D Edwards–Anderson model via Monte Carlo simulations performed by one of us recently.⁽¹²⁾ The advantage of numerical simulations compared to experiments is that while experimentally it is

very difficult to get direct information on the correlation function, in numerical simulations one can easily have access to both the correlation and response functions.

The correlation function is measured directly in the course of simulations starting from a random initial condition, which corresponds to a rapid temperature quench from the paramagnetic phase. The response function is measured in thermoremanent magnetization (TRM) experiments: the system is allowed to age for a time t_w in the presence of a small magnetic field h , then the magnetic field is cut off and the magnetization is recorded as a function of the time τ measured starting from t_w . We assume linear response conditions where the magnetization $M(\tau + t_w, t_w)$ is given by³

$$M(\tau + t_w, t_w) = h \int_0^{t_w} r(\tau + t_w, s) ds \quad (4)$$

Using (3), one can write

$$M(\tau + t_w, t_w) = \frac{h}{T} \int_{C(\tau + t_w, 0)}^{C(\tau + t_w, t_w)} \bar{x}(\tau + t_w, q) dq \quad (5)$$

and exploiting the monotonicity of C this time with respect to τ , we choose τ such that $C(\tau + t_w, t_w) = q$ and write with obvious meaning of the symbols

$$M(q, t_w) = \frac{h}{T} \int_{C(\tau + t_w, 0)}^q \bar{x}(\tilde{\tau}(q, t_w) + t_w, q') dq' \quad (6)$$

For infinite t_w , assuming loss of memory of the initial condition, $\lim_{t_w \rightarrow \infty} C(\tau + t_w, 0) \rightarrow 0$, one would have $M(q) = (h/T) \int_0^q dq' x(q')$. In the following we will present simulation data for the function

$$\chi(q, t_w) = \frac{T}{h} M(q, t_w) \xrightarrow{t_w \rightarrow \infty} \chi(q) \quad (7)$$

in the 3D Edwards–Anderson model. Simulation data for the corresponding function in the Sherrington–Kirkpatrick model have been given in ref. 9. In order to understand our findings, let us discuss some simple scenarios for the function $\chi(q)$.

³ Note that we use a notation in which both the time arguments of M are measured starting from the quenching time $t = 0$. The standard notation would be $M(\tau, t_w)$.

1. *Ergodic behavior in the whole phase space.* In this case $q_{EA} = 0$ and $x(q)$ is equal to one in the whole interval $0 \leq q \leq 1$ and one finds the classical FDT result

$$\chi(q) = q \tag{8}$$

typical, e.g., of paramagnetic systems.

2. *Ergodic behavior in a confined component.* Here the system relaxes to a nonzero q_{EA} and the dynamics remains confined to a single valley; then $x(q) = \Theta(q - q_{EA})$ and

$$\chi = \Theta(q - q_{EA})(q - q_{EA}) \tag{9}$$

Such behavior is found, e.g., in ferromagnets in the low-temperature phase, where q_{EA} is equal to the square of the magnetization and this would also be the prediction for a spin-glass scenario like that proposed by Fisher and Huse.⁽⁴⁾

3. *Mean-field aging behavior.* In this case two scenarios are found in the literature. In models with one step of replica symmetry breaking

$$\begin{aligned} x(q) &= x \Theta(q_{EA} - q) + \Theta(q - q_{EA}) \\ \chi(q) &= x \Theta(q_{EA} - q)q + \Theta(q - q_{EA})\{q - (1 - x)q_{EA}\} \end{aligned}$$

while in models with continuous replica symmetry breaking x is an increasing function from zero at $q = 1$ to one for $q = q_{EA}$ and stays equal to that value for $q > q_{EA}$. Correspondingly,

$$\chi(q) = \Theta(q_{EA} - q) \int_0^q dq' \tilde{x}(q') + \Theta(q - q_{EA}) \left\{ q - q_{EA} + \int_0^{q_{EA}} dq' x(q') \right\} \tag{10}$$

In the SK model near T_c one finds⁽⁹⁾ the linear shape $x(q) = 2aq$ with $a = 1/2$ and one obtains

$$\chi(q) = \Theta(q_{EA} - q)aq^2 + \Theta(q - q_{EA})(q - q_{EA} + aq_{EA}^2)$$

Let us turn now to the presentation of the simulation data. We stress that at finite times, $C(t, s)$ and $r(t, s)$ are regular functions, and the possible singularities in $x(q)$ and χ should be smoothed in some crossover region. We use the data obtained in ref. 12, doing some additional runs where necessary. For completeness let us recall the definition of the model that we investigate: it is the three-dimensional Edwards–Anderson model defined by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - h \sum_i S_i \tag{11}$$

where $\langle ij \rangle$ are nearest-neighbor pairs on a simple cubic lattice, $S_i = \pm 1$ are Ising spins, J_{ij} are quenched random variables taking on the values $+1$ and -1 with equal probability, and h is an external magnetic field. In this model a phase transition has been observed at $T_c \approx 1.2$ ⁽¹⁴⁾ (see, however, ref. 15 for a different point of view). We use single-spin-flip heat-bath dynamics with parallel sublattice update and calculate the spin-autocorrelation function $C(\tau, t_w)$ (in zero field) and the thermoremanent magnetization $M(\tau + t_w, t_w)$ as defined in (4). The field h applied for a time t_w before starting the measurement is small ($h=0.1$), and we checked by looking at $h=0.05$ and $h=0.2$, too, that we are in the linear response regime. Thus $\chi(\tau + t_w, t_w) = T/h M(\tau + t_w, t_w)$ is the magnetic relaxation function occurring in linear response theory. The lattice size used is $N=32^3$ and we made sure that finite-size effects were not significant. All data are averaged over at least 128 samples (i.e., different realizations of the disorder).

In Fig. 1 we show a picture, analogous to that presented in ref. 13, that clearly shows the violation of the FDT relation between magnetization

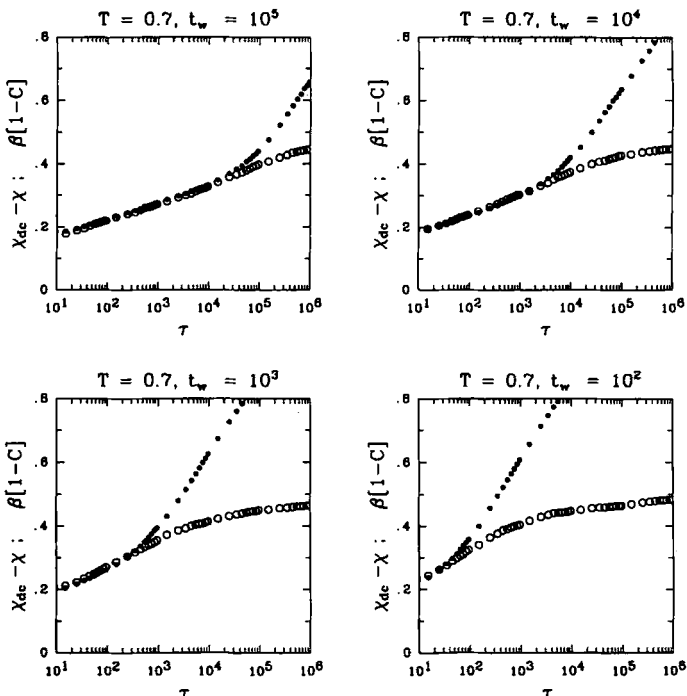


Fig. 1. The quantities $\chi_{dc} - \chi(\tau + t_w, t_w)$ (\circ) and $\beta[1 - C(\tau + t_w, t_w)]$ (\bullet) versus time t for different waiting times. χ_{dc} , the dc susceptibility, is a single fit parameter for all waiting times. The temperature is $T=0.7$. Note that for the FDT to hold both curves have to be identical.

and correlation function as a function of time. As long as $\tau \ll t_w$ the FDT relation is fulfilled,

$$\chi_{dc} - \chi(\tau + t_w, t_w) = \beta\{1 - C(\tau + t_w, t_w)\} \tag{12}$$

where χ_{dc} is the equilibrium dc susceptibility (see, e.g., ref. 3). For $\tau \gg t_w$ this relation is obviously violated.

In Fig. 2 we present the function $\chi(q, t_w)$ for different waiting times and temperatures $T=0.8, 1, 1.5, 2$. It is clearly seen in the $T=2.0$ plot that after a short transient, χ tends to the paramagnetic function $\chi(q) = q$. In the plot of the $T=1.5$ data we can see that the system has not equilibrated even after the largest waiting time $t_w = 10^5$. At low temperature we clearly recognize a t_w -dependent linear part in χ at large q . The slope of the linear part is indeed 1, as shown in Fig. 3, where we display $\chi(q, t_w) - q$ for $T=0.8$. From Figs. 2 and 3 one can extract an effective time-dependent EA parameter $q_{EA}(t_w)$ as the value of q at which $\chi(q)$ starts to depart from linearity. In this way we estimate at $T=0.8$ for $t_w = 10^3, 10^4$, and 10^5 the

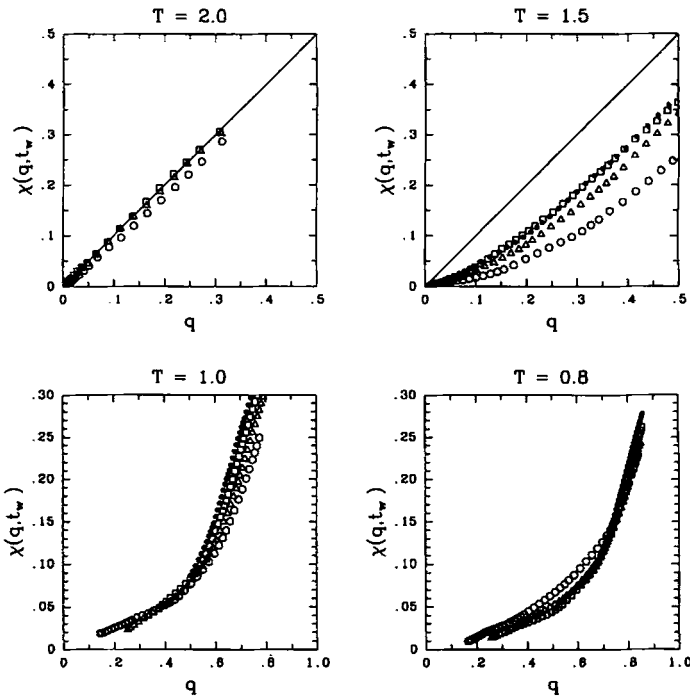


Fig. 2. The function $\chi(q, t_w)$ versus q for various temperatures. The waiting times are $t_w = 10^2$ (\circ), 10^3 (Δ), 10^4 (\square), and 10^5 (\bullet).

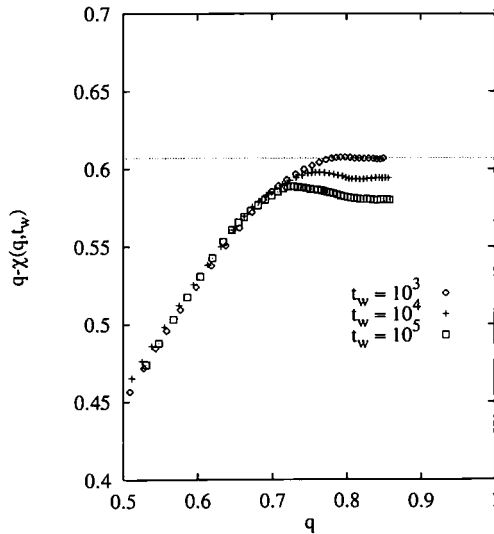


Fig. 3. The function $q - \chi(q, t_w)$ versus q for $T = 0.8$ and different waiting times. The function $q - \chi(q, t_w)$ should be constant as long as the FDT is fulfilled. The line is only a guide for the eye.

values $q_{EA} = 0.78, 0.75,$ and $0.72,$ respectively. It is clear that these data do not allow for any extrapolation.

The small- q part of the curves can be reasonably fitted with an arc of parabola $\chi(q) = aq^2$; for $t_w = 10^3, 10^4,$ and 10^5 the value of a at $T = 0.8$ is roughly constant and equal to $a = 0.2$. A linear fit of the kind $\chi(q) = xq$ gives much poorer results. This seems to indicate a scenario more similar to that of SK-like continuous replica symmetry breaking than that of a one-step replica symmetry breaking.

In Fig. 4 finally we present $\chi(q)$ as a function of q for $t_w = 10^5$ and different temperatures. As expected, the apparent q_{EA} parameter grows for decreasing temperatures. On one hand one definitely still observes a slight dependence of $\chi(q, t_w)$ on the waiting time t_w , which means that rigorous statements on the limiting shape of $\chi(q)$ and hence of $x(q)$ hardly can be made. On the other hand we do not observe any tendency of the curves $\chi(q, t_w)$ to approach a form like (9) that is characteristic for a system with only two pure states [note that this would imply that the whole small- q part, i.e., $q < q_{EA}$, of $\chi(q, t_w)$ has to come down to zero].

We leave to the reader to judge if our data can be interpreted as an indication for a nontrivial $x(q)$ in three dimensions. However, the 3D EA model is known to be only marginally critical; therefore it would be highly desirable to perform the same kind of investigation in four dimensions,

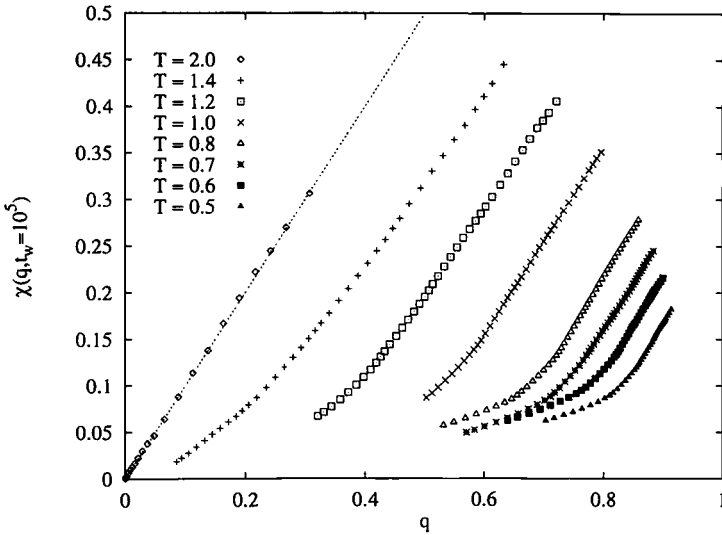


Fig. 4. $\chi(q, t_w)$ versus q for different temperatures at $t_w = 10^5$.

where a nontrivial *static* $P(q)$ has already been reported from a finite-size scaling analysis.⁽¹⁶⁾

Concluding, we have analyzed in this paper the data for the correlation and the response functions in the light of a recent mean-field theory of aging phenomena. We have shown that at least insofar as the quantity $\chi(q)$ is concerned, the behavior of the 3D EA model at the time scale we investigate agrees qualitatively with a mean-field-like behavior. One clearly sees a separation of the dynamics into a quasiequilibrium part, analogous to an equilibrium dynamics where the FD relation is respected, and an aging part where the FD ratio takes values different from zero and one. Rough estimates indicate that $\chi(q)$ grows linearly with q for small q , a behavior reminiscent of the SK model. The time scales to which we have access prevent us from probing the asymptotic behavior of the system, and even from proving that aging phenomena do not gradually disappear for increasing waiting times. This question is related to the one long debated of the existence of a sharp phase transition in the model, and more general in 3D short-range spin glasses. Although of fundamental theoretical importance, due to the slowness of the relaxation process, it is certainly not the most interesting one from an experimental point of view. It could well be the case that even if the transition is absent and the aging is interrupted after some very long time, the mechanisms responsible for aging in mean field could be relevant for the 3D physics on experimental times.

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