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Out-of-equilibrium dynamics in a Gaussian trap model

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Abstract

The violations of the fluctuation–dissipation theorem are analysed for a trap model with a Gaussian density of states. In this model, the system reaches thermal equilibrium for long times after a quench to any finite temperature and therefore all ageing effect are of a transient nature. For not too long times after the quench it is found that the so-called fluctuation–dissipation ratio tends to a non-trivial limit, thus indicating the possibility for the definition of a timescale-dependent effective temperature. However, different definitions of the effective temperature yield distinct results. In particular, plots of the integrated response versus the correlation function strongly depend on the way they are constructed. Also the definition of effective temperatures in the frequency domain is not unique for the model considered. This may have some implications for the interpretation of results from computer simulations and experimental determinations of effective temperatures.

1. Introduction

The out-of-equilibrium dynamics of glasses and disordered systems has been studied quite intensively in the last decade; see e.g. [1]. One reason for the interest in this area lies in the fact that glassy systems usually do not reach thermal equilibrium within experimentally accessible times when cooled to low temperatures. In such a situation the question as to whether there is a possibility for characterizing the non-equilibrium state of the system naturally arises. In particular, it would be extremely helpful if some of the tools of statistical physics could be extended to non-equilibrium situations. One of the efforts of quantifying the deviations from thermal equilibrium is concerned with extensions of the fluctuation–dissipation theorem (FDT) relating the response of the system to the two-time correlation function. In equilibrium, this relation is determined by the thermodynamic temperature. For non-equilibrium systems, the deviations from the FDT can in some cases be used for the introduction of a timescale-dependent effective temperature T_{eff} [2]. A variety of model-calculations and numerical simulations have been performed to analyse the behaviour of T_{eff} obtained this way; for reviews see [3, 4]. Recently, also some experimental investigations of the violations of the FDT have been performed; see e.g. [5]. One typically finds a behaviour in which T_{eff} exceeds the bath

temperature by a certain amount. This makes sense as the typical preparation of the system is given by a quench from a high temperature into a glassy phase.

There are, however, still some open questions regarding the usefulness of the interpretation of the effective temperatures obtained from FDT violations. For instance, for a meaningful definition of a temperature, T_{eff} should be independent of the dynamical variable used for its calculation. In the case that so-called neutral variables [6] are used, T_{eff} is often found to be independent of the variable in some long-time limit. Another question is concerned with the relaxation of T_{eff} to the bath temperature when the system reaches thermal equilibrium on some timescale. This point has been investigated in some recent papers [7–9] with the result that some care has to be taken in the determination of T_{eff}. Apart from these model calculations the relation of T_{eff} towards the bath temperature has also been observed in simulations [10].

In the present paper, I will consider another model in which the system reaches equilibrium for long times after a quench, namely a trap model with a Gaussian distribution of trap energies [11]. The same model has been introduced earlier as an approximation to a random walk model [12] and was termed 'energy master equation' then. It was shown in [12] that this model is able to reproduce some features that are observed in the relaxation of supercooled liquids and glasses. Furthermore, recently it was demonstrated that some results of simulations on models of supercooled liquids can (at least partly) be interpreted in terms of a Gaussian trap model [13–15]. Some features of the ageing behaviour of the populations of the traps have already been discussed in [7]. There it was shown that after a quench from an (infinitely) high temperature the distribution of populations as a function of the time elapsed after the quench first narrows and then broadens again, in qualitative accord with some observations in computer simulations [16]. It should, however, be mentioned that there are hints from simulations that for deep quenches the system explores regions of phase space that are not visited in equilibrium [16, 17]. Such effects cannot be captured by the simple trap model.

In the following section, I will briefly recall the derivation of the fluctuation–dissipation relations for trap models [18–20]. In section 3 the results of model calculations are presented and discussed. The paper closes with some conclusions in section 4.

2. Fluctuation–dissipation relations for trap models

The derivation of the fluctuation–dissipation relations for arbitrary continuous-time Markov processes has been given in [20]. Usually one assumes a situation in which the system under consideration is quenched from a high temperature T_0 to a low temperature T in the beginning of the experimental protocol. After a time t_{w}, called the waiting time, has elapsed after the quench, some dynamical quantities are monitored. In the present context, the correlation function of some dynamical variable $M(t)$,

$$C(t, t_{\text{w}}) = \langle M(t)M(t_{\text{w}}) \rangle = \int \mathrm{d}\epsilon \int \mathrm{d}\epsilon' M(\epsilon)M(\epsilon')G(\epsilon, t|\epsilon', t_{\text{w}})p(\epsilon', t_{\text{w}}) \tag{1}$$

and the response to a field applied at time t_{w}, $H(t) = H\delta(t - t_{\text{w}})$, conjugate to M,

$$R(t, t_{\text{w}}) = \left. \frac{\delta \langle M(t) \rangle}{\delta H(t_{\text{w}})} \right|_{H=0} \tag{2}$$

are of particular importance. In the above expressions, the values of ϵ are meant to represent the trap energies. $M(\epsilon)$ is the value the dynamical variable M acquires in the trap with energy ϵ and $G(\epsilon, t|\epsilon', t_{\text{w}})$ is the conditional probability to find the system in trap ϵ at time t, provided it was in trap ϵ' at time t_{w}. The populations $p(\epsilon', t_{\text{w}})$ evolve from the initial populations $p(\epsilon, t = 0)$, typically equilibrium populations at the starting temperature T_0, via $p(\epsilon, t_{\text{w}}) = \int \mathrm{d}\epsilon' G(\epsilon, t_{\text{w}}|\epsilon', 0)p(\epsilon', 0)$. For a stationary Markov process, the conditional

probability $G(\epsilon, t|\epsilon', t_w)$ is time-translational invariant, $G(\epsilon, t|\epsilon', t_w) = G(\epsilon, t - t_w|\epsilon', 0) \equiv G(\epsilon, t - t_w|\epsilon')$, and obeys a master equation [21]:

$$\frac{\partial}{\partial t} G(\epsilon, t|\epsilon') = -\int d\epsilon'' \, W(\epsilon''|\epsilon) G(\epsilon, t|\epsilon') + \int d\epsilon'' \, W(\epsilon|\epsilon'') G(\epsilon'', t|\epsilon') \quad (3)$$

with $W(\epsilon|\epsilon')$ denoting the rates for a transition from ϵ' to ϵ. In order to calculate the linear response to a field one has to fix the dependence of the transition rates on the field H. Following Ritort [18], I use the following form of multiplicatively perturbed transition rates:

$$W^{(H)}(\epsilon|\epsilon') = W(\epsilon|\epsilon') e^{\beta H[\gamma M(\epsilon) - \mu M(\epsilon')]} \quad (4)$$

where γ and μ are arbitrary parameters and $\beta = 1/T$ (with the Boltzmann constant set to unity). If $\mu + \gamma = 1$ holds additionally, then the rates $W^{(H)}(\epsilon|\epsilon')$ obey detailed balance also in the presence of the field, provided the $W(\epsilon|\epsilon')$ do so. In all following calculations the unperturbed transition rates will be chosen according to

$$W(\epsilon|\epsilon') = \eta(\epsilon)\kappa(\epsilon') \qquad \text{with } \kappa(\epsilon') = \kappa_\infty e^{\beta\epsilon'} \quad (5)$$

as is usual for the trap model [11, 12, 22]. Note, however, that other choices have also been considered; see e.g. [23]. As already mentioned above, I will only consider the trap model with a Gaussian density of states, $\eta(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\epsilon^2/(2\sigma^2)}$. In this case, the system reaches equilibrium for long times regardless of the initial conditions. The equilibrium populations are given by $p^{eq}(\epsilon) = \lim_{t\to\infty} G(\epsilon, t|\epsilon_0, t_0) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(\epsilon-\bar{\epsilon})^2/(2\sigma^2)}$ with the temperature-dependent mean energy $\bar{\epsilon} = -\beta\sigma^2$ [12]. Note that the variance σ is temperature independent.

The details of the calculation of the linear response according to equation (2) have been presented in [18–20]. As a result, it is found that for mean-field trap models with a dynamical variable M that obeys a distribution with zero mean, $\langle M \rangle = 0$, and unit variance, $\langle M^2 \rangle = 1$, the fluctuation–dissipation relation can be written as

$$R(t, t_w) = \beta \left[\gamma \frac{\partial \Pi(t, t_w)}{\partial t_w} - \mu \frac{\partial \Pi(t, t_w)}{\partial t} \right]. \quad (6)$$

Here, the correlation function

$$\Pi(t, t_w) = \int d\epsilon \, e^{-\kappa(\epsilon)(t-t_w)} p(\epsilon, t_w) \quad (7)$$

gives the probability that the system has not left the trap occupied at t_w in the following time interval $(t - t_w)$ [11].

In equilibrium, all quantities are time-translational invariant and one has

$$R_{eq}(t) = -\beta(\gamma + \mu) \frac{d\Pi_{eq}(t)}{dt} \quad (8)$$

which for $\mu = 1 - \gamma$ is just the well known FDT. As mentioned above, the system always reaches equilibrium for $t_w \to \infty$. Therefore, all ageing effects are of a transient nature. This behaviour is similar to what one expects for structural glasses cooled not too low below the calorimetric glass transition temperature. In the present paper, the quenches are performed in the following way. In the beginning, the system is prepared in thermal equilibrium at the initial temperature T_0, i.e. $p_{T_0}^{eq}(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(\epsilon-\bar{\epsilon}_0)^2/(2\sigma^2)}$ with $\bar{\epsilon}_0 = -\beta_0\sigma^2$. The following time evolution is calculated at the working temperature T, $p_T(\epsilon, t_w) = \int d\epsilon' \, G_T(\epsilon, t_w|\epsilon', 0) p_{T_0}^{eq}(\epsilon)$, where $G_T(\epsilon, t_w|\epsilon', 0)$ is the solution of equation (3) with the transition rates (5) evaluated for $\beta = 1/T$.

The violations of the FDT in out-of-equilibrium situations can be characterized by the so-called fluctuation–dissipation ratio (FDR):

$$X(t, t_w) = \frac{T R(t, t_w)}{\partial_{t_w} \Pi(t, t_w)} \quad (9)$$

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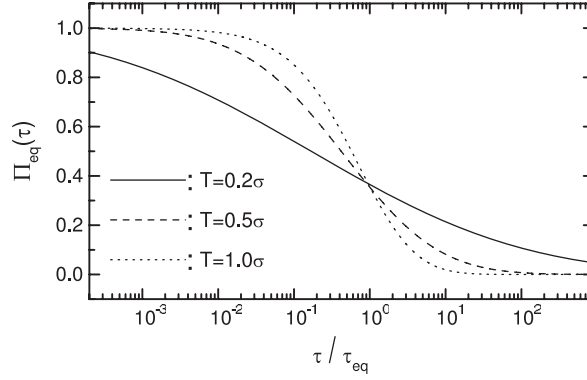
Figure 1. $\Pi_{eq}(\tau)$ versus τ for various temperatures.

which also allows the definition of a timescale-dependent effective temperature $T_{eff}(t, t_w) = T/X(t, t_w)$, the detailed behaviour of which has been discussed for a variety of models [3].

Another way to define an effective temperature has been proposed and applied in experimental determinations of FDT violations [2, 5]:

$$T_{eff}(\omega, t_w) = \frac{\omega C(\omega, t_w)}{\chi''(\omega, t_w)} \tag{10}$$

relating the Fourier transform of the correlation function (spectral density) to the dissipative part of the susceptibility. Of course, one would assume the various definitions to yield identical results. In the next section, different definitions will be compared and the differences will be discussed for the Gaussian trap model.

3. Results and discussion

I will start with a brief discussion of the equilibrium properties of the correlation function $\Pi(t, t_w)$. As already mentioned above, the system reaches equilibrium for long times after a quench has been performed, i.e. in the limit $t_w \to \infty$. According to equation (7), in this limit one has for $\tau = (t - t_w) < \infty$

$$\Pi_{eq}(\tau) = \int d\epsilon \, e^{-\kappa(\epsilon)\tau} p^{eq}(\epsilon). \tag{11}$$

This function is plotted in figure 1 as a function of τ/τ_{eq} for various temperatures, where τ_{eq} is the relaxation time determined as the $1/e$ decay time of $\Pi_{eq}(\tau)$. It is evident that the decay becomes broader with decreasing temperature. This means that in this model time–temperature superposition does not hold in equilibrium. Without showing the results here, I only mention that the values for the relaxation time τ_{eq} and the stretching parameter β_{eq} in a Kohlrausch fit to Π_{eq}, $\Pi_{eq}(\tau) \sim \exp[-(\tau/\tau_{eq})^{\beta_{eq}}]$, roughly follow the expressions given by Monthus and Bouchaud [11], $\ln(\tau_{eq}) \sim (1/T)^2$ and $\beta_{eq} \sim [1 + (a/T)]^{-1/2}$, where a is a constant.

In order to see in which time range ageing effects can be observed in $\Pi(t, t_w)$ for finite t_w, in figure 2(a) I show $\Pi(t_w + \tau, t_w)$ as a function of the measuring time τ for a quench from infinite temperature, $\beta_0 = 0$, to various working temperatures. It is seen that the decay times $\tau(t_w)$ span a much broader range at low temperatures than at high temperatures. A closer look additionally reveals the fact that the decay is broader for small and large waiting times than for intermediate t_w. The origin of this behaviour lies in the waiting-time-dependent width of the distribution of the population, $p(\epsilon, t_w)$; cf the more detailed discussion on this point in [7].

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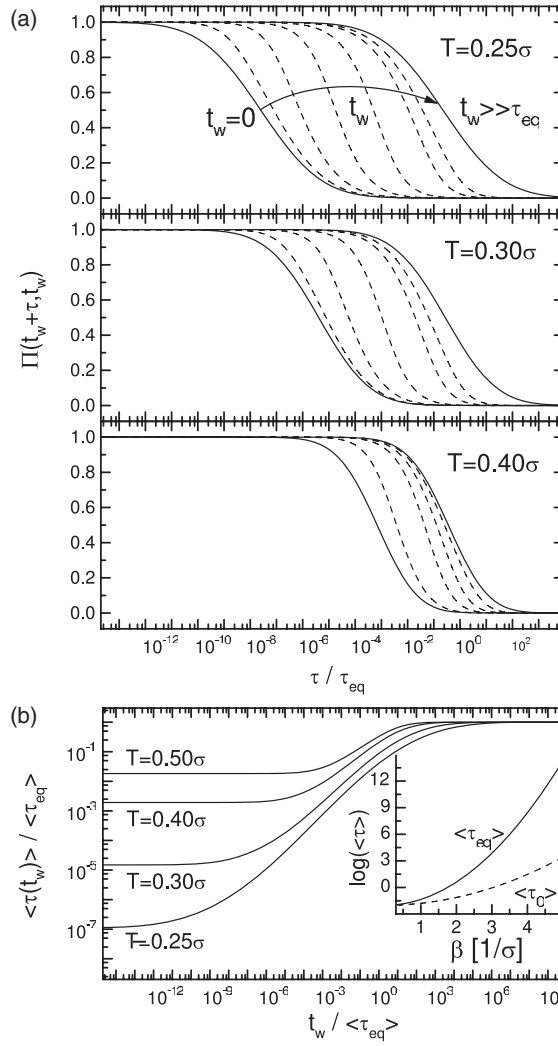
Figure 2. (a) $\Pi(t_w + \tau, t_w)$ versus measuring time τ, scaled to the equilibrium relaxation time τ_{eq} ($1/e$ decay time) for a quench from $T_0 = \infty$. (b) $\langle \tau(t_w) \rangle$ versus $t_w/\langle \tau_{eq} \rangle$ showing the time window in which ageing effects are to be expected. The inset shows the mean relaxation times $\langle \tau_0 \rangle = \langle \tau(0) \rangle$ and $\langle \tau_{eq} \rangle = \langle \tau(\infty) \rangle$ as a function of inverse temperature.

The time window in which significant ageing effects are to be expected can most easily be quantified by considering the mean relaxation time,

$$\langle \tau(t_w) \rangle = \int d\tau \, \Pi(t_w + \tau, t_w),$$

which does not depend on the width of the actual decay. The mean relaxation times for a quench from $T_0 = \infty$ to various temperatures are shown in figure 2(b). The difference of the mean relaxation time directly after the quench, $\langle \tau_0 \rangle = \langle \tau(0) \rangle = \kappa_\infty^{-1} \exp(\beta^2 \sigma^2 / 2)$, and the equilibrium mean relaxation time, $\langle \tau_{eq} \rangle = \langle \tau(\infty) \rangle = \kappa_\infty^{-1} \exp(3\beta^2 \sigma^2 / 2)$, shown in the inset in figure 2(b), gives a measure for the 'ageing time window' at a given temperature.

As is exemplified in figure 3(a), the overall time window for visible ageing effects diminishes not only with increasing final working temperature, but also with lower initial
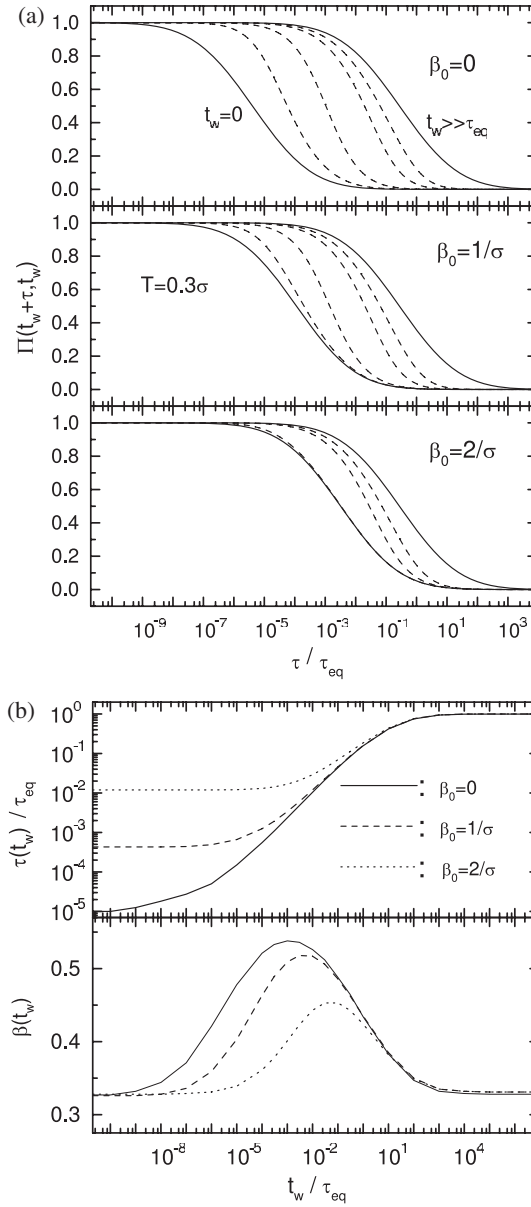
Figure 3. (a) $\Pi(t_w + \tau, t_w)$ versus τ/τ_{eq} for quenches from various $T_0 = 0$, σ, 0.5σ and $\log_{10}(t_w/\tau_{eq}) = -15, -5, -3, -1, 1, 5$. (b) $\tau(t_w)$ (upper panel) and $\beta(t_w)$ (lower panel) versus t_w/τ_{eq} as obtained from fits to a Kohlrausch function, $\exp[-(\tau/\tau(t_w))^{\beta(t_w)}]$.

temperature T_0. It is evident that the effect of lowering T_0 is similar to measuring the correlation at a higher working temperature for a given T_0. In figure 3(b) the relaxation time $\tau(t_w)$ and the stretching parameter $\beta(t_w)$ as obtained from Kohlrausch fits to $\Pi(t_w + \tau, t_w)$, $\Pi(t_w + \tau, t_w) \sim \exp[-(\tau/\tau(t_w))^{\beta(t_w)}]$, are shown. One can see that the overall spread in relaxation time diminishes with decreasing T_0 and that $\tau(t_w)$ approaches τ_{eq} at the working temperature T on the timescale of τ_{eq} itself. This is because there is no other timescale present in the model. The stretching parameter $\beta(t_w)$ first increases and then decreases again as a
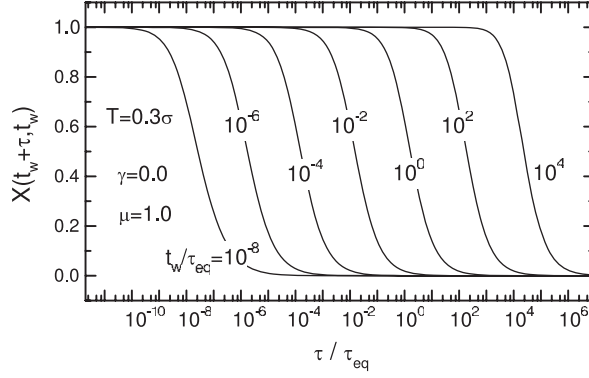
Figure 4. The FDR $X(t_w + \tau, t_w)$ versus τ/τ_{eq} for a quench from $T_0 = \infty$ to 0.3σ and $\gamma = 0$, $\mu = 1$ for various waiting times t_w.

function of the waiting time, similar to what has been found earlier in a free-energy model for the primary relaxation of viscous liquids [20]. Note that in the limit of short and long t_w the $\beta(t_w)$-values, $\beta(0) = \beta(\infty)$, are the same because in the present model the width σ of $\eta(\epsilon)$ and $p^{eq}(\epsilon)$ are independent of temperature.

Next, we turn to a discussion of the FDR, equation (9), which is calculated from the fluctuation–dissipation relation, equation (6). For long waiting times one finds

$$X(t, t_w) = \gamma + \mu \qquad \text{for } t_w \gg \tau_{eq} \tag{12}$$

as expected because the system is in equilibrium. Furthermore, the equal-time value also yields the same result,

$$X(t, t) = \lim_{(t-t_w)\to 0} X(t, t_w) = \gamma + \mu. \tag{13}$$

This can easily be seen from the fact that for small time differences one has $\partial_{t_w} \Pi(t, t_w) = -\partial_t \Pi(t, t_w)$. For finite t_w and long times, however, the FDR reaches a non-trivial limiting value

$$X_\infty(t_w) = \lim_{(t-t_w)\to\infty} X(t, t_w) = \gamma \tag{14}$$

independent of $T_0 > T$. This result is very similar to the one obtained in [9]. It is interesting to compare the result with the corresponding expression for the trap model with an exponential density of states, where it is found that the long-time limit of $X_\infty(t_w)$ tends towards γ, $X_\infty = \lim_{t_w \to \infty} X_\infty(t_w)$ [18]. Thus, apparently, the model with a Gaussian density of states resembles some features of the model with an exponential one for intermediate waiting times. If interpreted in terms of a timescale-dependent effective temperature, $T/X_\infty(t_w) = 1/\gamma$, one finds that it can be higher ($\gamma < 1$) or smaller ($\gamma > 1$) than the bath temperature T. It should be mentioned, however, that one typically will have $\gamma \leqslant 1$. For instance, in a 'force model', one would assume the bias induced by the external field to be symmetric and therefore $\gamma = \mu = 1/2$.

The detailed behaviour of the FDR is shown in figure 4, where I plotted $X(t_w + \tau, t_w)$ versus the measuring time τ for various t_w and $\gamma = 0$ for a quench from $T_0 = \infty$ to $T = 0.3\sigma$. It is seen that $X(t_w + \tau, t_w)$ starts from the short-time value $X(t_w, t_w) = 1$ and decays to its long-time limit, equation (14). This decay takes place on the timescale $(\tau/t_w) \sim 1$ as is to be expected for a model with a single timescale. For very long t_w, the decay of X will not be observed due to the long measuring times required. If one starts with lower T_0 the main

difference is that the decay from $X = 1$ to $X = \gamma$ for a given t_w takes place at somewhat later measuring times τ. This is because for smaller T_0 the system is closer to equilibrium for a given t_w. Thus, one can roughly compare X for the lower T_0 and a given t_w with the corresponding one for the higher T_0 but a longer t_w.

Instead of computing $X(t, t_w)$ directly, the FDR or the effective temperature is usually obtained from a so-called fluctuation–dissipation (FD) plot, i.e. a plot of the integrated response $\chi(t, t_w) = \int_{t_w}^{t} ds\, R(t, s)$ versus the correlation function $\Pi(t, t_w)$ [2, 3]. The FDR then is extracted as the slope in such an FD plot. It has been pointed out earlier that such plots have to be constructed with some care in the general case [6]. In some situations a plot of $\chi(t_w + \tau, t_w)$ versus $\Pi(t_w + \tau, t_w)$ with τ as the curve parameter and fixed t_w does not necessarily give the correct FDR. This is only ensured if t_w is used as the curve parameter due to the fact that according to the definition of the integrated response one has $R(t, t_w) = -\frac{\partial \chi(t, t_w)}{\partial t_w}$. The reason is that in general the different derivatives $\partial_{t_w} \Pi(t, t_w)$ and $\partial_t \Pi(t, t_w)$ cannot be interchanged. For some models with transient ageing behaviour, it has indeed been found that the former construction yields wrong results [8, 9]. Also for the Gaussian trap model, FD plots with τ as the curve parameter yield wrong results for the FDR. This fact is exemplified in figure 5(a), where such FD plots for different temperatures and $t_w = 10^{-15}\tau_{eq}$ are shown. The initial temperature was chosen as $T_0 = \infty$. The inset shows the temperature dependence of the slopes extracted from these plots via a linear regression in the interval $0.3 < \Pi < 0.7$. Note that all slopes are larger than $X_{\infty}(t_w) = \gamma = 0.5$. The situation is very similar to the one in a free-energy model for glassy relaxation discussed in detail in [9].

In figure 5(b), an FD plot with t_w as the curve parameter and various values of the time t is shown for $\gamma = 0$ (upper panel) and $\gamma = 1/2$ (lower panel). It is evident that in this case the limiting slopes coincide with $X_{\infty}(t_w)$, equation (14). However, it is also clear that the curves change continuously until this limiting slope is reached.

Therefore, similar to the case of the trap model with an exponential density of states, it appears that only the limiting slope $X_{\infty}(t_w)$ may be a useful candidate for the definition of an effective temperature [6]. Additionally, the detailed behaviour of the curves also depends on the initial temperature T_0, as can be seen from figure 5(c), which shows FD plots for various T_0 and a fixed time $t = 10^{-4}\tau_{eq}$ for $\gamma = 0$, $\mu = 1$. The limiting value for the slope is the same, as already pointed out above.

From the above discussion it appears that the quantity $T/X_{\infty}(t_w)$ may serve as a t_w-dependent effective temperature in the Gaussian trap model. As already noted in the previous section, there are other possible definitions of effective temperatures, in particular the one given in equation (10), $T_{eff}(\omega, t_w) = \frac{\omega C(\omega, t_w)}{\chi''(\omega, t_w)}$. Here, the natural way to define the Fourier transform is with respect to the measuring time [24, 25]:
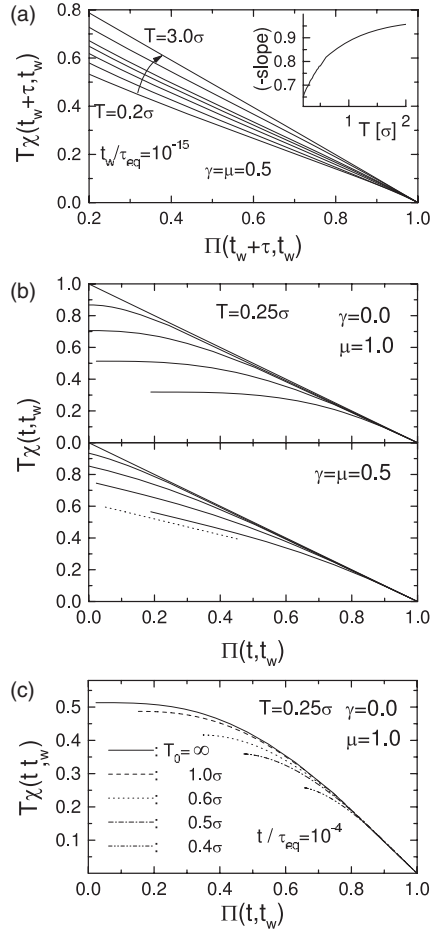
$$C(\omega, t_w) = \mathrm{Re} \int_0^{\infty} d\tau\, \Pi(t_w + \tau, t_w) e^{i\omega\tau}$$
$$\chi''(\omega, t_w) = \mathrm{Im} \int_0^{\infty} d\tau\, R(t_w + \tau, t_w) e^{i\omega\tau} \tag{15}$$

which is similar to the definition used in most experiments. It can be shown analytically that $T_{eff}(\omega, t_w)$ defined this way has the following limiting behaviour:

$$\lim_{t_w \to \infty} T_{eff}(\omega, t_w) = \lim_{\omega \to \infty} \lim_{t_w \to 0} T_{eff}(\omega, t_w) = \frac{T}{\mu + \gamma}, \tag{16}$$

as expected. However, the low-frequency limit is given by

$$\lim_{\omega \to 0} \lim_{t_w \to 0} T_{eff}(\omega, t_w) = \frac{T}{\mu + \gamma e^{2(\sigma/T)^2}}, \tag{17}$$

Figure 5. (a) Plot of $T\chi(t_w + \tau, t_w)$ versus $\Pi(t_w + \tau, t_w)$ (FD plot) with the measuring time τ as the curve parameter and fixed waiting time, $t_w = 10^{-15}\tau_{eq}$, for a quench from $T_0 = \infty$ to $T = 0.2, 0.3, 0.4, 0.5, 0.6, 1.0, 3.0\sigma$ from bottom to top. Here, $\gamma = \mu = 1/2$. The inset shows the slopes extracted from these plots via a linear regression for the data in the interval $0.3 < \Pi < 0.7$. (b) Plot of $T\chi(t, t_w)$ versus $\Pi(t, t_w)$ (FD plot) for a quench from $T_0 = \infty$ to 0.25σ and times $\log_{10}(t/\tau_{eq}) = -6, -4, -2, 0, 6$ from bottom to top. In the upper panel $\gamma = 0$, $\mu = 1$ has been chosen, i.e. $X_\infty(t_w) = 0$, and in the lower panel $\gamma = \mu = 1/2$ ($X_\infty(t_w) = 1/2$, dotted line). (c) $T\chi(t, t_w)$ versus $\Pi(t, t_w)$ for a quench from $T_0 = \infty, 1.0\sigma, 0.5\sigma$, and 0.4σ to $T = 0.25\sigma$ and $t/\tau_{eq} = 10^{-4}$, $\gamma = 0$, $\mu = 1$.

which is different from $T/X_\infty(t_w)$. For $\mu = 1$ and $\gamma = 0$ no deviations from the equilibrium FDT can be observed at all. When considered as a function of frequency, $T_{eff}(\omega, t_w)$ starts from the low-frequency limit $T/(\mu + \gamma e^{2(\sigma/T)^2})$ and roughly at $\omega t_w \sim 1$ smoothly crosses over to the high-frequency limit $T/(\mu + \gamma)$. The main difference from T/X is that the low-frequency limit is usually much smaller than the bath temperature T. An obvious reason for this discrepancy lies in the definition of the Fourier transform. The definition of the FDR involves only the partial derivative $\partial_{t_w}\Pi(t, t_w)$, whereas $\omega C(\omega, t_w)$ according to equation (15) corresponds to the Fourier transform of $\partial_t\Pi(t, t_w)$. Thus, the situation appears to be very similar to the one met when considering the different ways of constructing FD plots discussed above. There is, however, one difference. For the present model it is not at all clear that a definition of an effective

temperature via the Fourier transform of $\Pi(t, t_{\mathrm{w}})$ and $R(t, t_{\mathrm{w}})$ is related to the FDR in a direct manner. This is due to the fact that one has to consider the Fourier transform of $R(t, t_{\mathrm{w}}) = \beta X(t, t_{\mathrm{w}}) \partial_{t_{\mathrm{w}}} \Pi(t, t_{\mathrm{w}})$, which in general will give a convolution instead of a simple product.

It is tempting to use an alternative definition of the Fourier transform [2], $\hat{C}(\omega, t) = \mathrm{Re} \int_0^t \mathrm{d}s \, \Pi(t, s) \mathrm{e}^{-i\omega(t-s)}$ and $\hat{\chi}''(\omega, t) = \mathrm{Im} \int_0^t \mathrm{d}s \, R(t, s) \mathrm{e}^{-i\omega(t-s)}$, for which one can see that $\omega \hat{C}(\omega, t)$ is related to the Fourier transform of $\partial_{t_{\mathrm{w}}} \Pi(t, t_{\mathrm{w}})$. One then has $\hat{T}_{\mathrm{eff}}(\omega, t) = \frac{\omega \hat{C}(\omega,t)}{\hat{\chi}''(\omega,t)}$. However, this definition implies that one considers the situation $\omega t \gg 1$, in order for the oscillatory part of the functions involved to be negligible. As one can show analytically that $\hat{T}_{\mathrm{eff}}(\omega, t \to \infty) = \hat{T}_{\mathrm{eff}}(\omega \to \infty, t) = T/(\gamma + \mu)$, this condition means that the relevant small-frequency limit is hard to reach in practice, in particular because the relaxation takes place on the scale $\omega t \sim 1$.

4. Conclusions

In the present paper I have considered the ageing behaviour of the correlation function and the linear response in a Gaussian trap model. As in this model equilibrium is reached for long waiting times after a quench ($t_{\mathrm{w}} \to \infty$), all ageing effects are of a transient nature. The time window in which ageing effects can be observed expands with decreasing working temperature T if a quench from a fixed high temperature T_0 is considered. If T is kept fixed and T_0 is increased the 'ageing time window' also increases.

If the waiting time is chosen to be longer than the equilibrium relaxation time ($1/e$ decay time), $t_{\mathrm{w}} \gg \tau_{\mathrm{eq}}$, the two-time quantities like the correlation function $\Pi(t, t_{\mathrm{w}})$ and the response function $R(t, t_{\mathrm{w}})$ approach their equilibrium values and only depend on the time difference $(t - t_{\mathrm{w}})$. In this situation the FDT is obeyed. For short waiting times, on the other hand, one has an explicit dependence of $\Pi(t, t_{\mathrm{w}})$ and $R(t, t_{\mathrm{w}})$ on both times and the functions no longer are time-translational invariant. In this situation strong violations of the FDT are observed. In particular, for $t_{\mathrm{w}} < \tau_{\mathrm{eq}}$ the FDR $X(t, t_{\mathrm{w}})$ tends to a non-trivial long-time limit $X_\infty(t_{\mathrm{w}}) = \gamma$, cf equation (14), independent of $T_0 > T$. The constant γ is determined by the coupling of the system's dynamics to an external field via the transition rates $W^{(H)}(\epsilon'|\epsilon)$, cf equation (4). The only possible temperature dependence of $X_\infty(t_{\mathrm{w}})$ stems from a T-dependence of γ. The value for $X_\infty(t_{\mathrm{w}})$ coincides with that found for the trap model with an exponential density of states [18], albeit for long waiting times.

The FDR can be used for the definition of a timescale-dependent effective temperature, $T/X(t, t_{\mathrm{w}})$. Usually, the effective temperature is extracted from FD plots, which can be constructed in different ways. As has been pointed out [6], the correct way to construct FD plots is to use t_{w} as the curve parameter for fixed t. If FD plots are constructed this way, the limiting slope coincides with $X_\infty(t_{\mathrm{w}})$. The fact that these plots are curved indicates that not the function $X(t, t_{\mathrm{w}})$ as a whole but only the limiting value $X_\infty(t_{\mathrm{w}})$ may be used for a meaningful definition of an effective temperature. If alternatively FD plots with the measuring time as curve parameter for different $t_{\mathrm{w}} < \tau_{\mathrm{eq}}$ are considered, one finds that one can define a slope in these plots which, however, does not coincide with $X(t, t_{\mathrm{w}})$, and furthermore shows some artificial temperature dependence. A similar problem occurs when the definition of an effective temperature in the frequency domain is considered. The usual definition of the Fourier transform, equation (15), yields an effective temperature that is distinct from what one finds from the FDR. In this case, similarly as for the FD plots, one reason is that one cannot interchange the derivatives with respect to the earlier and the later time in the correlation function.

In the recent past FD plots have been constructed from computer simulations of model supercooled liquids [4, 26, 27]. For the model of a fragile liquid one finds that the FDT

is obeyed for large values of the correlation and then the slope changes to a smaller value indicating an effective temperature larger than the bath temperature [4, 26]. For a strong liquid, however, one finds an effective temperature smaller than the bath temperature [27]. These plots have been constructed with the measuring time as the curve parameter and fixed waiting times.

Given the fact that the Gaussian trap model is apparently able to capture some important features of the dynamics observed in computer simulations on supercooled liquids, it is tempting to speculate that FD plots with the waiting time as the curve parameter might look different to the ones published so far. Therefore, it would be interesting to calculate FD plots from simulation data the correct way and compare the results to the previous findings.

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References

[1] Bouchaud J-P, Cugliandolo L F, Kurchan J and Mezard M 1998 *Spin Glasses and Random Fields*
      ed A P Young (Singapore: World Scientific)
[2] Cugliandolo L F, Kurchan J and Peliti L 1997 *Phys. Rev.* E **55** 3898
[3] Crisanti A and Ritort F 2003 *J. Phys. A: Math. Gen.* **36** R181
[4] Barrat J-L 2003 *J. Phys.: Condens. Matter* **15** S1
[5] Grigera T S and Israeloff N E 1999 *Phys. Rev. Lett.* **83** 5038
      Bellon L, Ciliberto S and Laroche C 2001 *Europhys. Lett.* **53** 511
      Bellon L and Ciliberto S 2002 *Physica* D **168/169** 325
      Bonn D and Kegel W K 2003 *J. Chem. Phys.* **118** 2005
      Buisson L, Ciliberto S and Garcamartin A 2003 *Europhys. Lett.* **63** 603
      Abou B and Gallet F 2004 *Phys. Rev. Lett.* **93** 160603
[6] Fielding S and Sollich P 2002 *Phys. Rev. Lett.* **88** 050603
      Sollich P, Fielding S and Mayer P 2002 *J. Phys.: Condens. Matter* **14** 1683
[7] Diezemann G 2005 *J. Chem. Phys.* **123** 204510
[8] Diezemann G 2006 *J. Non-Cryst. Solids* at press
[9] Diezemann G and Böhmer R 2006 *J. Chem. Phys.* **124** 214507
[10] Sciortino F and Tartaglia P 2001 *Phys. Rev. Lett.* **86** 107
[11] Monthus C and Bouchaud J-P 1996 *J. Phys. A: Math. Gen.* **29** 3847
[12] Dyre J C 1995 *Phys. Rev.* B **51** 122276
[13] Denny R A, Reichman D R and Bouchaud J-P 2003 *Phys. Rev. Lett.* **90** 025503
[14] Doliwa B and Heuer A 2003 *Phys. Rev.* E **67** 031506
[15] Heuer A, Doliwa B and Saksaengwijit A 2005 *Phys. Rev.* E **72** 021503
[16] Saika-Vovoid I and Sciortino F 2004 *Phys. Rev.* E **70** 041202
[17] Mossa S and Sciortino F 2004 *Phys. Rev. Lett.* **92** 045504
[18] Ritort F 2003 *J. Phys. A: Math. Gen.* **36** 10791
[19] Sollich P 2003 *J. Phys. A: Math. Gen.* **36** 10807
[20] Diezemann G 2005 *Phys. Rev.* E **72** 011104
      Diezemann G 2006 *Phys. Rev.* E **73** 039907 (erratum)
[21] van Kampen N G 1981 *Stochastic Processes in Physics and Chemistry* (Amsterdam: North-Holland)
[22] Bouchaud J-P 1992 *J. Physique* I **2** 1705
      Bouchaud J-P, Vincent E and Hammann J 1994 *J. Physique* I **4** 139
      Bouchaud J-P and Dean D S 1995 *J. Physique* I **5** 265
[23] Barrat A and Mezard M 1995 *J. Physique* I **5** 941
[24] Garriga A and Ritort R 2005 *Phys. Rev.* E **72** 031505
[25] Ritort F and Sollich P 2003 *Adv. Phys.* **52** 219
[26] Kob W and Barrat J-L 1999 *Physica* A **263** 234
      Kob W and Barrat J-L 2000 *Eur. Phys. J.* B **13** 319
[27] Scala A, Valeriani C, Sciortino F and Tartaglia P 2003 *Phys. Rev. Lett.* **90** 115503