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Fluctuation-dissipation relations and effective temperatures in simple non-mean field systems

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Abstract

We give a brief review of violations of the fluctuation-dissipation theorem (FDT) in out-of-equilibrium systems; in mean field scenarios the corresponding fluctuation-dissipation (FD) plots can, in the limit of long times, be used to define a *effective temperature* T_{eff} that shares many properties of the true thermodynamic temperature T . We discuss carefully how correlation and response functions need to be represented to obtain meaningful limiting FD plots in *non-mean field* systems. A minimum requirement on the resulting effective temperatures is that they should be independent of the observable whose correlator and response are being considered; we show for two simple models with glassy dynamics (Bouchaud's trap model and the Glauber–Ising chain at zero temperature) that this is generically not the case. Consequences for the wider applicability of effective temperatures derived from FD relations are discussed; one intriguing possibility is that at least the limit of the FDT violation factor for well separated times may generically be observable-independent and so could yield a meaningful T_{eff} .

1. Introduction: fluctuation-dissipation relations and effective temperatures

One of the core ideas of statistical mechanics is that *equilibrium* states can be accurately described in terms of only a small number of thermodynamic variables, such as temperature and pressure. For glassy systems, which can remain far from equilibrium on very long timescales, no similar simplification exists *a priori*; the whole past history of a sample is in principle required to specify its state at a given time. This complexity makes the theoretical analysis of glasses very awkward, and one is driven instead to look for a description of out-of-equilibrium

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states in terms of a few effective thermodynamic parameters. The focus of the present paper is on one such parameter, the *effective temperature*; this can be defined on the basis of fluctuation-dissipation (FD) relations between correlation and response functions and has proved to be very fruitful in mean field systems [1].

The use of FD relations to quantify the out-of-equilibrium dynamics in glassy systems is motivated by the occurrence of *ageing* [2]: the timescale of response to an external perturbation increases with the age (time since preparation) t_w of the system. As a consequence, time translational invariance (TTI) and the equilibrium fluctuation-dissipation theorem (FDT) [3] relating correlation and response functions break down. To quantify this, consider the autocorrelation function for a generic observable m of a system, defined as

$$C(t, t_w) = \langle m(t)m(t_w) \rangle - \langle m(t) \rangle \langle m(t_w) \rangle. \quad (1)$$

The associated ‘impulse response’ function can be defined as

$$R(t, t_w) = \left. \frac{\delta \langle m(t) \rangle}{\delta h(t_w)} \right|_{h=0}$$

and gives the linear response of $m(t)$ to a small impulse in its conjugate field h at time t_w . An equivalent way of characterizing the linear response is via the ‘step response’ function

$$\chi(t, t_w) = \int_{t_w}^t dt' R(t, t') \quad (2)$$

which tells us how m responds to a small step $h(t) = h\Theta(t - t_w)$ in the field. In spin glasses, this response function would be called the zero-field cooled response because the field is only switched on a certain ‘waiting time’ t_w after preparation of the system (e.g. by cooling) at time $t = 0$.

Now, in *equilibrium*, $C(t, t_w) = C(t - t_w)$ by TTI (similarly for R and χ), and the FDT reads

$$-\frac{\partial}{\partial t_w} \chi(t - t_w) = R(t, t_w) = \frac{1}{T} \frac{\partial}{\partial t_w} C(t - t_w) \quad (3)$$

with T the thermodynamic temperature (we set $k_B = 1$). A parametric ‘FD plot’ of χ versus C is thus a straight line of slope $-1/T$. In the ageing case, the violation of FDT can be measured by an FD ratio, $X(t, t_w)$, defined through [4, 5]

$$-\frac{\partial}{\partial t_w} \chi(t, t_w) = R(t, t_w) = \frac{X(t, t_w)}{T} \frac{\partial}{\partial t_w} C(t, t_w). \quad (4)$$

In equilibrium, due to TTI, the derivatives $\partial/\partial t_w$ in the FDT (3) could equally be replaced by $-\partial/\partial t$; one could therefore argue that a similar replacement could be made in (4), leading to a different definition of $X(t, t_w)$. However, the latter would make rather less sense, since in a situation without TTI only the t_w -derivative of $\chi(t, t_w)$ is directly related to the impulse response $R(t, t_w)$. Adopting therefore the definition (4), one sees that values of X different from unity mark a violation of FDT. In glasses, these can persist even in the limit of long times, indicating strongly non-equilibrium behaviour even though one-time observables of the system—such as entropy and average energy—may have already settled to essentially stationary values.

Remarkably, the FD ratio for several *mean field* models [4, 5] assumes a special form at long times: taking $t_w \rightarrow \infty$ and $t \rightarrow \infty$ at constant $C = C(t, t_w)$, $X(t, t_w) \rightarrow X(C)$ becomes a (nontrivial) function of the single argument⁴ C . If the equal-time correlator $C(t, t)$ also

⁴ This definition is not quite as stringent as requiring that $X(t, t_w)$ be a function of $C(t, t_w)$ only, at long times t_w and t . For some coarsening models at criticality one finds, for example, that $X(t, t_w) = f(t_w^a C(t, t_w))$ for long times, in terms of a scaling function $f(\cdot)$ and a positive exponent a [6]; X is therefore not a function of C alone. Nevertheless, making t and t_w large at constant C , one finds a nontrivial function $X(C)$ which in this case is discontinuous, $X(C) = f(\infty)$ for $C > 0$ and $X(C) = f(0)$ for $C = 0$.

approaches a constant C_0 for $t \rightarrow \infty$, it follows that

$$\chi(t, t_w) = \frac{1}{T} \int_{C(t, t_w)}^{C_0} dC X(C). \quad (5)$$

Graphically, this limiting non-equilibrium FD relation is obtained by plotting χ versus C for increasingly large times; from the slope $-X(C)/T$ of the limit plot, an *effective temperature* [1] can be defined as $T_{\text{eff}}(C) = T/X(C)$.

In the most general ageing scenario, a system displays dynamics on several characteristic timescales, one of which may remain finite as $t_w \rightarrow \infty$, while the others diverge with t_w . If, due to their different functional dependence on t_w , these timescales become infinitely separated as $t_w \rightarrow \infty$, they form a set of distinct ‘time sectors’; in mean field, $T_{\text{eff}}(C)$ can then be shown to be *constant* within each such sector [5]. In the short-time sector ($t - t_w = O(1)$), where $C(t, t_w)$ decays from C_0 to some plateau value, one generically has quasi-equilibrium with $T_{\text{eff}} = T$, giving an initial straight line with slope $-1/T$ in the FD plot. The further decay of C (on ageing timescales $t - t_w$ that grow with t_w) gives rise to one of three characteristic shapes: (i) in models which statically show one-step replica symmetry breaking (RSB), e.g. the spherical p -spin model [4], there is only one ageing time sector and the FD plot exhibits a second straight line, with $T_{\text{eff}} > T$. (ii) In models of coarsening and domain growth, e.g. the $O(n)$ model at large n , this second straight line is flat, and hence $T_{\text{eff}} = \infty$ [7]. (iii) In models with an infinite hierarchy of time sectors (and infinite step RSB in the statics, e.g. the SK model) the FD plot is instead a continuous curve [5].

T_{eff} has been interpreted as a timescale-dependent non-equilibrium temperature, and within mean field has been shown to display many of the properties associated with a thermodynamic temperature [1]. For example (within a given time sector), it is the reading which would be shown by a thermometer tuned to respond on that timescale. Furthermore—and of crucial importance to its interpretation as a temperature—it is independent of the observable⁵ m used to construct the FD plot [1].

While the above picture is well established in mean field, its status in non-mean field models is less obvious. To check its validity, one must demonstrate: (a) that a limiting FD plot exists, (b) that it gives effective temperatures that are independent of the observable–field pair used to calculate C and χ , and (c) that the effective temperature is constant within a given time sector, i.e. the same for all timescales differing only by factors of order unity. One then expects FD plots similar to those for mean field systems, composed either of a set of straight lines, or of a continuous curve in the case of an infinite number of distinct ageing time sectors. Of course, full independence of the effective temperature from the observable considered may be too strong a requirement for non-mean field systems, but one would at least expect independence within a large class of sufficiently ‘neutral’ observables; we return to this point in section 4.

Encouragingly, molecular dynamics (MD) and Monte Carlo (MC) simulations of binary Lennard-Jones mixtures [9], as well as MC simulations of frustrated lattice gases [10] (which loosely model structural glasses, whose phenomenology is similar to that of the p -spin model) show a limiting plot of type (i). Oscillator models with MC dynamics show similar plots, but the initial short-time regime where one has effective equilibrium is absent and one finds only a single straight line [11]. MC simulations of the Ising model with conserved and non-conserved order parameter in dimensions $d = 2$ and 3 show a plot of type (ii) [12]. And MC

⁵ This applies to a wide class of observables, but has not to our knowledge been established in complete generality. The restriction arises because the observables that are commonly used in mean field models are defined in terms of random fields or couplings, and are therefore uncorrelated with the energy of the system. It is possible that for other variables, which *are* correlated with the energy, different effective temperatures would be obtained (S Franz and F Ritort, Private communication). This effect is observed explicitly in oscillator models with MC dynamics [8].

simulations of the Edwards–Anderson model in $d = 3$ and 4 [13] give a plot of type (iii). The majority of existing studies, however, do not show that T_{eff} is independent of observable (notable exceptions being [9, 10]) since they consider just one observable–field pair. In the Backgammon model (see e.g. [14] for a summary of results), several observables have recently been considered and differences in the FD ratios found; however, these differences only occur in sub-leading terms which decay to zero at long times, and so it is not clear how seriously this observable-dependence needs to be taken.

Below, we therefore give some results for two models for which FD relations can be calculated for a broad range of observables; our aim is to clarify the status of FD-derived effective temperatures in non-mean field systems. First, however, we pause briefly to discuss the appropriate representation of FD plots in such systems. As explained above, for mean field systems the existence of a limiting relation (5) between response χ and correlation C ensures that parametric plots of χ versus C converge, for long times, to a limiting FD plot whose negative slope directly gives $X(C)/T$. Equation (5) implies that the plots can be produced either with t as the curve parameter, holding the earlier time t_w fixed, or vice versa. Since it is normally easier to fix the time t_w at which a field is switched on and measure the resulting response as a function of t —rather than observing the response at fixed t to fields switched on at a range of earlier times t_w —the first version is the one that is conventionally used [4, 5].

In general, however, it is clear that the definition (4) ensures a slope of $-X(t, t_w)/T$ for a parametric χ – C plot *only* if t_w is used as the parameter, with t being fixed. This issue becomes particularly important when—for the particular observable chosen—the equal-time correlator $C(t, t)$ diverges or decreases to zero for $t \rightarrow \infty$, instead of approaching a constant value. A series of ‘raw’ FD plots at increasing t will then either grow or shrink in scale indefinitely, preventing the existence of a limiting FD plot for $t \rightarrow \infty$. It therefore appears reasonable to *normalize* the FD plot. The normalization factor must be the same for the χ -axis and the C -axis and must be independent of t_w , in order to preserve the connection between X and the slope of the plot. To ‘attach’ the plot to a definite point on the C -axis, it is thus sensible to normalize by $C(t, t)$, plotting $\tilde{\chi}(t, t_w) = \chi(t, t_w)/C(t, t)$ versus $\tilde{C}(t, t_w) = C(t, t_w)/C(t, t)$. In this representation, a limiting FD plot *may* be approached as t is increased. If this is the case, then $X(t, t_w)$ converges to a nontrivial limit for large times, but now at a constant value of the *normalized* correlator \tilde{C} (rather than of C itself). Also, *if a limiting plot exists*, it can be obtained from plots of $\tilde{\chi}$ versus \tilde{C} that use *either* t or t_w as the curve parameter; the normalization still has to be performed with $C(t, t)$ and not with $C(t_w, t_w)$, however, in order to retain the link between X and the slope of the limit plot.

One final benefit of the method of producing FD plots discussed above—normalize by $C(t, t)$, and use t_w as the curve parameter—is that the plots for the two types of response function most frequently considered are trivially related. We have worked above with the ‘switch-on’ (or zero-field cooled) response function (2); a common alternative is the ‘switch-off’ (or thermo-remanent) response, defined for a field switched on at time 0 and off again at time t_w :

$$\chi_{-}(t, t_w) = \int_0^{t_w} dt' R(t, t') = \chi(t, 0) - \chi(t, t_w). \quad (6)$$

With t_w being used as the curve parameter, the FD plots of χ versus C and χ_{-} versus C are then trivially related (by a reflection about the horizontal axis and a vertical shift); the same remains true after normalization of the curves by $C(t, t)$. If, on the other hand, one were to follow the naive approach of using t as the curve parameter—keeping t_w fixed—and normalizing by $C(t_w, t_w)$, then the plots for χ and for χ_{-} are not related in any obvious way and can in fact have very different shapes [15].

We end this section with a brief comment on a recent proposal [16] to construct FDT plots from the response and the *disconnected* correlation function

$$C_{\text{dis}}(t, t_w) = \langle m(t)m(t_w) \rangle$$

as opposed to the *connected* one (1) used above. This can avoid the normalization problem in some cases: if, for example, one is dealing with a systems of spins $s_i = \pm 1$, and m is a staggered magnetization with a random field, then C_{dis} reduces to a spin–spin autocorrelation function and so is automatically normalized at equal times, $C_{\text{dis}}(t, t) = 1$. While apparently convenient, use of C_{dis} in FD plots appears to us to have little theoretical justification. A serious drawback is that FD plots constructed from C_{dis} are no longer invariant under simple affine transformations of the observable, $m' = am + b$. This seems to us to violate the physical intuition that such trivially related observables should not be able to reveal significantly different glassy physics. We would therefore advocate use of the connected correlation function (1) throughout; this ensures that affine transformations of observables, as defined above, leave all FD plots invariant (up to a trivial overall scale factor of a^2). This point was also made in a very recent investigation of out-of-equilibrium FD relations in simple glassy spin models [17]. Of course, if the observable is such that it has no drift, i.e. $\langle m(t) \rangle = \text{constant}$, then disconnected and connected correlation functions can be used interchangeably, since they differ only by a trivial additive constant. This may be the case for sufficiently ‘neutral’ observables (or could in fact be part of the criterion for deciding whether an observable is neutral); see the discussion in section 4.

2. Model system 1: Bouchaud’s trap model

Trap models [18–20] are obvious candidates for a study of FD violation in systems with glassy dynamics. Popular as alternatives to the microscopic spin models discussed above, they capture ageing within a simplified single particle description. The simplest such model [18] comprises an ensemble of uncoupled particles exploring a spatially unstructured landscape of (free) energy traps by thermal activation. The tops of the traps are at a common energy level and their depths E have a ‘prior’ distribution $\rho(E)$ ($E > 0$). A particle in a trap of depth E escapes on a timescale $\tau(E) = \tau_0 \exp(E/T)$ and hops into another trap, the depth of which is drawn at random from $\rho(E)$. The probability, $P(E, t)$, of finding a randomly chosen particle in a trap of depth E at time t thus obeys

$$(\partial/\partial t)P(E, t) = -\tau^{-1}(E)P(E, t) + Y(t)\rho(E) \quad (7)$$

in which the first (second) term on the right-hand side represents hops out of (into) traps of depth E , and $Y(t) = \langle \tau^{-1}(E) \rangle_{P(E,t)}$ is the average hopping rate. The solution of (7) for initial condition $P_0(E)$ is

$$P(E, t) = P_0(E)e^{-t/\tau(E)} + \rho(E) \int_0^t dt' Y(t')e^{-(t-t')/\tau(E)} \quad (8)$$

from which $Y(t)$ has to be determined self-consistently. For the specific choice of prior distribution $\rho(E) \sim \exp(-E/T_g)$, the model shows a glass transition at a temperature T_g . This can be seen as follows: at a temperature T , the equilibrium Boltzmann state (if it exists) is $P_{\text{eq}}(E) \propto \tau(E)\rho(E) \propto \exp(E/T)\exp(-E/T_g)$. For temperatures $T \leq T_g$ this is unnormalizable, and cannot exist; the lifetime averaged over the prior, $\langle \tau \rangle_\rho$, is infinite. Following a quench to $T \leq T_g$, the system never reaches a steady state, but instead ages: in the limit $t_w \rightarrow \infty$, $P(E, t_w)$ is concentrated entirely in traps of lifetime $\tau = O(t_w)$. The model thus has just one characteristic timescale, which grows linearly with the age t_w . In contrast, for $T > T_g$ all relaxation processes occur on timescales $O(\tau_0)$. In what follows, we rescale all energies such that $T_g = 1$, and also set $\tau_0 = 1$.

To study FD violation one can extend the model as follows [21]: to each trap we assign, in addition to its depth E , a value for an (arbitrary) observable m ; by analogy with spin models we refer to m as magnetization. The trap population is then characterized by the joint prior distribution $\sigma(m|E)\rho(E)$, where $\sigma(m|E)$ is the distribution of m across traps of given fixed energy E . We focus on the non-equilibrium dynamics after a quench at $t = 0$ from $T = \infty$ to $T < 1$; the initial condition is thus $P_0(E, m) = \sigma(m|E)\rho(E)$. The subsequent evolution is governed by

$$(\partial/\partial t)P(E, m, t) = -\tau^{-1}(E, m)P(E, m, t) + Y(t)\sigma(m|E)\rho(E) \quad (9)$$

where the activation times are modified, in the presence of a small field h conjugate to m , according to $\tau(E, m) = \tau(E)\exp(mh/T)$. Other choices of $\tau(E, m)$ that maintain detailed balance are possible [20, 22]; we adopt this particular one because, in the spirit of the unperturbed model, it ensures that the jump rate between any two states depends only on the initial state, and not the final one.

Let us outline briefly the calculation of correlation and response function for the observable m . The autocorrelation function is (in the absence of a field, i.e. $h = 0$)

$$C(t, t_w) = \int dm dm_w dE dE_w m m_w P(E_w, m_w, t_w)[P(E, m, t|E_w, m_w, t_w) - P(E, m, t)] \quad (10)$$

in which the ‘propagator’ $P(E, m, t|E_w, m_w, t_w)$ is the probability that a particle with magnetization m_w and energy E_w at time t_w subsequently has m and E at time t . The key simplification in the calculation is that this can be related back to the known distribution $P(E, m, t)$:

$$P(E, m, t|E_w, m_w, t_w) = \delta(m - m_w)\delta(E - E_w)e^{-(t-t_w)/\tau(E_w)} + \int_{t_w}^t dt' \tau^{-1}(E_w)e^{-(t'-t_w)/\tau(E_w)} P(E, t - t')\sigma(m|E). \quad (11)$$

The first term corresponds to the particle not having hopped at all since t_w (first term) or having first hopped at t' (second term) into another trap; after a hop the particle evolves as if ‘reset’ to time zero since it selects its new trap from the prior distribution $\sigma(m|E)\rho(E)$, which describes the initial state of the system. We also have $P(E, m, t) = \sigma(m|E)P(E, t)$ since at zero field the unperturbed dynamics is recovered. Substituting these relations into (10) and integrating over m and m_w , one obtains an exact integral expression for C . This is expressible as the sum of two components: the first depends only on the mean $\bar{m}(E)$ of the fixed energy distribution $\sigma(m|E)$ and the second only on its variance, $\Delta^2(E)$. This of course makes sense, since the correlation function only measures statistics of m up to second order.

To find the corresponding response function, one can use the relation [21]

$$T \frac{\partial}{\partial t_w} \chi(t, t_w) = \frac{\partial}{\partial t} C(t, t_w) + \frac{\partial}{\partial t} \langle m(t) \rangle \langle m(t_w) \rangle \quad (12)$$

in which $\langle m(t) \rangle = \langle \bar{m}(E) \rangle_{P(E,t)}$ is the global mean of m . Equation (12) is a slight generalization of the results of [22, 23]; it is exact for any Markov process in which the effect of the field on the transition rate between any two states depends only on the initial state and not the final one. Substituting the expression for C into (12), and integrating over t_w with the boundary condition $\chi(t_w, t_w) = 0$, one finds a closed expression for χ . For convenience, we rescale the field $h \rightarrow Th$ in the following, thus absorbing a factor $1/T$ into the definition of the response function. In this way, the slope of the FD plot of χ versus C , or of their normalized analogues, becomes $-X = -T/T_{\text{eff}}$ ($= -1$ in equilibrium).

Using the exact results described above, C and χ have been calculated for a number of different distributions $\sigma(m|E)$, each specified by given functional forms of $\bar{m}(E)$ and $\Delta^2(E)$ [21]. Each form effectively corresponds to a distinct physical identity of the observable m . For example $\sigma(m|E) = \delta(m - E)$ implies $m = E$, in which case $h = -\delta T/T$. For simplicity, we confined ourselves to distributions either of zero mean (but non-zero variance) or of zero variance (but non-zero mean). Even for these simpler observables m , the equal-time correlator $C(t, t)$ can depend strongly on t ; this is in contrast to the spin models often considered in mean field studies, where $C(t, t)$ is automatically normalized. The following plots are therefore of the normalized correlation and response functions, \tilde{C} and $\tilde{\chi}$; as explained above, these are obtained by dividing the raw quantities by the equal-time correlator $C(t, t)$ at the *later* time.

For the first class of observables (with zero mean $\bar{m}(E)$), we considered a variance $\Delta^2(E) = \exp(En/T)$ for various values of the exponent n , generalizing the results of [22] for $n = 0$. The equal-time correlator is then $C(t, t) = \int dE P(E, t) \exp(nE/T)$. For large t , its scaling behaviour can be deduced from that of $P(E, t)$, and depends on the value of n : for $n < T - 1$, $C(t, t)$ is sensitive only to shallow traps (the population of which depletes in time as t^{T-1} due to ageing, giving $C(t, t) \sim t^{T-1}$) and one correspondingly expects the two-time correlator to decay on timescales $t - t_w = O(1)$, probing only quasi-equilibrium behaviour. In contrast, for $T - 1 < n < T$ one finds that $C(t, t)$ is dominated by the contribution from traps with depths E such that $\tau(E) = O(t)$; this results in the scaling $C(t, t) \sim t^n$. For such n , the two-time correlator will decay on ageing timescales $t - t_w = O(t_w)$, and we expect strong violation of equilibrium FDT. The numerical results confirm the above predictions. For values of $n < T - 1$ (not shown) the normalized FD plot approaches a straight line of equilibrium slope -1 at long times $t \rightarrow \infty$. In the regime $T - 1 < n < T$ (figure 1), equilibrium FDT is strongly violated, as expected, but a limiting *non-equilibrium* FD plot is nevertheless approached at long times. This can be proved analytically by showing that \tilde{C} and $\tilde{\chi}$ share the same scaling variable $(t - t_w)/t_w$ in this limit. The slope of each plot varies continuously with \tilde{C} . In contrast to mean field, this is not due to an infinite hierarchy of time sectors; the variation is in fact continuous across the single time sector $t - t_w = O(t_w)$. More seriously, different observables give different plots. One has to be slightly careful here: observable-independence requires that $X(t, t_w)$, as a function of the long *times* t and t_w , be independent of the observable considered. The limiting FD plots, however, give X as a function of \tilde{C} rather than of t and t_w . One thus has to convert the results for X derived from different observables back into the time domain before comparing them. In our case this means comparing the $X(\tilde{C})$ values corresponding to a fixed value $(t - t_w)/t_w$; such a comparison reveals that the values of X do indeed differ among the observables considered.

In [21], we also considered observables defined by a fixed energy distribution $\sigma(m|E)$ with zero variance and mean $\bar{m}(E) = \exp(En/2T)$; in this case m is a deterministic functions of E . Here too, we found that for $n < T - 1$ the limiting FD plot is of equilibrium form, while for $T - 1 < n < T$ (figure 2) a non-equilibrium FD plot is approached as $t \rightarrow \infty$, with a shape dependent (here very obviously) on the observable m . Note that the response function can now change sign from positive to negative for increasing time separation $t - t_w$. This is not untypical for activated dynamics, and can be understood as follows: suppose for simplicity that $n > 0$. Then $\bar{m}(E)$ increases with E and so in equilibrium the application of a positive field conjugate to m would increase E and thus m on average, giving the conventional *positive* response which we observe for t close to t_w . On the other hand, since the application of the field effectively increases the depth of all traps it also slows down the out-of-equilibrium relaxation of E and m to larger values, thus giving a *negative* response for large $t - t_w$.

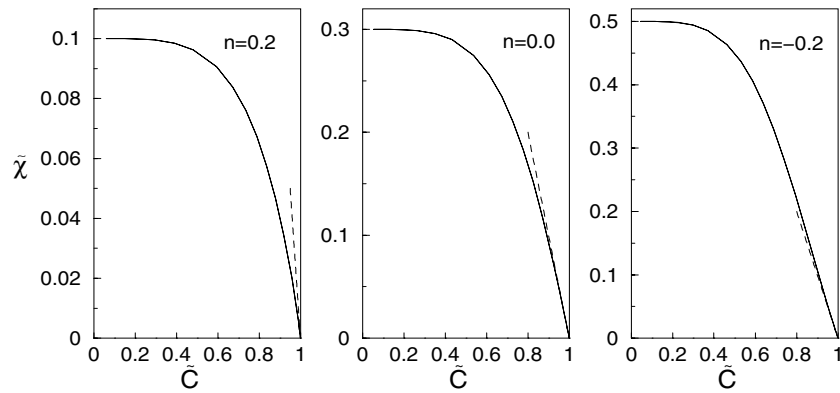


Figure 1. FD plots of $\tilde{\chi}$ versus \tilde{C} for a distribution $\sigma(m|E)$ of variance $\exp(nE/T)$ (but zero mean) for $n = 0.2, 0.0, -0.2$; $T = 0.3$. For each n data are shown for times $t = 10^6, 10^7$; these are indistinguishable, confirming that the limiting FD plot has been attained. Dashed curve: the predicted asymptote $\tilde{\chi} = 1 - \tilde{C}$ for $t \rightarrow \infty$ and $\tilde{C} \rightarrow 1$ (from [21]).

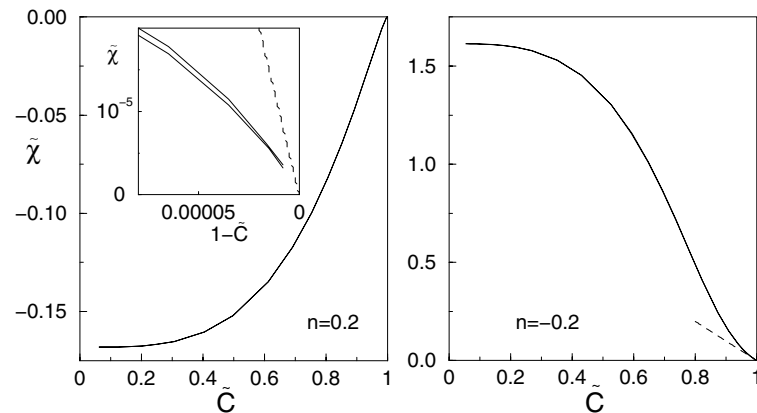


Figure 2. FD plots of $\tilde{\chi}$ versus \tilde{C} for a distribution with mean $\exp(nE/2T)$ (but zero variance), for $n = 0.2, -0.2$; $T = 0.3$. Curves are shown for times $t = 10^6, 10^7$, but are indistinguishable except for the zoom-inset on the left-hand side (upper curve: $t = 10^7$). Dashed curve: the predicted asymptote $\tilde{\chi} = 1 - \tilde{C}$ for $t \rightarrow \infty$, $\tilde{C} \rightarrow 1$ (from [21]).

Observables with a power law dependence of the mean, $\bar{m}(E) = E^p$, were also considered, with zero variance $\Delta^2(E) = 0$ as before so that $m = \bar{m}(E)$ is a deterministic function of E . Then $p = 1$ corresponds to energy–temperature FD, since the observable is energy ($m = E$) and the conjugate field is, apart from trivial scale factors, the temperature. Interestingly, in this case no limiting plot exists. This is because the amplitude of the correlator remains finite as $t \rightarrow \infty$, while the response function, for any fixed value of \tilde{C} , diverges as $\ln t$.

A final observation to be made from figures 1 and 2 is that, whenever a limiting FD plot exists for the observables considered here, its slope in the limit of well separated times ($t \gg t_w$, corresponding to $\tilde{C}(t, t_w) \rightarrow 0$) is always $X_\infty = 0$.

3. Model system 2: Glauber–Ising chain at zero temperature

As the second model system, we consider a chain of N spins s_i with the Ising Hamiltonian $H = -J \sum_i s_i s_{i+1}$. The time evolution is assumed to be given by Glauber dynamics; this means that at each time step a spin i is chosen randomly and its state assigned to $s_i = \pm 1$ with probability proportional to the Boltzmann factor $\exp(-H/T)$ for the new configuration. Time is scaled so that each spin is updated once, on average, per unit time.

When this system is quenched to a low temperature from a random initial state, corresponding to equilibrium at $T = \infty$, the dynamics will progressively line up neighbouring spins with each other and alternating domains of up and down spins will grow (coarsen) until they reach the equilibrium domain length $\xi_{\text{eq}} \sim \exp(2J/T)$ at a time $\tau_{\text{eq}} \sim \exp(4J/T)$. In the limit of $T \rightarrow 0$, these scales grow to infinity and the systems remains out of equilibrium at any finite time; this will be the limit of interest to us. Since the Ising spin chain has a phase transition to an ordered ferromagnetic state at $T = 0$, one can regard the out-of-equilibrium dynamics for $T \rightarrow 0$ as critical coarsening [6]. Physically, however, this is somewhat different from coarsening at a finite-temperature critical point, since in the Ising chain the growing domains are not critical but have the structure of either of the ordered phases (spins all up or all down).

The FD relations for the Glauber–Ising chain have been studied previously for the case of the spin–spin autocorrelation (see [24]; a brief summary of the results can be found in [6]). It is a simple matter to extend the calculation to a somewhat more general class of observables, defined as

$$m = \sum_i \epsilon_i s_i \quad (13)$$

where the ϵ_i are quenched random variables with zero mean and translation-invariant covariances $[\epsilon_i \epsilon_j] = q_{j-i}$; here $[\dots]$ denotes the average over the quenched disorder. The corresponding perturbation in the Hamiltonian is $-hm$, as usual, so that the local field acting on each site is $h\epsilon_i$. With different choices of the correlation function one can then interpolate between the two extremes of a uniform field ($q_k = 1$, in which case m is the conventional magnetization) and a locally random field ($q_k = \delta_{k0}$, the case treated in [24]).

Because $\langle s_i(t) \rangle = 0$, m as defined by (13) also has an average of zero at all times. Using the known results for the two-time spin–spin correlation function [24], $C_{ij}(t, t_w) = \langle s_i(t) s_j(t_w) \rangle$, which can be written as $C_{ij}(t, t_w) = c_{j-i}(t, t_w)$ due to translation invariance, one then has for the autocorrelation function of m (scaled by N to get a quantity of order unity)

$$C(t, t_w) = \frac{1}{N} \sum_{ij} \epsilon_i \epsilon_j c_{j-i}(t, t_w) = \sum_k \left(\frac{1}{N} \sum_l \epsilon_l \epsilon_{l+k} \right) c_k(t, t_w) = \sum_k q_k c_k(t, t_w) \quad (14)$$

where in the last step we have used that in the limit of an infinitely large system the spatial average of $\epsilon_l \epsilon_{l+k}$ becomes identical to the quenched average $[\epsilon_l \epsilon_{l+k}] = q_k$. The scaled response function of m to its conjugate field is obtained similarly as $R(t, t_w) = \sum_k q_k r_k(t, t_w)$, where the translationally invariant response function $r_{j-i}(t, t_w)$ gives the response of a spin at site i and time t to a local field applied at site j at time t_w . Using the exact solutions for $c_k(t, t_w)$ and $r_k(t, t_w)$, one can thus evaluate the correlation and response functions of m , at least in principle.

Before giving the results, let us briefly discuss what behaviour one would expect. We can define a correlation length of the random fields $h_i = h\epsilon_i$ as $\xi_h = \sum_{k=-\infty}^{\infty} q_k$. This length needs to be compared with the growing spin–spin correlation length $\xi(t)$ of the coarsening system, which is of the same order as the typical domain length. For early times the field is essentially uniform on the lengthscale of the spin correlations ($\xi(t) \ll \xi_h$) and so we expect to

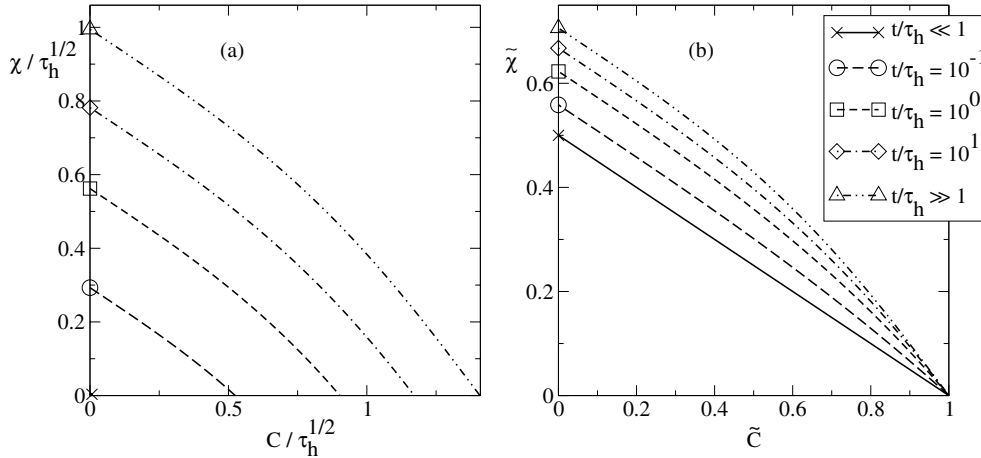


Figure 3. FD plots for Glauber–Ising chain, for a linear observable (13) with fields ϵ_i that have a Lorentzian covariance function $q_k = q(k/\xi_h)$ with $q(x) = 1/(1 + x^2)$. (a) Raw, unnormalized, response and correlation functions. The constant factor $1/\tau_h^{1/2}$ only serves to remove the trivial scaling of the amplitude of these functions with the field correlation length $\xi_h = \tau_h^{1/2}$. Curves are for increasing ratios of t/τ_h as shown in the legend. (b) FD plots of the normalized correlation and response, \tilde{C} and $\tilde{\chi}$. The normalization shows that in the limit $t/\tau_h \ll 1$ one obtains a straight line of negative slope $X = 1/2$, exactly as in the long time limit for *uniform* fields; see figure 4.

see behaviour corresponding to the uniform field limit. For late times, the field correlations are much more short-ranged than those of the spins ($\xi(t) \gg \xi_h$); across each typical spin domain, the ϵ_i change signs many times and we expect qualitatively the same effects as for completely uncorrelated fields. The crossover between these two regimes takes place when $\xi(t) \approx \xi_h$. Since the growth of $\xi(t)$ is driven by the random-walk motion of the domain walls, it scales as $\xi(t) \sim t^{1/2}$, and thus the crossover time is of order $\tau_h = \xi_h^2$.

To simplify the theoretical analysis, it is convenient to look at the limit where all times (t , t_w and τ_h) are large compared to unity. This then also implies that the field correlation length ξ_h is large, so that we can write $q_k = q(k/\xi_h)$, where $q(x)$ is a smooth function of the scaled distance $x = k/\xi_h$. We leave all details of the calculation to a forthcoming publication and display only the results.

In figure 3(a) we show the unnormalized (except for a constant scale factor) FD plot for the case of a Lorentzian field correlation function $q(x) = 1/(1 + x^2)$. As before, the earlier time t_w is used as the curve parameter and t is held constant for each curve. As t increases, the amplitude of both correlator and response initially grows, but eventually saturates for $t \gg \tau_h$. For such long times, the FD plot is identical to that for uncorrelated fields [24] as predicted, with negative slope $X = 1$ for t close to t_w , corresponding to quasi-equilibrium, and $X = X_\infty = 1/2$ in the limit of well separated times $t \gg t_w$. For shorter times $t \ll \tau_h$, on the other hand, the FD plot is a straight line of slope $X = 1/2$ throughout; this is more easily seen once correlation and response are normalized by $C(t, t)$ as in figure 3(b). As we will see very shortly, and consistent with our expectations, the FD plot in this regime, i.e. before the crossover at $t \approx \tau_h$, is identical to that obtained for uniform fields.

Figure 4 shows the limiting ($t \rightarrow \infty$) FD plots for a range of field correlation functions $q(x)$. At one extreme, we have the case of uniform fields ($q(x) = 1$), giving a straight line of negative slope $X = 1/2$. At the other extreme, all field correlation functions $q(x)$ for which a finite correlation length can be defined have the same limit plot as for uncorrelated fields.

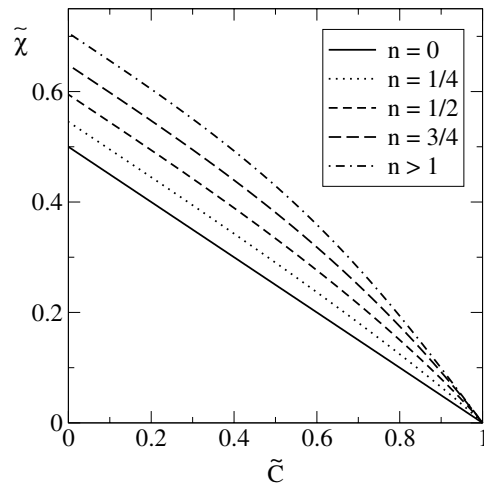


Figure 4. Limiting FD plots for the Glauber–Ising chain, for different asymptotic behaviours $q(x) \sim x^{-n}$ of the field correlation function; the value of n is shown in the legend. For $n \rightarrow 0$ one has the case of uniform fields, which gives a straight line of negative slope $X = 1/2$. The opposite extreme $n \geq 1$ corresponds to correlation functions with a finite correlation length; these all give the same limit plot, identical to that for entirely uncorrelated fields. Values of n between 0 and 1 give nontrivial intermediate FD plots. Note that the negative slope X of all plots is, in the limit of well separated times, $X_\infty = 1/2$.

Because we defined the correlation length above as $\xi_h = \sum_{k=-\infty}^{\infty} q_k$, the scaled correlation function must obey $\int dx q(x) < \infty$ for a finite correlation length to exist; this requires that $q(x)$ decay faster than x^{-1} for large x . Correlation functions $q(x)$ which decay asymptotically as $q(x) \sim x^{-n}$ with $0 < n < 1$ give intermediate FD plots, whose shape is determined only by the asymptotic decay exponent n . Results for several values of n between 0 and 1 are shown in figure 4; they demonstrate clearly that even among the relatively restricted class of observables defined by (13), nontrivially different limiting FD plots exist which give different results for the FD ratio X . Intriguingly, however, the limit of X for strongly separated times $t \gg t_w$, is $X_\infty = 1/2$ for *all* observables considered here.

4. Discussion

Let us summarize our findings. For the trap model, on the basis of exact relations for correlation and response functions, we have studied FD relations in the glass phase for a broad class of observables m . For observables which indeed probe the ageing regime, equilibrium FDT is violated; in most cases, a limiting non-equilibrium FD plot is approached at long times. In contrast to mean field, this plot depends strongly on the observable. It furthermore has a slope which varies continuously across the single time sector $t - t_w = O(t_w)$. This shows that in this simple, paradigmatic model of glassy dynamics, the mean field concept of an FD-derived effective temperature T_{eff} cannot be applied. One may dismiss the trap model as too abstract for this to be of general relevance; but by placing traps onto a d -dimensional lattice and allowing hops only to neighbouring traps, a more ‘physical’ model (of diffusion in the presence of disorder) can be obtained. Recent work [20] shows the scaling of correlation functions to be unaffected by this modification; since (12) would also continue to hold, the results for the trap model should be qualitatively unchanged.

Our results for the Glauber–Ising chain were qualitatively similar. There, we restricted ourselves to observables that are linear in the spin variables; again, exact results for the correlation and response functions of such observables can be obtained. Limiting FD plots always exist, but depend nontrivially on the observable. Except for the case where the observable is the magnetization (and the corresponding perturbation therefore a uniform field), the slope of the limit plots varies continuously; as in the trap model, this variation takes place within a single time sector $t - t_w = O(t_w)$.

The results above demonstrate that the idea of an effective temperature T_{eff} derived from FD relations does not apply straightforwardly to generic non-mean field models. Could the concept nevertheless be rescued? One difficulty in the two models considered was the non-uniqueness of the limiting FD plots. One could argue that in order to probe an inherent T_{eff} characterizing the non-equilibrium dynamics, the statistical properties of the observable must not change significantly across the phase space regions visited during ageing. (In coarsening models, similar arguments have been used to exclude observables correlated with the order parameter [12].) Applying this idea to the trap model, where the typical trap depth E increases without bound for $t \rightarrow \infty$, a ‘neutral’ observable would presumably require that $\bar{m}(E)$, $\Delta^2(E) \rightarrow \text{const.}$ as $E \rightarrow \infty$; with this restriction we indeed get a unique limiting FD plot. In the Glauber–Ising chain, the energy $E = \langle H \rangle$ decreases towards the ground state energy E_0 during coarsening. A neutral observable might then be one whose properties within a *microcanonical* ensemble at given E do not change significantly as $E \rightarrow E_0$. It is easy to see that, for our observables (13), this criterion again produces a limiting FD plot: It only allows field correlation functions with a finite correlation length—which all give the same limit plot, namely that for uncorrelated fields—while other observables have a variance which diverges as $E \rightarrow E_0$. The selection of neutral observables may in fact obviate the normalization problem for FD plots discussed in detail in this paper: if an observable has a variance $C(t, t)$ which either converges to zero or diverges as t increases, then this in itself implies that its statistical properties change strongly while the system ages; conversely, for neutral observables $C(t, t)$ should approach a finite limit for $t \rightarrow \infty$.

Even if one can, by a judicious choice of a ‘neutral’ observable, produce a unique limiting FD plot and thus a unique FD ratio $X(t, t_w)$, one is still faced with the problem that X may—as in our cases—vary continuously across a single time-sector. This almost certainly makes X inappropriate for the definition of a meaningful effective temperature $T_{\text{eff}} = T/X$, since two thermometers probing timescales which differ only by factors of order unity should be required to measure the same temperature. There is, however, the intriguing possibility that the limit of X obtained for long times and large time separations, $X_\infty = \lim_{t_w \rightarrow \infty} \lim_{t \rightarrow \infty} X(t, t_w)$ may still correspond to a meaningful T_{eff} . In fact, in the two models considered here, X_∞ was the same for all observables considered, as long as limiting FD plots actually existed. These ideas should be explored in future work; we are currently in the process of calculating FD plots for *second order* observables such as $m = \sum_i \epsilon_i s_i s_{i+1}$ in the Glauber–Ising chain. If the same X_∞ results, this would strongly support the hypothesis that X_∞ is indeed observable independent.

Finally, it is of course likely that there are different classes of non-mean field systems as far as the concept of an effective temperature is concerned. One could conjecture that FD plots would provide a diagnostic tool here: the appearance of rounded FD plots like those shown above may signal that a system does not have a meaningful T_{eff} , while limiting FD plots consisting of two straight line segments—as found in simulations of some non-mean field models [9, 10, 12]—may indicate that a well-defined effective temperature does indeed exist. One of the main tasks ahead must be to develop physical criteria that allow us to predict to which of these two classes a given system belongs. It is probable that a strong separation of

the dynamics into fast and slow timescales will play a role (see e.g. [25,26]), but this may not be sufficient. The trap model is again instructive here: In the glass phase the fast processes (on timescales of order unity) do not contribute to the dynamics, and all relevant relaxation processes happen on slow timescales of the same order ($\sim t_w$). A naive timescale separation argument would then suggest that the FD plot should consist of a single straight line, with a non-equilibrium slope $X \neq 1$, while the exact results presented above show that the actual situation is rather more complicated.

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References

- [1] Cugliandolo L F, Kurchan J and Peliti L 1997 Energy flow, partial equilibration, and effective temperatures in systems with slow dynamics *Phys. Rev. E* **55** 3898–914
- [2] Bouchaud J P, Cugliandolo L F, Kurchan J and Mézard M 1998 Out of equilibrium dynamics in spin-glasses and other glassy systems *Spin Glasses and Random Fields* ed A P Young (Singapore: World Scientific)
- [3] Reichl L E 1980 *A Modern Course in Statistical Physics* (Austin, TX: University of Texas Press)
- [4] Cugliandolo L F and Kurchan J 1993 Analytical solution of the off-equilibrium dynamics of a long-range spin-glass model *Phys. Rev. Lett.* **71** 173–6
- [5] Cugliandolo L F and Kurchan J 1994 On the out-of-equilibrium relaxation of the Sherrington–Kirkpatrick model *J. Phys. A: Math. Gen.* **27** 5749–72
- [6] Godreche C and Luck J M 2002 Nonequilibrium critical dynamics of ferromagnetic spin systems: *J. Phys.: Condens. Matter* this issue (cond-mat/0109212)
- [7] Cugliandolo L F and Dean D S 1995 Full dynamical solution for a spherical spin-glass model *J. Phys. A: Math. Gen.* **28** 4213–34
- [8] Nieuwenhuizen T M 2000 Thermodynamic picture of the glassy state gained from exactly solvable models *Phys. Rev. E* **61** 267–92
- [9] Kob W and Barrat J L 2000 Fluctuations, response and aging dynamics in a simple glass-forming liquid out of equilibrium *Eur. Phys. J. B* **13** 319–33
- [10] Arenzon J J, Ricci-Tersenghi F and Stariolo D A 2000 Dynamics of the frustrated Ising lattice gas *Phys. Rev. E* **62** 5978–85
- [11] Bonilla L L, Padilla F G and Ritort F 1998 Aging in the linear harmonic oscillator *Physica A* **250** 315–26
- [12] Barrat A 1998 Monte Carlo simulations of the violation of the fluctuation-dissipation theorem in domain growth processes *Phys. Rev. E* **57** 3629–32
- [13] Marinari E, Parisi G, Ricci-Tersenghi F and Ruiz-Lorenzo J J 1998 Violation of the fluctuation-dissipation theorem in finite-dimensional spin glasses *J. Phys. A: Math. Gen.* **31** 2611–20
- [14] Godreche C and Luck J M 2002 Nonequilibrium dynamics of urn models *J. Phys.: Condens. Matter* this issue Also available as Godreche C and Luck J M 2001 *Preprint* cond-mat/0109213
- [15] Fielding S M 2000 *PhD Thesis* University of Edinburgh
- [16] Crisanti A, Ritort F, Rocco A and Sellitto M 2002 Is the Stillinger and Weber decomposition relevant for coarsening models? *J. Phys.: Condens. Matter* this issue
- [17] Buhot A and Garrahan J P 2001 Fluctuation-dissipation relations in the activated regime of simple strong-glass models *Preprint* cond-mat/0111035
- [18] Bouchaud J P 1992 Weak ergodicity breaking and aging in disordered-systems *J. Phys. (France) I* **2** 1705–13
- [19] Monthus C and Bouchaud J P 1996 Models of traps and glass phenomenology *J. Phys. A: Math. Gen.* **29** 3847–69
- [20] Rinn B, Maass P and Bouchaud J P 2000 Multiple scaling regimes in simple aging models *Phys. Rev. Lett.* **84** 5403–6
- [21] Fielding S M and Sollich P 2001 Observable-dependence of fluctuation-dissipation relations and effective temperatures *Preprint* cond-mat/0107627
- [22] Bouchaud J P and Dean D S 1995 Aging on Parisis tree *J. Phys. (France) I* **5** 265–86

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- [23] Sasaki M and Nemoto K 1999 Aging phenomena of magnetization in a hierarchical diffusion model *J. Phys. Soc. Japan* **68** 1148–61
 - [24] Godreche C and Luck J M 2000 Response of non-equilibrium systems at criticality: exact results for the Glauber–Ising chain *J. Phys. A: Math. Gen.* **33** 1151–70
 - [25] Leuzzi L and Nieuwenhuizen T M 2002 Exactly solvable model glass with a facilitated dynamics *J. Phys.: Condens. Matter* this issue (cond-mat/0110030)
 - [26] Garriga A 2002 Zeroth law in structural glasses: An example *J. Phys.: Condens. Matter* this issue