Fluctuation-dissipation relations in ageing and driven non-mean field glass models

Suzanne M. Fielding* and Peter Sollich[†]

*Polymer IRC and Department of Physics & Astronomy, University of Leeds, Leeds LS2 9JT, United Kingdom †Department of Mathematics, King's College London, Strand, London, WC2R 2LS, United Kingdom

Abstract. We study the fluctuation-dissipation theorem (FDT) in the glass phase of (1) Bouchaud's trap model and (2) its driven counterpart, the "soft glassy rheology" model. We incorporate into the models an arbitrary observable m and obtain its correlation and response functions in closed form. A limiting non-equilibrium FDT plot (of correlator vs. response) is approached at long times for most choices of m. In contrast to standard mean field models, however, the plot, in general, (i) depends non trivially on the observable, (ii) has a continuously varying slope (even though there is a single scaling of relaxation times with age) and (iii) differs in the ageing and driven regimes. Despite this, all plots share the same limiting slope for well separated times, suggesting that a meaningful non-equilibrium effective temperature could apply in this limit. Beyond the trap model, we discuss more generally the status of FD temperatures in such non-mean field systems.

INTRODUCTION

Glasses relax very slowly at low temperatures. They thus stay far from equilibrium long after preparation, and show ageing [1]: the time scale for response to perturbations (or decay of correlations) increases with the time t_w since the temperature quench, eventually exceeding any experimental time scale. Time translational invariance is lost. Because of this sluggishness, glasses are highly susceptible to external driving, which typically stabilises a non-equilibrium steady (TTI) state of apparent age $O(1/\dot{\gamma})$, for drive-rate $\dot{\gamma}$ [2].

Let $C(t,t_{\rm w})=\langle m(t)m(t_{\rm w})\rangle-\langle m(t)\rangle\langle m(t_{\rm w})\rangle$ be the autocorrelation function for an observable $m,\ R(t,t_{\rm w})=\delta\langle m(t)\rangle/\delta h(t_{\rm w})|_{h=0}$ the linear response of m(t) to a small impulse in its conjugate field h at time $t_{\rm w}$, and $\chi(t,t_{\rm w})=\int_{t_{\rm w}}^t dt'\,R(t,t')$ the response to a field step $h(t)=h\Theta(t-t_{\rm w})$. In equilibrium, $C(t,t_{\rm w})=C(t-t_{\rm w})$ by TTI (similarly for R and χ), and the FDT reads $-\frac{\partial}{\partial t_{\rm w}}\chi(t-t_{\rm w})=R(t,t_{\rm w})=\frac{1}{T}\frac{\partial}{\partial t_{\rm w}}C(t-t_{\rm w})$, with T the thermodynamic temperature. (We set $k_{\rm B}=1$.) A parametric FDT plot of χ vs. C is thus a straight line of slope -1/T.

Out of equilibrium, FDT violation is measured by a fluctuation-dissipation ratio (FDR), X, defined by [3]

$$-\frac{\partial}{\partial t_{w}}\chi(t,t_{w}) = R(t,t_{w}) = \frac{X(t,t_{w})}{T}\frac{\partial}{\partial t_{w}}C(t,t_{w}). \quad (1)$$

In ageing systems, violation $(X \neq 1)$ can persist even at long times $t_w \to \infty$, indicating far from equilibrium behaviour even when one-time quantities, e.g. entropy

have settled to stationary values. Similarly, driven glasses can violate FDT even for weak driving, $\dot{\gamma} \rightarrow 0$.

Remarkably, however, the FDR for several mean field models [3] assumes a special form at long times (ageing case). Taking $t_w \to \infty$ at constant $C = C(t, t_w), X(t, t_w) \to X(C)$ becomes a (nontrivial) function of the single argument C. If the equal-time correlator C(t,t) also approaches a constant C_0 for $t \to \infty$, it follows that

$$\chi(t,t_{\rm w}) = \int_{C(t,t_{\rm w})}^{C_0} dCX(C)/T. \tag{2}$$

A limiting non-equilibrium FDT plot is then obtained by plotting χ vs. C for increasingly large times; from its slope -X(C)/T, an effective temperature [4] can be defined as $T_{\rm eff}(C) = T/X(C)$. An equivalent FD relation has been suggested to hold in slowly driven glasses [4] with $T_{\rm eff}(C,\dot{\gamma}\to 0) = T_{\rm eff}(C,t_{\rm w}\to \infty)$.

In the most general ageing scenario, a system evolves on several characteristic time scales, each with its own functional dependence on t_w . If these become infinitely separated as $t_w \to \infty$, they form distinct 'time sectors'. In mean field, $T_{\rm eff}(C)$ is *constant* in each sector [3]. It has thus been interpreted as a time scale dependent non equilibrium temperature, and shown to have many of the properties of a thermodynamic temperature (e.g. in controlling of heat flow) [4]. Of crucial importance to its interpretation as a temperature, it is *independent* of the observable m used to construct the FD plot.

While this picture is well established in mean field, evidence beyond mean field is limited. Limiting FD plots were found in, e.g., Refs. [5, 6]. Observable indepen-

dence is largely unestablished, but see Ref. [5] for encouraging results. Evidence for equivalent ageing and driven FD plots is limited, but has been found in models of supercooled liquids [7]. In this work, therefore, we study a simple non-mean field model for which FD plots can be calculated for arbitrary observables, allowing detailed study of whether the mean field picture applies [8].

TRAP MODEL

The (undriven) trap model [9] comprises an ensemble of uncoupled particles exploring a landscape of energy traps by thermal activation. The traps descend from a common level, with depths E chosen from a 'prior' distribution $\rho(E)$ (E>0). A particle in a trap of depth E escapes on a time scale $\tau(E)=\tau_0\exp(E/T)$ and hops into another trap, with a depth chosen randomly 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

$$\partial_t P(E,t) = -\tau^{-1}(E)P(E,t) + Y(t)\rho(E)$$
 (3)

in which the first (second) term on the RHS represents hops out of (into) traps of depth E, and $Y(t) = \left\langle \tau^{-1}(E) \right\rangle_{P(E,t)}$ is the average hop rate. For a prior distribution $\rho(E) \sim \exp\left(-E/T_g\right)$ the model shows a glass transition at a temperature T_g , because for $T \leq T_g$ the equilibrium state $P_{\rm eq}(E) \propto \tau(E)\rho(E) \propto \exp\left(E/T\right)\exp\left(-E/T_g\right)$ is unnormalizable and the average lifetime $\left\langle \tau \right\rangle_{\rho}$ is infinite. Following a quench to $T \leq T_g$, the system cannot equilibrate and instead ages. At large times $t_w \to \infty$ a scaling limit is reached with $P(\tau,t_w) = [T/\tau(E)]P(E,t_w)$ concentrated on traps of lifetime $\tau = O(t_w)$. The model thus has just one characteristic time scale, growing linearly with age. We set $T_g = 1$, $\tau_0 = 1$.

To study FDT we assign to each trap a generic observable m. The landscape 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 a fixed energy E. We consider non-equilibrium dynamics after a quench at t=0 from $T=\infty$ to T<1. The initial condition is thus $P_0(E,m)=\sigma(m|E)\rho(E)$, with subsequent evolution

$$\partial_t P(E, m, t) = -\frac{P(E, m, t)}{\tau(E, m)} + Y(t)\rho(E)\sigma(m|E) \quad (4)$$

where the activation times are modified by a small field h as $\tau(E,m) = \tau(E) \exp(mh/T)$. (Other choices of $\tau(E,m)$ that maintain detailed balance are also possible [10, 11].)

To find the autocorrelation function C for m at h = 0 we need the probability that a particle with m_w and energy E_w at time t_w subsequently has m and E at time t:

$$P(E, m, t|E_{\rm w}, m_{\rm w}, t_{\rm w}) =$$

$$\delta(m - m_{\rm w})\delta(E - E_{\rm w})e^{-(t - t')/\tau(E_{\rm w})}P(E_{\rm w}, m_{\rm w}, t_{\rm w}) + \int_{t_{\rm w}}^{t} dt' \frac{e^{-(t' - t_{\rm w})/\tau(E_{\rm w})}}{\tau(E_{\rm w})}P(E, t - t')\sigma(m|E).$$
 (5)

The first (second) term on the RHS corresponds to a particle not having hopped since t_w (first having hopped at t'). After hopping the particle evolves as if "reset" to time zero since it selects its new trap from the prior distribution, which also describes the initial state. From Eqn. 5, an exact expression for $C(t,t_w)$ can be found.

To find the response function, we proved

$$T\frac{\partial}{\partial t_{w}}\chi(t,t_{w}) = \frac{\partial}{\partial t}C(t,t_{w}) + \frac{\partial}{\partial t}\langle m(t)\rangle\langle m(t_{w})\rangle \quad (6)$$

in which $\langle m(t) \rangle = \langle \overline{m}(E) \rangle_{P(E,t)}$ is the global mean of m. This generalizes the results of [11, 12] to non-zero means. We rescale the field $h \to Th$, absorbing a factor 1/T into the response function. The slope of the FDT plot is then $-X = -T/T_{\rm eff}$ (= -1 in equilibrium).

Our expressions for C and χ each comprise two additive components, depending separately on the mean $\overline{m}(E)$ and variance $\Delta^2(E)$ of $\sigma(m|E)$. Using them, we numerically calculated C and χ for several different distributions $\sigma(m|E)$, each specified by given functional forms of $\overline{m}(E)$ and $\Delta^2(E)$. For simplicity, we considered only distributions of zero mean (but non-zero variance); or of zero variance (but non-zero mean).

As expected, the decay of C in general depends on the waiting time t_w : TTI is lost. For any observable m that is correlated with E, the equal-time correlator C(t,t) can also depend on t (either decaying or diverging). While Eqn. 2 implies that an FD plot can be produced either with t as the curve parameter (at fixed t_w), or vice versa, Eqn. 1 in general only ensures a slope of $-X(t,t_{\rm w})/T$ with $t_{\rm w}$ as the parameter. This issue is important if, as here, C(t,t) is time dependent, requiring pre-normalisation of χ and C to ensure a limiting FD plot of time independent size. 1 To preserve the connection between X and the slope, the normalisation factor must be the same for χ and C, and independent of t_w . We therefore use C(t,t), rather than $C(t_w,t_w)$, denoting the normalized quantities by $\tilde{\chi}$ and \tilde{C} . A limiting plot may then be approached at long times. If so, either t_w or t could be used as the curve parameter. We choose $t_{\rm w}$, because this ensures that FD plots constructed with the switch-on or switch-off response functions are trivially related, as discussed more fully in Ref. [13].

For zero mean observables, $\overline{m}(E) = 0$, we consider a variance $\Delta^2(E) = \exp(En/T)$. For different values of n, the correlator probes different moments of the prior

¹ This issue has not arisen in mean field studies, where variables are usually sufficiently "neutral" that $C(t,t) \to \text{const.}$

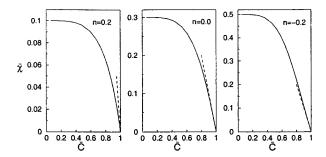


FIGURE 1. FDT plots of $\tilde{\chi}$ vs \tilde{C} for a distribution $\sigma(m|E)$ of variance $\exp(nE/T)$ (but zero mean) for n=0.2, 0.0, -0.2; T=0.3. For each n data are shown for times $t=10^6, 10^7$; these are indistinguishable, confirming that a limit FDT plot has been attained. Dashed: asymptote $\tilde{\chi}=1-\tilde{C}$ for $t\to\infty$ and $\tilde{C}\to 1$.

distribution $\rho(E)$. For n < T - 1, it is sensitive only to shallow traps and decays on time scales $t - t_w = O(1)$, probing only quasi-equilibrium behaviour and so yielding an FD plot that is a straight line of slope -1 as $t \to \infty$. In contrast ², for T - 1 < n < T the correlator is dominated by traps with $\tau(E) = O(t)$, and decays on ageing time scales $t - t_w = O(t_w)$. Equilibrium FDT is then violated. A limiting non-equilibrium FD plot is nevertheless approached at long times (Fig. 1) since \tilde{C} and $\tilde{\chi}$ then share the same scaling variable $(t-t_{\rm w})/t_{\rm w}$. The slope of each plot varies continuously with \bar{C} . In contrast to mean field, this is not due to an infinite hierarchy of time sectors: the variation occurs across the single time sector $t-t_{\rm w}=O(t_{\rm w})$. More seriously, different observables give different plots: at a fixed value of \tilde{C} the slopes -X depend on n. For variables with zero variance and mean $\overline{m}(E) = \exp(En/2T)$ we again find FDT violation for T - 1 < n < T (Fig. 2) with a limiting non-equilibrium plot that depends (now obviously) on m.

The concept of a non equilibrium FD temperature is therefore not straightforward in the trap model. Can it nonetheless be rescued? One difficulty is the non-uniqueness of the FD plots. Observable dependent FD plots have also been found in the zero-temperature Glauber-Ising chain (ZTGIC) [13, 14], for different correlation lengths of the applied field, h. One could argue that to probe an inherent $T_{\rm eff}$, the properties of the observable must not change much across the phase space regions visited during ageing. Applying this to the trap model, where the typical trap depth E increases without bound for $t \to \infty$, a "neutral" observable requires $\Delta^2(E), \overline{m}(E) \to \text{const.}$ as $E \to \infty$. With this restriction, we do indeed get a unique FD plot. The same is true for the ZTGIC, for neutral (random) fields.

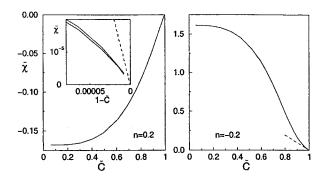


FIGURE 2. FDT plots of $\tilde{\chi}$ vs \tilde{C} for a distribution with mean $\exp(nE/2T)$ (but zero variance), for n=0.2,-0.2; T=0.3. Curves are shown for times $t=10^6, 10^7$, but are indistinguishable except for the zoom-inset on the left (upper: $t=10^7$). Dashed: predicted asymptote $\tilde{\chi}=1-\tilde{C}$ for $t\to\infty$, $\tilde{C}\to1$.

Even with a judicious choice of neutral observable, however, X still varies continuously across the single time sector in the trap model. Two thermometers probing time scales that differ only by a factor of order unity would thus measure different (and so meaningless) effective temperatures. Similarly rounded plots are seen in the ZTGIC [13, 14]. There is, however, the possibility that the limit of X obtained at large time separation $X_{\infty} = \lim_{t_w \to \infty} \lim_{t \to \infty} X(t, t_w)$ may still give a meaningful T_{eff} . Indeed, in the trap model $X_{\infty} = 0$ is the same for all variables considered; the ZTGIC also has $X_{\infty} = 0$ for domain wall variables (but $X_{\infty} = 1/2$ for spin variables) [14].

We now turn to the driven model, as first defined to study "soft glassy rheology". Each particle is assigned a local elastic "strain" l and "stress" kl. (We set k=1.) After any hop, l resets to zero. Between hops, $\dot{l}=\dot{\gamma}$, the external strain rate. A particle in a trap of depth E strained by l sees a reduced energy barrier $E-\frac{1}{2}l^2$, so

$$[\partial_t + \dot{\gamma}\partial_l]P(E,l,t) = -\tau^{-1}(E)e^{l^2/2T}P + Y(t)\rho(E)\delta(l).$$
(7)

In the glass phase, steady driving ($\dot{\gamma} = \text{const.}$) interrupts ageing and restores a steady state. In the limit $\dot{\gamma} \to 0$, the steady state distribution $P_{\infty}(E) = \int dl \, P_{\infty}(E, l)$ approaches a scaling state with all relaxation times $O(1/\dot{\gamma})$.

In our study of driven FDT, we focus on neutral observables, $\overline{m}(E) = 0$ and $\Delta^2(E) = \text{const.}$ For these, the autocorrelation function

$$C(t,\dot{\gamma}) = \int_{\dot{\gamma}t}^{\infty} dl \int_{0}^{\infty} dE \, P_{\infty}(E,l) \tag{8}$$

where $P_{\infty}(E,l) = \lim_{t\to\infty} P(E,l,t)$, which can be calculated exactly. (Because TTI is restored, C and χ do not depend explicitly upon the waiting time t_w , so we have set $t_w = 0$.) Eqn. 8 can be understood by noting that

² The regime n > T is meaningless: It gives $C(t,t) = \infty \forall t$.

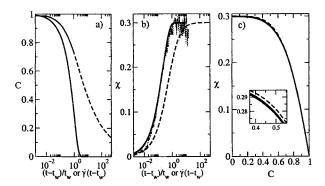


FIGURE 3. a) Correlator and b) response vs. scaled time for the neutral observable $\Delta^2(E) = 1$: driven (solid lines); ageing (dashed). Waiting times (or inverse driving rates) 10^3 , 10^4 , 10^5 , 10^6 are shown (but indistinguishable). c) FD plots: driven (solid); ageing (dashed). For the driven case, driving rate decreases downwards at fixed C. Temperature T = 0.3.

only particles that have not hopped since time t = 0 (i.e. those with strains $l \ge \dot{\gamma}t$) contribute to the correlator. The switch-on response function can be shown to be

$$\chi(t,\dot{\gamma}) = \int_0^\infty dE \int_0^\infty dl \, \frac{\left[P_\infty(E,l) - P_\infty(E,l+\dot{\gamma}t)\right]}{\dot{\gamma}\tau(E)} I(l,T)$$
(9)

in which $I(l,T) = \int_0^l ds \exp\left(\frac{s^2}{2T}\right)$.

Using these expressions, we evaluated $C(t,\dot{\gamma})$ and $\chi(t,\dot{\gamma})$ numerically. The results are shown in Fig. 3a,b (with simulation results as a check). In the limit $\dot{\gamma} \to 0$, $t \to 0$ at fixed $\dot{\gamma}t$, $C(t,\dot{\gamma})$ and $\chi(t,\dot{\gamma})$ depend on t and $\dot{\gamma}$ only through the scaling variable $\dot{\gamma}t$, as expected.

Although the scaling functions $C(\dot{\gamma}t)$ and $\chi(\dot{\gamma}t)$ both differ strongly from their ageing counterparts $C(\frac{t-t_w}{t_w})$, $\chi(\frac{t-t_{\rm w}}{t_{\rm w}})$ (compare solid and dashed lines in Fig. 3) the ageing and driven FD relations are remarkably similar (Fig. 3c). Both start with a quasi-equilibrium slope $-X(C=1) \equiv \chi'(C=1) = -1$ and finish with slope $\chi'(C=0) = 0$ at intercept $\chi(C=0) = T$. Between these limits, these is little discernible difference between the ageing and driven plots. This non-trivial result is consistent with the predictions of Cugliandolo et al., that the relationship between correlation and response should be the same in ageing and weakly driven glasses. Despite this, the inset of Fig. 3c, does reveal a small discrepancy. To investigate this further, we examined the behaviour of $X \equiv -\chi'(C)$ in the limit $C \to 0$, finding $X \sim C^{1/T}$ in the ageing case, but $C \sim X^T [\log(1/X)]^{(T-1)/2}$ in the driven case. Therefore, the driven and ageing FD plots are only equivalent to within minor logarithmic corrections. Finally, this similarity of ageing and driven FD relations is not robust with respect to non-neutrality of observable, or to driving mechanisms that respect detailed balance [8].

CONCLUSIONS

We have shown that the mean field concept of a non equilibrium FD temperature is not straightforward in the trap model. FD plots, in general, (i) depend on observable, (ii) have a slope varying continuously across a single time sector, (iii) differ in the ageing and driven cases. Nonetheless, *neutral* observables do all share a unique (observable independent) FD plot, which is the same (to within logs) for ageing and driven systems. Although the slope of the plot varies continuously, there remains the intriguing possibility that the limit of X obtained for large time separations $X_{\infty} = \lim_{t_{\rm w} \to \infty} \lim_{t \to \infty} X(t, t_{\rm w})$ may still corresponds to a meaningful $T_{\rm eff}$. Indeed, for the trap model, X_{∞} is the same (zero) for all variables considered; this value even holds in trap models with slow dynamics arising from entropy rather than energy barriers [15].

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