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Effective temperatures in a simple model of non-equilibrium, non-Markovian dynamics

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Abstract. The concept of effective temperatures in nonequilibrium systems is studied within an exactly solvable model of non-Markovian diffusion. The system is coupled to two heat baths which are kept at different temperatures: one ('fast') bath associated with an uncorrelated Gaussian noise and a second ('slow') bath with an exponential memory kernel. Various definitions of effective temperatures proposed in the literature are evaluated and compared. The range of validity of these definitions is discussed. It is shown in particular, that the effective temperature defined from the fluctuation-dissipation relation mirrors the temperature of the slow bath in parameter regions corresponding to a separation of time scales. On the contrary, quasi-static and thermodynamic definitions of an effective temperature are found to display the temperature of the fast bath in most parameter regions.

1. Introduction

Recent years have witnessed enormous efforts in understanding glassy systems by studying a broad variety of model systems. At the same time, it has been found that various other systems like colloids, granular materials, etc. share several features of typical phenomenology of glassy systems. Therefore, a common macroscopic description of glassy systems would be extremely helpful. However, unlike equilibrium thermodynamics, there is no general, well-established framework for a macroscopic description available today that works out of equilibrium.

A key role in the macroscopic description of glassy systems could be played by the concept of effective temperature [1, 2]. Based on the fluctuation-dissipation relation (FDR) [1], the effective temperature is supposed to govern the slow, not equilibrated degrees of freedom, while the short time dynamics and the equilibrated degrees of freedom are governed by the bath temperature. Subsequent molecular dynamics simulations [3, 4] on a supercooled model fluid during aging or in shear flow are in agreement with this picture. However, it has been argued that non-linear generalizations of the fluctuation-dissipation theorem (FDT) out of equilibrium could spoil the interpretation of effective temperatures from FDR [5]. The authors emphasize that "Physical interpretations of the several temperatures and their relation to experimental probes and to their mutual relation in non-equilibrium steady states are needed." (p. 2014 in [5]). In addition, more recent molecular dynamics simulations [6] found that effective temperatures should sometimes be defined from static FDR rather than from the dynamical one, as was done in [3, 4]. The authors of [6] conclude their study with a "puzzle: when should one use static linear response and when should one use a time-dependent relation?". For a review on the numerical evidence of effective temperatures see also [7]. Up to now, experimental investigations of effective temperatures in

glassy systems are not conclusive. Experiments on spin glasses in the aging regime [8] and self-diffusion of granular material in a Couette cell [9] have shown some evidence in favor of the existence of an effective temperature as introduced in [1]. In dense colloidal suspensions, very recent experiments [10] found no deviation from the FDT, while an effective temperature could be measured in a colloidal glass of laponite [11, 12]. Most experiments, however, involve frequencies that are rather high compared to the inverse relaxation time. Earlier experiments on an aging colloidal glass [13] observed violations of the FDT in electrical but not in rheological studies.

In view of these controversies, it seems appropriate to resort to simplified model systems, where the validity of effective temperature concepts can be studied in more detail. It has been found, that mean-field spin glasses with one-step replica symmetry breaking scheme do allow the definition of an effective temperature from the FDR [14], while those with continuous replica symmetry breaking do not [7]. Field-theoretic calculations on the critical dynamics of spin models show, that the effective temperature defined from the FDR does depend on the variables considered [15, 16]. Also in the Ising chain with Glauber dynamics and dynamical trap models, a meaningful effective temperature cannot be defined from the FDR [17]. A slightly different perspective was taken in [18, 19, 20], where Brownian particles coupled to two heat baths at different temperatures were studied. The aim of the present study is to derive and compare different static as well as dynamic definitions of effective temperatures in these systems and discuss their range of validity.

This paper is organized as follows. The model of non-Markovian diffusion in the presence of two heat baths is introduced in Sec. 2. In Sec. 3, the model is simplified by considering the overdamped limit. From the exact solution of the model, different definitions of effective temperatures are evaluated and compared in Sec. 4. Some conclusions are offered in Sec. 5.

2. Model

Consider a particle of mass m at position x with velocity v moving in a potential $V(x)$ under the influence of two thermal baths. One bath is held at temperature T_{slow} . Its influence on the dynamics of the particle is described by the retarded friction coefficient (memory kernel) $\Gamma(t)$. The other bath is kept at temperature T_{fast} . Contrary to the first, slow bath, the correlation time of the second bath is small enough, so that the particle experiences an instantaneous friction described by the friction coefficient Γ_0 . The equations of motion read

$$\begin{aligned} \dot{x} &= v \\ m\dot{v} &= -\frac{\partial V}{\partial x} - \int_0^t ds \Gamma(t-s)v(s) - \Gamma_0 v(t) + \xi(t) + \eta(t). \end{aligned} \quad (1)$$

The fast bath is modelled as Gaussian white noise with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(s) \rangle = 2T_{\text{fast}}\Gamma_0\delta(t-s)$, whereas the random force due to the slow bath is characterized by $\langle \xi(t)\xi(s) \rangle = T_{\text{slow}}\Gamma(t-s)$. We choose units such that Boltzmann's constant $k_B \equiv 1$. The model (1) generalizes earlier work on non-Markovian diffusion [21] by including a second heat bath at a different temperature.

The diffusion equation (1) is difficult to study in general due to its non-Markovian character. For the special case of an exponential memory function,

$$\Gamma(t) = \frac{1}{\alpha} \exp[-t/(\alpha\gamma)], \quad (2)$$

it is possible to map the non-Markovian dynamics (1) onto a Markovian process in an extended state space [21],

$$\dot{x} = v$$

$$\begin{aligned}
m\dot{v} &= -\frac{\partial V}{\partial x} + z(t) - \Gamma_0 v(t) + \eta(t) \\
\dot{z} &= -\frac{1}{\alpha}v(t) - \frac{1}{\alpha\gamma}z(t) + \zeta(t)
\end{aligned} \tag{3}$$

where ζ is a Gaussian white noise with

$$\langle \zeta(t)\zeta(s) \rangle = \frac{2T_{\text{slow}}}{\alpha^2\gamma}\delta(t-s). \tag{4}$$

Equations (3) together with the noise correlators specify the model to be considered in the present study.

3. The overdamped limit

Formally, the model of non-Markovian diffusion introduced in Sec. 2 can be mapped onto a system of two coupled Brownian particles, each equipped with its own heat bath. In order to further simplify the analysis, we here consider the overdamped limit $m\dot{v} \rightarrow 0$ where the inertia term can be dropped. In the overdamped limit, the time evolution equations (3) simplify to

$$\begin{aligned}
\Gamma_0\dot{x} &= -\frac{\partial V}{\partial x} - \Gamma(0)x(t) + \Gamma(t-t_0)x(t_0) + \eta(t) + h(t) \\
h(t) &= -\int_{t_0}^t ds \frac{\partial \Gamma(t-s)}{\partial t} x(s) + \zeta(t)
\end{aligned} \tag{5}$$

These equations are studied also in [19]. In [19], the initial time is set $t_0 \rightarrow -\infty$, thus $\Gamma(t-t_0)x(t_0) \rightarrow 0$ and the term depending on the initial condition is absent.

Employing again the exponentially decaying memory function (2), closed, Markovian time evolution equations for x and h are obtained. In a generalized notation ¹, the resulting time evolution equations take the form

$$\begin{aligned}
\dot{x}_1 &= -\frac{1}{\Gamma_1}\frac{\partial U}{\partial x_1} + \nu_1 x_2 + \eta_1(t) \\
\dot{x}_2 &= -\frac{\kappa_2}{\Gamma_2}x_2 + \nu_2 x_1 + \eta_2(t)
\end{aligned} \tag{6}$$

where the Gaussian white noise is characterized by $\langle \eta_i(t) \rangle = 0$ and $\langle \eta_i(t)\eta_j(s) \rangle = 2T_i\Gamma_i^{-1}\delta_{ij}\delta(t-s)$. In Eq. (6), we have neglected the transient term $\Gamma(t-t_0)x(t_0)$, which is justified for times t long enough or for the initial condition $x(t_0) = 0$. Although Eqs. (6) are very similar to those studied in [19], we point out the important difference that the memory function (2) does not satisfy $\dot{\Gamma}(0^+) = 0$ as is assumed in [19].

Only for the special case $\Gamma_1\nu_1/T_1 = \Gamma_2\nu_2/T_2$ (in terms of the original parameters, this condition reduces to $T_{\text{slow}} = T_{\text{fast}}$) is the equilibrium distribution function corresponding to (6) a Boltzmann distribution, $p_{\text{eq}}(x_1, x_2) \propto \exp(-U(x_1)/T_1 - \kappa_2 x_2^2/T_2 + \nu_1 \Gamma_1 x_1 x_2/T_1)$. In that case, the marginal distribution $f_{\text{eq}}(x_1) = \int_{-\infty}^{\infty} dx_2 p_{\text{eq}}(x_1, x_2)$ is given by $f_{\text{eq}}(x_1) \propto \exp(-U(x_1)/T_1 + \kappa_{21} x_1^2/2T_2)$ where $\kappa_{21} = (\Gamma_2\nu_2)^2/\kappa_2$. Thus, the coupling to x_2 leads to a shifted equilibrium distribution, that can be described by a repulsive harmonic potential of strength κ_{21} . In case the potential $U(x_1)$ is itself harmonic, $U(x_1) = \kappa_1 x_1^2/2$, the shifted equilibrium distribution f_{eq} is of the same form as the uncoupled equilibrium distribution but with a renormalized spring coefficient. If instead one insists on the equilibrium form $f_{\text{eq}}(x_1) \propto$

¹ The original model is recovered if the following identifications are made: $x_1 = x$, $x_2 = h$, $U = V + (2\alpha)^{-1}x^2$, $\kappa_2 = \alpha$, $\Gamma_1 = \Gamma_0$, $\Gamma_2 = \alpha^2\gamma$, $\nu_1 = 1/\Gamma_0$, $\nu_2 = 1/(\alpha^2\gamma)$, $T_1 = T_{\text{fast}}$, $T_2 = T_{\text{slow}}$.

$\exp(-U(x_1)/T_{\text{eq}})$, an effective temperature ² is defined by $T_{\text{eq}} = T_1/[1 - \Gamma_1\Gamma_2\nu_1\nu_2(\kappa_1\kappa_2)^{-1}]$. In terms of the original variables, U is harmonic if the potential V in (1) is harmonic, $V(x) = \kappa_{1,0}x^2/2$. Thus, $\kappa_1 = \kappa_{1,0} + \alpha^{-1}$ and the corresponding identification of an effective temperature equals the bath temperature $T_{\text{eq}} = T_1$ as it should, since in this case the condition $\Gamma_1\nu_1/T_1 = \Gamma_2\nu_2/T_2$ reduces to $T_{\text{fast}} = T_{\text{slow}}$. It is interesting to note, that the same effective temperature T_{eq} is obtained by adiabatic elimination, if x_2 is assumed to vary much faster than x_1 [2]. Then, the assumption $\kappa_1/\Gamma_1 \ll \kappa_2/\Gamma_2$ replaces the condition $\Gamma_1\nu_1/T_1 = \Gamma_2\nu_2/T_2$.

Yet another approach to obtain effective temperatures is to employ the Quasi-Equilibrium Approximation (QEA) which is used successfully in many areas of statistical physics [22, 23]. Following the standard procedure [22], extremizing the entropy functional $S[p] = -\int dx_1 dx_2 p \ln p$ subject to the constraints of fixed moments $M_0 = \langle 1 \rangle$, $M_1 = \langle x_1^2 \rangle$, $M_2 = \langle x_2^2 \rangle$, $M_3 = \langle x_1 x_2 \rangle$, the quasi-equilibrium distribution is found to be given by $p^*(x_1, x_2) = \exp(\lambda_0 + \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_1 x_2)$. The Lagrange multipliers λ_i are chosen such that the constraints are satisfied identically. In equilibrium, p^* reduces to p_{eq} . Out of equilibrium, p^* approximates the true non-equilibrium state by equilibrating all degrees of freedom except for the macroscopic variables M_i . The quasi-equilibrium entropy S^* is defined by $S^*(M) = S[p^*]$ and satisfies $dS^* = \sum_j \lambda_j dM_j$. Within the QEA, the temperature is defined as $T_{\text{QEA}}^{-1} \equiv \partial S^*/\partial U$. For simplicity, we will assume a harmonic potential, $V(x) = \kappa_{1,0}x^2/2$. Then, the effective temperature within the QEA is given by $T_{\text{QEA}}^{-1} = (2/\kappa_1)\lambda_1$. Thanks to the simplicity of the model, the Lagrange multipliers can be evaluated explicitly by performing Gaussian integrals. The resulting expression for T_{QEA} is

$$T_{\text{QEA}} = \kappa_1 (\langle x_1^2 \rangle - \langle x_1 x_2 \rangle^2 / \langle x_2^2 \rangle). \quad (7)$$

In the uncoupled case, $\langle x_1 x_2 \rangle = 0$, Eq. (7) reduces to the equipartition theorem and $T_{\text{QEA}} = T_1$.

In the following section, we evaluate and compare different definitions of effective temperatures derived from the exact solution in case of harmonic potentials.

4. Exact solution for harmonic forces

For the harmonic potential $U(x_1) = \kappa_1 x_1^2/2$, $\kappa_1 = \kappa_{1,0} + 1/\alpha$, Eqs. (6) are stochastic differential equations of the narrow-sense linear type that can be solved exactly by transformation to normal coordinates. The solution reads

$$x_i(t) = \sum_{\alpha=+,-} b_{i,\alpha} X_\alpha(t) \quad (8)$$

where the coefficients $b_{i,\alpha}$ are defined by $b_{1,+} = -a_-/(a_+ - a_-)$, $b_{1,-} = a_+/(a_+ - a_-)$, $b_{2,+} = 1/(a_+ - a_-)$, $b_{2,-} = -1/(a_+ - a_-)$ and

$$X_\alpha(t) = e^{-(t-t_0)c_\alpha} X_\alpha(t_0) + \int_{t_0}^t ds e^{-(t-s)c_\alpha} \eta_\alpha(s). \quad (9)$$

The noise terms appearing in Eq. (9) are related to those in (6) by $\eta_\alpha(t) = \eta_1(t) + a_\alpha \eta_2(t)$. The eigenvalues associated with Eqs. (6) are given by

$$c_\pm = \frac{1}{2} \left(\frac{\kappa_1}{\Gamma_1} + \frac{\kappa_2}{\Gamma_2} \right) \mp \frac{1}{2} \sqrt{D} \quad (10)$$

² Note, that $T_{\text{eq}} \neq T_1$ if even both baths are at the same temperature $T_1 = T_2$ since the effective temperature mimics the effect of the coupling on the equilibrium state. Therefore, quantities that depend only on x_1 but not on x_2 , show equilibrium expectation values corresponding to T_{eq} rather than T_1 .

with $D = (\kappa_1/\Gamma_1 - \kappa_2/\Gamma_2)^2 + 4\nu_1\nu_2$. The coefficients a_{\pm} introduced above are defined by $a_{\pm} = (\kappa_1/\Gamma_1 - c_{\pm})/\nu_2$. Note, that the special case $\nu_2 = 0$ has to be treated separately. In that case, the time evolution equation for x_2 can be solved independently of x_1 , resulting in an additional noise term in form of an Ornstein-Uhlenbeck process resulting from x_2 . In particular, one finds in this case, $c_{\pm} = \kappa_1/\Gamma_1$ and $a_{\pm} = -(\kappa_1/\Gamma_1 - \kappa_2/\Gamma_2)^{-1}\nu_1$. In the uncoupled case, $\nu_1 = 0$, the eigenvalues reduce to the individual relaxation frequencies $c_+^0 = \kappa_2/\Gamma_2$ and $c_-^0 = \kappa_1/\Gamma_1$. In the coupled case, $\nu_1\nu_2 \neq 0$, stable solutions with positive eigenvalues c_{\pm} exist for $\kappa_1\kappa_2 > (\Gamma_1\nu_1)(\Gamma_2\nu_2)$. For $\nu_1\nu_2 < 0$ a further condition $|\kappa_1/\Gamma_1 - \kappa_2/\Gamma_2| > 2\sqrt{|\nu_1\nu_2|}$ is necessary in order to ensure real values of c_{\pm} . For the original parameters, $\nu_1 = 1/\Gamma_0 > 0$ and the stability condition reads $\kappa_1\alpha > 0$.

In the long-time ('static') limit, we find from the exact solution (8)

$$\langle x_i x_j \rangle_{\infty} = \sum_{\alpha, \beta} \frac{2b_{i,\alpha} b_{j,\beta}}{c_{\alpha} + c_{\beta}} \left(\frac{T_1}{\Gamma_1} + a_{\alpha} a_{\beta} \frac{T_2}{\Gamma_2} \right) \quad (11)$$

In the uncoupled case, $\nu_1 = 0$, the equipartition theorem $\tilde{\kappa}_1 \langle x_1^2 \rangle_{\infty} = T_1$ is recovered. Here and in the following, $\tilde{\kappa}_1 = \kappa_{1,0}$ refers to the bare spring constant of the original model. If, however, one considers Eqs. (6) as starting point, $\tilde{\kappa}_1 = \kappa_1$ is interpreted as the bare spring constant. Note, that in terms of the original model parameters, the uncoupled case $\nu_1 = 0$ corresponds to $\Gamma_0, \alpha \rightarrow \infty$. In the general case $\nu_1 \neq 0$, one might assume that some generalization of the equipartition theorem holds,

$$T_{\text{static}} = \tilde{\kappa}_1 \langle x_1^2 \rangle_{\infty} \quad (12)$$

with an effective ('static') temperature T_{static} . Note, however, that such an effective temperature results from an underlying canonical distribution function only for the special choice $\Gamma_1\nu_1/T_1 = \Gamma_2\nu_2/T_2$, as was demonstrated in Sec. 3. For this choice of parameters, $T_{\text{static}} = T_{\text{slow}}$. For a general choice of parameters, T_{static} denotes the effective temperature deduced from the equipartition theorem if we would not be aware of the coupling of x_1 to x_2 . A comparison of these and other definitions of effective temperatures is provided later.

Next, we consider possible definitions of effective temperatures from time-dependent FDR. The response of the system (6) to a time-dependent perturbation $f(t)$ is measured by the response functions

$$R_{i,1}(t, t') \equiv \left. \frac{\delta \langle x_j(t) \rangle_f}{\delta f(t')} \right|_{f=0} \quad (13)$$

Due to the simplicity of the model, the response functions are also obtained analytically,

$$R_{i,1}(t, t') = \Gamma_1^{-1} \sum_{\alpha=+,-} b_{i,\alpha} e^{-(t-t')c_{\alpha}} \Theta(t-t') \quad (14)$$

where $\Theta(t)$ denotes the unit step function. The response functions are causal, $R(t, t') = 0$ for $t < t'$, and time-translational invariant, $R_{i,1}(t, t') = R_{i,1}(t-t')$, as they should. The correlation functions are defined by

$$C_{i,j}(t, t') \equiv \langle x_i(t) x_j(t') \rangle - \langle x_i(t) \rangle \langle x_j(t') \rangle \quad (15)$$

Inserting the exact solution, Eqs. (8), (9), into (15), one obtains

$$C_{i,j}(t, t') = \sum_{\alpha, \beta} \frac{2b_{i,\alpha} b_{j,\beta}}{c_{\alpha} + c_{\beta}} \left(\frac{T_1}{\Gamma_1} + a_{\alpha} a_{\beta} \frac{T_2}{\Gamma_2} \right) \left[e^{-(t-t')c_{\alpha}} - e^{-(t-t_0)c_{\alpha}} e^{-(t'-t_0)c_{\beta}} \right] \quad (16)$$

where $t > t'$ has been assumed without loss of generality. Again, due to time-translational invariance $C_{i,j}(t, t') = C_{i,j}(t - t')$ holds. For the special choice of parameters corresponding to the original model, Eqs. (14) and (16) are equivalent to the equations given in [18]. Note, that the long time limit of the equal time correlation function reduces to $\lim_{t \rightarrow \infty} C_{i,j}(t, t) = \langle x_i x_j \rangle_\infty$. From Eq. (16) we observe that the decay of the correlation function is determined by the two eigenvalues c_\pm . This can be interpreted as a two-step process, where the initial, fast decay is described by the larger eigenvalue c_- , while the smaller eigenvalue c_+ governs the long time decay. Such an interpretation is particularly relevant if the two eigenvalues are well-separated.

The fluctuation-dissipation relation (FDR) is most conveniently expressed in terms of the integrated response function, defined by $\chi_{i,j}(t) = \int_{-\infty}^t ds R_{i,j}(s)$. Integrating Eq. (14) over time differences one obtains

$$\chi_{i,1}(t) = \Gamma_1^{-1} \sum_{\alpha=+,-} \frac{b_{i,\alpha}}{c_\alpha} (1 - e^{-tc_\alpha}). \quad (17)$$

In equilibrium, one can prove under quite general assumptions the validity of the FDT,

$$\tilde{\chi}_{i,j}(t) = \frac{1}{T} [1 - \tilde{C}_{i,j}(t)] \quad (18)$$

where $\tilde{\chi}_{i,j}(t) \equiv \chi_{i,j}(t)/C_{i,j}(t=0)$ and $\tilde{C}_{i,j}(t) \equiv C_{i,j}(t)/C_{i,j}(t=0)$. In the present case, the FDT holds identically in the uncoupled case $\nu_1 = 0$. For $\nu_1 \neq 0$, however, the FDT is violated for the system studied here, as can be seen directly by comparing Eqs. (16) and (17). It was proposed in [1], that a meaningful effective temperature can be defined from the FDR by

$$-T_{\text{eff}}^{-1} = \frac{d\chi_{i,j}}{dC_{i,j}}. \quad (19)$$

For short times, the effective temperature defined from Eq. (19) coincides with T_1 , as is readily shown by expanding the exponentials in Eqs. (16) and (17) to first order in tc_α . For long times, the time dependence of both the correlation and response function is dominated by the smallest eigenvalue. In this regime, the effective temperature defined from Eq. (19) is given by

$$T_{\text{eff}}^{\text{long}} = \left(\frac{\kappa_1}{\Gamma_1} + \frac{\kappa_2}{\Gamma_2} \right)^{-1} \left(T_1 \left[c_+ + \frac{\kappa_2}{\Gamma_2} \right] + T_2 \frac{\Gamma_1 \nu_1}{\Gamma_2 \nu_2} \left[c_- - \frac{\kappa_2}{\Gamma_2} \right] \right) \quad (20)$$

Finally, we introduce also the effective temperature $T_\infty^{-1} = \chi_{1,1}(t \rightarrow \infty)/C_{1,1}(0)$, $C_{1,1}(0) = \langle x_1^2 \rangle_\infty$, introduced in [6]. This temperature, defined from the 'static' limit of the FDR, was found to be useful when the definition (20) was problematic [6]. From the long time limit of (17) we find

$$T_\infty = T_{\text{static}}(\kappa_1/\tilde{\kappa}_1) [1 - \Gamma_1 \Gamma_2 \nu_1 \nu_2 (\kappa_1 \kappa_2)^{-1}] \quad (21)$$

where T_{static} is the static, effective temperature defined in (12). Note, that T_∞ is well-defined since we assumed $\kappa_1 \kappa_2 > (\Gamma_1 \nu_1)(\Gamma_2 \nu_2)$ above. Within the original model, $T_\infty = T_{\text{static}}$ holds which is directly verified inserting the original model parameters.

Table 1 summarizes the different definitions of effective temperature considered here.

In Fig. 1, the integrated response $\chi_{1,1}(t)$ is plotted in a parametric plot, versus the correlation function $C_{1,1}(t)$. Parameters are chosen as $\gamma = \Gamma_0 = T_{\text{fast}} = 1$, $\kappa_{1,0} = T_{\text{slow}} = 2$. The values of α are varied between $1 \leq \alpha \leq 10$. From Fig. 1 one observes a cross-over from the short time regime with $T_{\text{eff}} = T_1$ to the long time regime with T_{eff} given by (20). This scenario has been found also for spin glass systems [1] and in molecular dynamics simulations of sheared model-glasses [4]. For increasing coefficients α or $\kappa_{1,0}$, T_{eff} increases and the cross-over is shifted to later times. For increasing γ , T_{eff} increases as well, however, the cross-over point is not shifted.

Table 1. Overview of different definitions of effective temperatures.

symbol	effective temperature from	defined in
T_{QEA}	quasi-equilibrium approximation	(7)
T_{static}	equipartition theorem	(12)
T_{eff}	FDR	(19)
$T_{\text{eff}}^{\text{long}}$	long-time limit of the FDR	(20)
T_{∞}	'static' limit of the FDR	(21)

The time evolution of the effective temperature (19) is shown in Fig. 2, where T_{eff} is calculated with the help of the time derivatives of Eqs. (16) and (17). Equilibrium initial conditions for the uncoupled system were chosen. Figure 2 shows the approach of the effective temperature to its long time asymptotic value (19). For the present choice of parameters, the asymptotic value is approached for times $t \gtrsim 1$, while T_{eff} remains close to the bath temperature T_1 for short times.

Figures 3, 4 show a comparison of different definitions of effective temperatures for several model parameters. We observe that for increasing α , or γ or $\kappa_{1,0}$, the static temperatures all approach the temperature T_{fast} of the fast bath, while the effective temperature from the long-time asymptotics of the FDR approaches the temperature T_{slow} of the slow bath. Only in case of very strong friction coefficient Γ_0 associated with the fast bath, does T_{eff} fail to approach T_{slow} .

5. Conclusion

The concept of effective temperatures has been studied within an exactly solvable model of non-Markovian dynamics for a harmonic oscillator coupled to two heat baths held at different temperatures. For parameter ranges ($\alpha \gg 1$, or $\gamma \gg 1$, or $\kappa_{1,0} \gg 1$) corresponding to a separation of time scales of the fast and slow bath, it has been found that the effective temperature $T_{\text{eff}}^{\text{long}}$ defined from the long-time limit of the fluctuation-dissipation relation (FDR) indeed approaches the temperature of the slow heat bath. This result is therefore consistent with the proposition [1] of $T_{\text{eff}}^{\text{long}}$ as a useful definition of effective temperatures out of equilibrium. For intermediate values of the parameters, when the separation of time scales is not achieved, the effective temperature $T_{\text{eff}}^{\text{long}}$ is intermediate between the temperature of the slow and fast heat bath. Only in the unlikely case of a friction coefficient Γ_0 associated with the fast bath, larger than the friction γ associated with the slow bath, $T_{\text{eff}}^{\text{long}}$ approaches the temperature of the fast bath, while the quasi-equilibrium temperature is somewhat higher.

In comparison, other, static effective temperature definitions yield results that are much more difficult to rationalize. In most cases, the temperature of the fast bath is obtained from these definitions. However, in some cases, values intermediate between T_{slow} and T_{fast} are obtained even when time scales are well separated (see e.g. figures 3 and 4, panels b and c, for T_{static} or T_{QEA}).

We finally mention that a breakdown of the effective temperature from the long-time limit of the FDR can be observed in the model (6) for particular choices of the parameters that are, however, inconsistent with the original model 5. For couplings $\nu_1 < 0$, $\nu_2 > 0$, $\Gamma_1 < \Gamma_2$ and $T_1 > T_2$, there are parameter ranges where an overshoot in the response function χ is observed together with a corresponding undershoot in the correlation function C . There, the parametric plot χ versus C continues to negative values of C and $\chi(C)$ becomes multi-valued. Approaching this regime, the plot χ versus C flattens more and more, which makes the application of (19) difficult. A similar situation was observed for some observables in molecular dynamics

simulations [6].

The present study confirms and extends previous results [23] that several, non-equivalent effective temperatures can be defined. In the model system considered here, which could be taken as a model for an internal degree of freedom in a slowly driven system, the definition that appears to have the most sensible behavior is associated with the long time limit of the fluctuation dissipation ratio.

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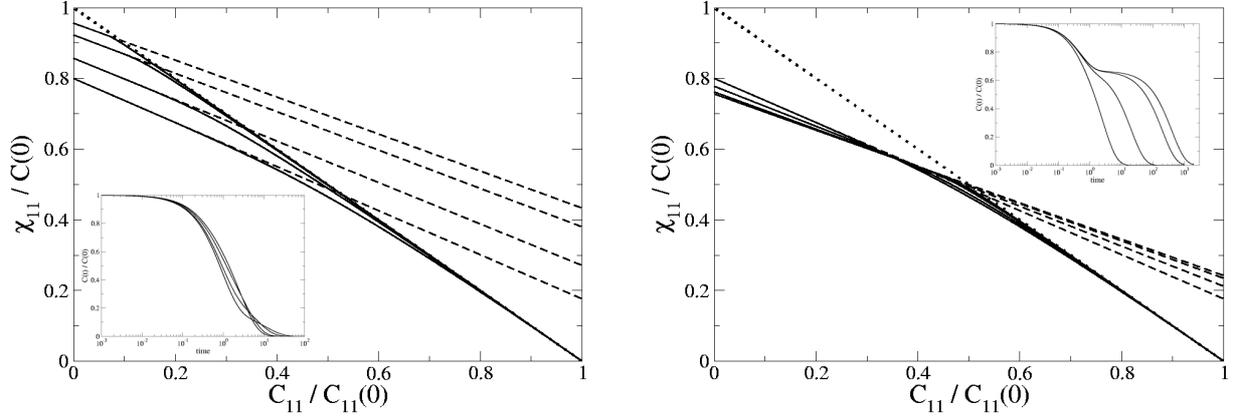


Figure 1. The integrated response function (17) is plotted versus the correlation function (16). Dashed lines have inverse slopes calculated from Eq. (20). The inset shows the time evolution of the normalized correlation function for the same parameters. The parameters have been chosen as $\alpha = \gamma = \Gamma_0 = \kappa_{1,0} = \kappa_2 = 1$, $T_{\text{fast}} = 1$, and $T_{\text{slow}} = 2$ if not stated otherwise. In the left figure, the values of α from bottom to top are $\alpha = 1, 2, 5, 10$, while γ varies from top to bottom on the far left of the right figure as $\gamma = 1, 2, 10, 100$.

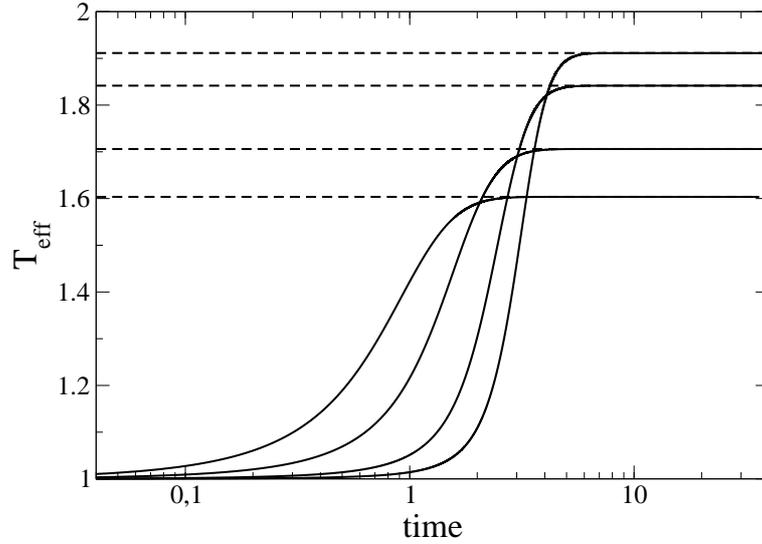


Figure 2. The time evolution of the effective temperature defined from the time-dependent FDR, Eq. (19), is shown on a logarithmic time scale. The same values of the parameters as in Fig. 1 (left panel) are used. Dashed lines are the long-time effective temperatures calculated from Eq. (20).

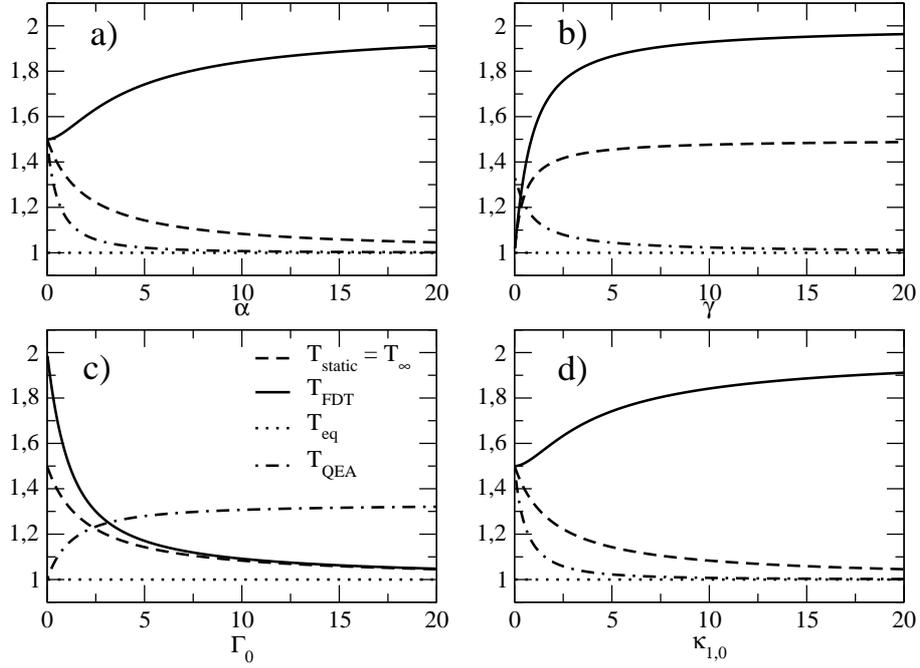


Figure 3. Different definitions of effective temperatures are shown as a function of model parameters α, γ, Γ_0 , and $\kappa_{1,0}$. The remaining parameters are chosen as in Fig. 1, with $\alpha = 1$ and $\gamma = 100$.

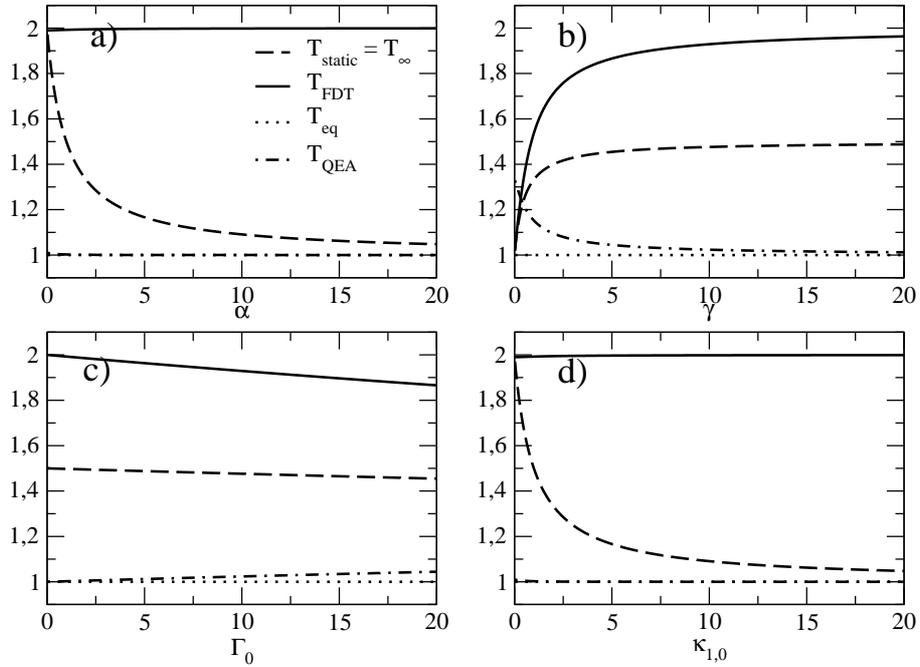


Figure 4. Different definitions of effective temperatures are shown as a function of model parameters α, γ, Γ_0 , and $\kappa_{1,0}$. The remaining parameters are chosen as in Fig. 1, with $\alpha = 1$ and $\gamma = 100$.