Fluctuation-dissipation relations for Markov processes

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(Received 5 April 2005; published 12 July 2005)

The fluctuation-dissipation relation is calculated for stochastic models obeying a master equation with continuous time. In the general case of a nonstationary process, there appears to be no simple relation between the response and the correlation. Also, if one considers stationary processes, the linear response cannot be expressed via time-derivatives of the correlation function alone. In this case, an additional function, which has rarely been discussed previously, is required. This so-called asymmetry depends on the two times also relevant for the response and the correlation and it vanishes under equilibrium conditions. The asymmetry can be expressed in terms of the propagators and the transition rates of the master equation but it is not related to any physical observable in an obvious way. It is found that the behavior of the asymmetry strongly depends on the nature of the dynamical variable considered in the calculation of the correlation and the response. If one is concerned with a variable which randomizes with any transition among the states of the system, the asymmetry vanishes in most cases. This is in contrast to the situation for other classes of variables. In particular, for trap models of glassy relaxation, the fluctuation-dissipation ratio strongly depends on the observable and the asymmetry plays a dominant role in the determination of this ratio also if only neutral variables are considered. Some implications of a nonvanishing asymmetry with regard to the definition of an effective temperature are discussed.

DOI: 10.1103/PhysRevE.72.011104 PACS number(s): 05.40.−a, 64.70.Pf, 61.20.Lc

I. INTRODUCTION

The out-of-equilibrium dynamics of stochastic models has gained intensive interest in the last decade. In particular, the deviations from the fluctuation dissipation theorem (FDT), relating the linear response to the two-time correlation function, have been investigated in great detail; for a recent review see [1]. In the past, much attention has been paid to study the behavior of the response and the correlation for models of glassy dynamics. While in equilibrium the FDT relates the response to the correlation in a unique way, this does not hold in out-of-equilibrium situations. The violations of the FDT usually are parameterized via the introduction of the so-called fluctuation-dissipation ratio (FDR) $X(t,t_w)$, which is defined via [1]

$$R(t,t_w) = \frac{X(t,t_w)}{T}\frac{\partial C(t,t_w)}{\partial t_w}. \tag{1}$$

Here, the correlation function of a dynamical quantity $M(t)$ is defined by $C(t,t_w)=\langle M(t)M(t_w)\rangle$ and the corresponding response to a field conjugate to $M(t)$ is $R(t,t_w)=\delta\langle M(t)\rangle/\delta H(t_w)|_{H=0}$ for $t\geq t_w$. In case that M is a so-called neutral variable [2], $X(t,t_w)$ is expected to be independent of M.

The FDR has been calculated for a variety of models and it has been found that in some cases $X(t,t_w)$ can be expressed as a function of the correlation alone, $X(t,t_w)=X(C)$. In this case, it is tempting to use $X(C)$ for the definition of an effective temperature $T_{\rm eff}$ characterizing the out-of-equilibrium state of the system [3]. Particularly, the long-time limit of X, X^∞, might be well suited for this purpose, as this has been found not to depend on the variable under consideration, provided a so-called fluctuation-dissipation (FD) plot, a plot of the integrated response versus the correlation, exists [2].

The FDR and the value of X^∞ has been calculated for different models with varying results. One class of models that has been considered is coarsening models [4], for which X^∞ is known to vanish [5]. Examples are the well-known spherical model [6,7] and the $O(N)$ model in the limit of large N [8], as well as the Ising models in one [9] or higher dimension [10]. For some discontinuous mean-field spin models a different behavior has been found [11]. In the context of glass-forming liquids, models which exhibit one-step replica symmetry breaking (1SB) are of particular interest. For these models, one finds $X(C)=1$ for short times, whereas $X(C)<1$ in the long-time sector, implying an effective temperature which is higher than the bath temperature. In addition to the analytical calculations, a number of molecular dynamics simulations have been performed on model glass-forming liquids; for a recent review see Ref. [12].

Some of the quoted models are soft-spin models and the stochastic dynamics is calculated from a Langevin equation. The classical treatment of FDT violations for stochastic models with Langevin dynamics has been given in Ref. [13], where various examples have been considered. In addition to models obeying a Langevin equation, the out-of-equilibrium dynamics of models with a dynamics determined by a master equation (ME) [14] have been investigated, in particular in the context of the aging dynamics in spin glasses. In this context also the function $A(t,t_w)$, which will be a central topic of the present paper, has been discussed [15,16]. Another simple model revealing glassy dynamics is Bouchauds trap model [17] and a number of investigations of the FDT violations have been presented [18–20].

In the present paper, I consider models for which the stochastic dynamics is described by a Markov processes with continuous time. Furthermore, I assume that the transition rates of the ME in the presence of a field are perturbed in a multiplicative manner [19]. In particular, it is not assumed that the transition rates obey the detailed balance condition. The behavior of the function $A(t,t_w)$ and its impliciations on the FDR will be discussed in detail for the trap model [17]. In order to explicitly calculate the response and the correlation, one has to assign values M_k to the states k. This can be done in a variety of different ways and I will consider two special choices. One class of variables randomizes completely with any transition among the states of the system. This type of variable is standard in the investigation of trap models. Another class of variables is chosen in such a way that there is no correlation to the transitions among the states at all. Even though in both cases the variables can be chosen as neutral, it will be shown that the behavior of all relevant dynamic quantities is quite different. In particular, the asymmetry vanishes for the first class of variables under very mild conditions whereas this is different for uncorrelated variables.

The outline of the paper is the following. In the next section the general formalism will be discussed and the FDR will be derived for arbitrary Markov processes with continuous time [21]. In addition, the choice of different dynamical variables is described. Section III is devoted to a detailed discussion of trap models. The trap model is chosen because one generally finds that $A(t,t_w)$ vanishes for these models [18–20]. Here, I will show that $A(t,t_w)=0$ holds only in the case of randomizing variables. Also the implications of a nonvanishing asymmetry on the FDR are discussed in detail. The paper closes with the conclusions in Sec. IV.

II. MASTER EQUATIONS AND FDT VIOLATIONS

A. General formalism

The time evolution of complex systems is often described in terms of Markov processes. Therefore in the present paper a stochastic dynamics according to a ME [14] is assumed. It should be pointed out that in the context of glassy systems one often is interested in a coarse grained description and that the coarse graining procedure may result in a nonstationary Markov process [1]. In order to keep the treatment as general as possible, in the following, I will treat the case of a nonstationary Markov process. The results obtained are then specialized to stationary processes in the next section.

In a discrete notation, let $G_{kl}(t,t_0)$ be the conditional probability to find the system in state k at time t provided it was in state l at time t_0 (Greens function). At this point it is not necessary to specify the meaning of the term "states" apart from the fact that it is the various realizations of the stochastic process under consideration. If continuous variables are considered, all sums in the following expressions are to be replaced by the corresponding integrals. Denoting the rates for a transition from state k to state l by $W_{lk}(t)[=W_{l\leftarrow k}(t)]$, the ME reads

$$\frac{\partial}{\partial t}G_{kl}(t,t_0) = -\sum_n W_{nk}(t)G_{kl}(t,t_0) + \sum_n W_{kn}(t)G_{nl}(t,t_0). \tag{2}$$

Only if the transition rates $W_{kl}(t)$ are time-independent the process considered is stationary. Note that the same ME is obeyed by the populations of state k, the one-time probabilities $p_k(t)$, $\dot{p}_k(t)=-\Sigma_n W_{nk}(t)p_k(t)+\Sigma_n W_{kn}(t)p_n(t)$. These populations are related to the $G_{kl}(t,t_0)$ via $p_k(t)=\Sigma_l G_{kl}(t,t_0)p_l(t_0)$. In addition to the ME, Eq. (2), one has the so-called "backwards equation," giving the propagation in the initial time [22]

$$\frac{\partial}{\partial t_0}G_{kl}(t,t_0) = \sum_n W_{nl}(t_0)[G_{kl}(t,t_0) - G_{kn}(t,t_0)]. \tag{3}$$

The $W_{kl}(t)$ can be related to the elements of the master-operator $\mathcal{W}(t)$ via [14]

$$\mathcal{W}(t)_{kl} = W_{kl}(t) - \delta_{kl}\sum_n W_{nl}(t). \tag{4}$$

Here $\mathcal{W}(t)_{kl}\geqslant 0$ holds for all $k\neq l$ and the sum rule

$$\sum_k \mathcal{W}(t)_{kl} = 0 \ \ \forall\, l \tag{5}$$

is fulfilled. The sum rule is a general property of the transition rates for any Markov process and it follows from the short-time behavior of $G_{kl}(t+\Delta t,t)=\delta_{kl}[1-\Sigma_n W_{nl}(t)\Delta t]+W_{kl}(t)\Delta t$ and $\Sigma_k G_{kl}(t+\Delta t,t)=1$. Equation (2) or (3) has to be solved with the initial condition $G_{kl}(t_0,t_0)=\delta_{kl}$, where δ_{kl} denotes the Kronecker symbol. In all calculations that follow it is assumed that the system is prepared in some initial state described by a fixed set of populations, $p_k^0=p_k(t=0)$ with $\Sigma_k p_k^0=1$. These populations evolve according to $p_k(t)=\Sigma_l G_{kl}(t,0)p_l^0$.

Central to the topic of the present paper is the two-time correlation function of a dynamic variable $M(t)$ of the system,

$$C(t,t_w) = \langle M(t)M(t_w)\rangle = \sum_{k,l} M_k M_l G_{kl}(t,t_w)p_l(t_w), \tag{6}$$

where M_k is the value of $M(t)$ in state k. In this expression, t_w denotes the time that has elapsed after the initial preparation of the system in the populations p_k^0. In the following $t\geqslant t_w$ will always be assumed. I only mention that cross-correlations can be treated in a similar way. If $\langle M(t)\rangle\neq 0$, it is advantageous to consider the connected correlation function $\hat{C}(t,t_w)=\langle M(t)M(t_w)\rangle-\langle M(t)\rangle\langle M(t_w)\rangle$.

In order to calculate the linear response of the system to a field conjugate to M applied at time t_w, $H(t)=H\delta(t-t_w)$,

$$R(t,t_w) = \left.\frac{\delta\langle M(t)\rangle}{\delta H(t_w)}\right|_{H=0}, \tag{7}$$

the dependence of the transition rates on the field H has to be fixed. In principle there is no restriction regarding this dependence. From equilibrium considerations one expects a Boltzmann-like dependence, $e^{\beta H M_k}$. This is because if the states k are determined by their energy E_k, one would expect a change according to $E_k\to(E_k-M_kH)$ [19]. However, these considerations are not sufficient to fix the dependence of the transition rates on the field. In the present paper, following Ritort [19], I choose the following form of multiplicatively perturbed transition rates:

$$W_{kl}^{(H)}(t) = W_{kl}(t)e^{\beta H X_{kl}} \quad \text{where } X_{kl} = \gamma M_k - \mu M_l. \tag{8}$$

Here, γ and μ are arbitrary parameters. The rates $W_{kl}^{(H)}(t)$ only fulfill detailed balance, if $\mu+\gamma=1$ holds. It has to be pointed out that other forms for $W_{kl}^{(H)}(t)$ than the one given in Eq. (8) might be appropriate in some cases. For the purpose of the calculation of the linear response any form of $W_{kl}^{(H)}(t)$ that can be expanded in linear order with respect to the field is acceptable.

The calculation of $R(t,t_w)$ is performed in the same way as it is usually done in linear response theory [23]. Time-dependent perturbation theory is used to calculate $G_{kl}^{(H)}(t,t_0)$ in linear order with respect to the field. The details of the calculation are presented in Appendix A. The response according to Eq. (7) follows from the difference $(\langle M(t)\rangle_H - \langle M(t)\rangle_0)$ in the limit of vanishing H. As detailed in Appendix A, the resulting expression for the response is given by a sum of two terms,

$$R(t,t_w) = R_\gamma(t,t_w) + R_\mu(t,t_w) \tag{9}$$

with

$$R_\gamma(t,t_w) = \beta\gamma \sum_{k,l,n} M_k M_l [G_{kl}(t,t_w) - G_{kn}(t,t_w)] W_{ln}(t_w) p_n(t_w),$$
$$R_\mu(t,t_w) = \beta\mu \sum_{k,l,n} M_k M_l [G_{kl}(t,t_w) - G_{kn}(t,t_w)] W_{nl}(t_w) p_l(t_w). \tag{10}$$

Next, one tries to relate the response to the time-derivatives $\partial_{t_w} C(t,t_w)$ and $\partial_t C(t,t_w)$ of the correlation function $C(t,t_w)$, Eq. (6). In the calculation of $\partial_{t_w} C(t,t_w) = \sum_{k,l} M_k M_l [\{\partial_{t_w} G_{kl}(t,t_w)\} p_l(t_w) + G_{kl}(t,t_w)\{\partial_{t_w} p_l(t_w)\}]$ one uses the backward equation, Eq. (3), for $\partial_{t_w} G_{kl}(t,t_w)$ and the ME, Eq. (2), for $\partial_{t_w} p_l(t_w)$. After a lengthy but straightforward calculation one finds that $R_\gamma(t,t_w)$ can be written in the form

$$R_\gamma(t,t_w) = \beta\gamma \left[\frac{\partial C(t,t_w)}{\partial t_w} - A_{\text{n.s.}}(t,t_w) \right], \tag{11}$$

where I defined the function

$$A_{\text{n.s.}}(t,t_w) = \sum_{k,l,n} M_k M_l G_{kn}(t,t_w) [W_{ln}(t_w) p_n(t_w) - W_{nl}(t_w) p_l(t_w)]. \tag{12}$$

This function also plays an important role in case of stationary Markov processes treated in the next section. Using the ME, Eq. (2), in the calculation of $\partial_t C(t,t_w) = \Sigma_{k,l} M_k M_l \{\partial_t G_{kl}(t,t_w)\} p_l(t_w)$ it becomes evident immediately that there is no relation to the response function in general. This is because in the expressions for the response given above, Eq. (10), only the transition rates evaluated at t_w, $W_{kl}(t_w)$, occur, whereas $\partial_t C(t,t_w)$ contains only terms involving $W_{kl}(t)$, cf. Eq. (2). It does not appear to be possible to relate $R_\mu(t,t_w)$ to a time-derivative of the correlation function in a way similar to Eq. (11). This means that there is no simple relation between the response and the correlation for nonstationary Markov processes. Instead one finds

$$R(t,t_w) = R_\mu(t,t_w) + \beta\gamma \left[\frac{\partial C(t,t_w)}{\partial t_w} - A_{\text{n.s.}}(t,t_w) \right]. \tag{13}$$

It is evident that one has to calculate the response and the correlation separately in order to determine the FDR. It should be mentioned that the FDR given in Eq. (13) cannot be compared directly to the corresponding expression given in Ref. [1] because there detailed balance has been assumed to hold also in the presence of the field. In addition, the expressions given in Ref. [1] have been derived using a discrete-time ME.

As a special case, consider a process which is such that equilibrium populations p_k^{eq} exist in the long-time limit and additionally detailed balance $W_{lk}(t_w) p_k^{eq} = W_{kl}(t_w) p_l^{eq}$ holds. In equilibrium (i.e., $t_w \to \infty$) one then finds from Eq. (13)

$$R(t,t_w) = \beta(\gamma + \mu) \partial_{t_w} C(t,t_w).$$

In order to show this, one uses $p_n(t_w \to \infty) = p_n^{eq}$ and $W_{ln}(t_w) p_n^{eq} = W_{nl}(t_w) p_l^{eq}$ in Eq. (10) for $R_\mu(t,t_w)$, which shows that $R_\mu(t,t_w) = R_\gamma(t,t_w)$ in this case. The same argument allows one to show that $A_{\text{n.s.}}(t,t_w)$ given in Eq. (12) vanishes in equilibrium.

Examples of nonstationary Markov-processes have been discussed in various fields of chemistry and physics, e.g., in the context of single molecule kinetics [24]. As a particularly simple example of a nonstationary process, in Appendix B, I consider a model for which the transition rates are chosen to be of the form $W_{kl}(t) = g(t) a_k$. In this case the ME can be solved analytically if all states $k = 1, 2, \ldots, N$ are connected with each other [25]. In this example one explicitly finds $R_\mu(t,t_w) = -\beta\mu [g(t_w)/g(t)] \partial_t C(t,t_w)$ demonstrating the importance of the inital time t_w. Thus even for this simple example $R_\mu(t,t_w)$ is not simply related to a time-derivative of the correlation. Only for long times one finds $R(t,t_w) = \beta(\gamma + \mu) \partial_{t_w} C(t,t_w)$ provided that $[g(t_w)/g(t)] \to 1$ in this case, cf. Appendix B.

B. Stationary Markov processes

For many models considered in the analytical treatment of glassy dynamics the corresponding stochastic processes are Markovian as well as stationary. For such processes the transition rates are independent of time, $W_{kl}(t) = W_{kl}$. The same holds for the transition rates in the presence of a field, cf. Eq. (8)

$$W_{kl}^{(H)} = W_{kl} e^{\beta H X_{kl}}; \quad X_{kl} = \gamma M_k - \mu M_l. \tag{14}$$

As a consequence of the time-independence of the W_{kl}, the Greens functions $G_{kl}(t_2,t_1)$ depend only on the difference of the times involved, $G_{kl}(t_2,t_1) = G_{kl}(t_2 - t_1)$.

All formulas of the last section hold also in this situation. A very important difference is that now there exists a simple relation between $R_\mu(t,t_w)$ and $\partial_t C(t,t_w)$, namely

$$R_\mu(t,t_w) = -\beta\mu \frac{\partial C(t,t_w)}{\partial t}. \tag{15}$$

In order to obtain this expression, one can use the fact that in case of a stationary Markov process the backwards equation, Eq. (3), can be cast into the form $\partial_\tau G_{kl}(\tau)=-\Sigma_n[G_{kl}(\tau)-G_{kn}(\tau)]W_{nl}$, which is an equation for the evolution in the second index of $G_{kl}(t)$ [22]. If this is used in the calculation of $\partial_t C(t,t_w)=\Sigma_{k,l}M_kM_l\{\partial_t G_{kl}(t-t_w)\}p_l(t_w)$, a comparison with the expression for $R_\mu(t,t_w)$ according to Eq. (10) with time-independent transition rates directly yields Eq. (15). The combination of the expressions (13) for stationary processes and Eq. (15) gives the FDR:

$$R(t,t_w)=\beta\left[\gamma\frac{\partial C(t,t_w)}{\partial t_w}-\mu\frac{\partial C(t,t_w)}{\partial t}-\gamma A(t,t_w)\right] \quad (16)$$

with

$$A(t,t_w)=\sum_{k,l,n}M_kM_lG_{kn}(t-t_w)[W_{ln}p_n(t_w)-W_{nl}p_l(t_w)]. \quad (17)$$

It is important to point out that Eq. (16) holds for arbitrary stationary Markov processes described by a continuous time ME. Additionally, the function $A(t,t_w)$ cannot be related to a time derivative of the correlation function and therefore the response is not determined by $C(t,t_w)$ alone in the general case. $A(t,t_w)$ plays a similar role as the asymmetry in the treatment of the response derived from a Langevin equation [13]. This is because the ME reduces to a Fokker-Planck equation in this case [26]. Therefore I will refer to $A(t,t_w)$ as asymmetry in the following. Of course, a relation between $R(t,t_w)$ and $\hat{C}(t,t_w)$ mentioned above is easily obtained from Eq. (16). If the system is prepared in an equilibrium state initially, $p_k^0=p_k^{eq}$, one has $p_l(t_w)=\Sigma_k G_{lk}(t_w)p_k^{eq}=p_l^{eq}$ and the detailed balance condition $W_{ln}p_n^{eq}=W_{nl}p_l^{eq}$ shows that $A_{eq}(t,t_w)\equiv 0$. Furthermore, the response and the correlation in this case are time-translational invariant, i.e., $C_{eq}(t,t_w)=C_{eq}(t-t_w)$ and $R_{eq}(t,t_w)=R_{eq}(t-t_w)$ and one thus finds

$$R_{eq}(t)=-\beta(\gamma+\mu)\frac{dC_{eq}(t)}{dt} \quad (18)$$

which for $\mu=1-\gamma$ is just the well-known FDT.

To the best of the authors knowledge, Eq. (16) has not been derived in this form before. However, equations similar to Eq. (16) have been given for various models in the literature. Hoffmann and Sibani [16] have derived Eq. (16) for the special case $\gamma=1$, $\mu=0$. Later on Bouchaud and Dean [18] gave a similar expression with, however, $A(t,t_w)=0$. Furthermore, Fielding and Sollich [2] derived Eq. (16) for the special case of $\gamma=0$, $\mu=1$. Additionally, it has recently been shown that in the special case of Ising spins the asymmetry can be expressed in the form of a special correlation function [27]. In that work also the choice for the transition rates in the presence of the field, Eq. (14), has been justified for $\gamma=\mu=1/2$.

As noted by Hoffmann and Sibani, $A(t,t_w)$ vanishes if the relaxation to equilibrium is determined by distribution functions that are equilibrated with respect to the states k and depend on time only parametrically. In order to see this explicitly let us assume that the initial conditions are such that one can write $p_k(t_w)=p_k^{eq}\delta_k(t_w)$ with unspecified functions $\delta_k(t_w)$. In this case Eq. (17) reads as

$$A(t,t_w)=\sum_{k,l,n}M_kM_lG_{kn}(t-t_w)W_{nl}p_l^{eq}[\delta_n(t_w)-\delta_l(t_w)],$$

which shows that $A(t,t_w)$ vanishes if $\delta_k(t_w)=\delta(t_w)\ \forall k$. Such a situation may be expected if the populations obey some scaling relations.

If Eq. (16) is compared to the more general relation for a nonstationary Markov process according to Eq. (13), one can see that formally the results are similar only in the special case $\mu=0$, i.e., if the field-dependence of the transition rates regarding the initial state of a transition vanishes.

Another remark concerns the transition rates in the presence of a field, $W_{kl}^{(H)}$, according to Eq. (14). As already mentioned in the previous section, these transition rates do not fulfill a detailed balance if $\mu\neq 1-\gamma$. This also holds if the unperturbed W_{kl} do obey the detailed balance condition $W_{kl}p_l^{(eq)}=W_{lk}p_k^{(eq)}$. Equation (14) with $\mu=1-\gamma$ has, for instance, been used by Bouchaud and Dean [18] in a study of the aging properties of the trap model [17]. Even though γ also in the case $\mu=1-\gamma$ in principle can take on any value, there often will be some guiding principle. For example, if the states k denote the energies in a canonical ensemble, one expects that γ can be determined from the dependence of the unperturbed W_{kl} on k and l. If, on the other hand, the W_{kl} are of a form allowing a Kramers-Moyal expansion [26], and therefore the ME has a well-defined Fokker-Planck equation as a limit, one would naturally choose $\gamma=\mu=1/2$.

However, it has to be pointed out that usually the states k are understood as metastable states or components [28] in connection with glassy systems. Then the corresponding free energies are to be viewed as coarse-grained quantities [1] and one does no longer have a strict relation of γ to the unperturbed W_{kl} and also the choice $\mu=1-\gamma$ is not guided by some underlying general principle. Furthermore, if the unperturbed transition rates do not fulfill detailed balance, one cannot even expect that the perturbed transition rates will. In addition, it has to be pointed out that the choice made for the perturbed transition rates in Eq. (14) itself is not the only possible one. In the linear regime, however, one expects the perturbed transition rates to depend on the unperturbed ones multiplied by the field amplitude H [27].

C. Choice of variables

Usually the dynamical quantity $M(t)$ is interpreted as some (generalized) magnetization in the context of the dynamics of glassy systems. In order to perform explicit calculations for some model one has to specify the definition of the $M(t)$ and their coupling to the dynamics. In the usual treatment of magnetic models one assumes that a "magnetization" M_k is assigned to the state k [2,16]. In practice one has to choose the dependence of the transition rates on the values of the M_k, i.e., one has to consider composite transition rates $W_{kl}(M_k|M_l)$ instead of the W_{kl}. In particular, one has to specify what happens to $M_l(t)$ in case of a $l\rightarrow k$ transition. In the following, I will consider two different classes of variables, defined by their coupling to the dynamics.

1. Uncorrelated variables

With this term I mean variables which are completely decoupled from the transitions among the various states k. This choice has, for example, been made by Koper and Hilhorst [29] in their treatment of the kinetic random energy model. For the composite transition rates $W_{kl}(M_k|M_l)$ this simply means that they are independent of the values of M_l and M_k in the initial and the destination state of the transition:

$$W_{kl}(M_k|M_l) = W_{kl}. \tag{19}$$

In order to calculate the correlation, the response, and the asymmetry according to Eqs. (6), (16), and (17), one has to replace W_{kl} in the expressions by $W_{kl}(M_k|M_l)$, use Eq. (19) and then average over the distribution of the M_k, to be denoted by $\sigma_k(M_k)$.

In calculating the averages some care has to be taken in performing multiple summations. For instance, in an abbreviated form one has

$$C(t,t_w) = \sum\nolimits_{k,l} \int dM_k \int dM_l \sigma_k(M_k)\sigma_l(M_l)M_kM_lC_{k,l}.$$

In such an expression, one has to treat the terms $k=l$ and $k \neq l$ separately and then perform the integrations. This way one finds

$$C(t,t_w) = \sum_k \langle \Delta M_k^2\rangle G_{kk}(t-t_w)p_k(t_w) + \sum_{k,l} \langle M_k\rangle\langle M_l\rangle G_{kl}(t-t_w)p_l(t_w) \tag{20}$$

with the moments $\langle M_k^n\rangle = \int dM_k\sigma_k(M_k)M_k^n$ and the variance $\langle \Delta M_k^2\rangle = \langle (M_k - \langle M_k\rangle)^2\rangle$. For the asymmetry $A(t,t_w)$ one finds

$$A(t,t_w) = \sum_{k,l} \langle \Delta M_k^2\rangle G_{kl}(t-t_w)[W_{kl}p_l(t_w) - W_{lk}p_k(t_w)] + \sum_{k,l,n} \langle M_k\rangle\langle M_l\rangle G_{kn}(t-t_w)[W_{ln}p_n(t_w) - W_{nl}p_l(t_w)]. \tag{21}$$

If even distribution functions, $\sigma_k(M_k)=\sigma_k(-M_k)$, for which $\langle M_k\rangle=0$ are chosen, the second term in the above expression for the correlation function vanishes and the same holds for the second term in Eq. (21). Note that the asymmetry $A(t,t_w)$ does not vanish for this choice of variables that are uncorrelated from the dynamics of the states k.

2. Randomizing variables

In contrast to the above choice, I now consider a class of variables that randomize completely whenever a $l \to k$ transition takes place. This means that after such a transition the value of M is drawn randomly from the distribution $\sigma_k(M_k)$, where k denotes the destination state of the transition. This scenario is realized if one chooses the composite transition rates according to

$$W_{kl}(M_k|M_l) = \sigma_k(M_k)W_{kl}. \tag{22}$$

Using the ME and this choice for the transition rates it can be shown that the solution for the conditional probability $G_{kl}(M_k,t|M_l)$ can be expressed in terms of the M-independent $G_{kl}(t)$ via

$$G_{kl}(M_k,t|M_l) = \delta_{kl}\delta_{M_k,M_l}e^{-\kappa_k t} + \sigma_k(M_k)[G_{kl}(t) - \delta_{kl}e^{-\kappa_k t}]. \tag{23}$$

Here, I used the abbreviation $\kappa_k = \sum_{l\neq k}\kappa_{lk}$ for the inverse lifetime of state k. Using Eq. (23), one finds the following expression for the correlation:

$$\Pi(t,t_w) = \sum_k \langle \Delta M_k^2\rangle e^{-\kappa_k(t-t_w)}p_k(t_w) + \sum_{k,l} \langle M_k\rangle\langle M_l\rangle G_{kl}(t-t_w)p_l(t_w), \tag{24}$$

which has been denoted by $\Pi(t,t_w)$ because for symmetric distributions $\sigma_k(M_k)=\sigma_k(-M_k)$ this coincides with the probability that the process has not jumped at all during the time-interval $(t-t_w)$, and this is exactly the function that usually is considered in the treatment of trap models [30]. In that case, $\Pi(t,t_w)$ can be considered as an intermediate scattering function in the limit of large scattering vectors. In the context of molecular rotations this has been termed a random jump correlation function [31,32].

The asymmetry is found to be given by

$$A_{\rm rand}(t,t_w) = \sum_{k,l,n} \langle M_k\rangle\langle M_l\rangle G_{kn}(t-t_w)[W_{ln}p_n(t_w) - W_{nl}p_l(t_w)] \tag{25}$$

from which it is evident that the asymmetry vanishes in the case of symmetric distributions $\sigma_k(M_k)=\sigma_k(-M_k)$.

In the usual treatment of trap models, it is assumed that the value of M_k is independent on the state k,

$$\langle M_k^n\rangle = \langle M^n\rangle. \tag{26}$$

This choice yields for the correlation

$$\Pi(t,t_w) = \langle M\rangle^2 + \langle \Delta M^2\rangle \sum_k e^{-\kappa_k(t-t_w)}p_k(t_w) \tag{27}$$

and for the asymmetry

$$A_{\rm rand}(t,t_w) = 0. \tag{28}$$

The last fact naturally explains why the asymmetry up to now has not been considered in the context of trap models. It should be noted that an explicit variable-dependence of the FDT and its implications for the definition of an effective temperature has been investigated by Fielding and Sollich [2]. These authors, however, chose $\gamma=0$ in their calculations and therefore the asymmetry did not appear and they obtained Eq. (16) with $\gamma=0$ in their derivation.

A remark concerning neutrality of the variables considered is in order. For both cases, randomizing and uncorrelated variables, one obtains so-called neutral variables if one assumes that M_k is independent of k and that the distribution $\sigma(M)$ is symmetric, $\sigma(M)=\sigma(-M)$ [19]. The actual calculations performed in the following are based on these assumptions.

III. TRAP MODELS

As already mentioned above, Bouchaud and Dean [18] derived Eq. (16) for a trap model, although with $A(t,t_w)=0$. This becomes clear from the fact that in the usual treatment of trap models variables are used, which I have termed as randomizing. Then for symmetric distributions $\sigma_k(M_k)=\sigma_k(-M_k)$, the asymmetry vanishes. Such distributions have been considered also by Monthus and Bouchaud (MB) [30] in their analytical treatment. Fielding and Sollich, on the other hand, considered the variable-dependence of the FDR in trap models [23] and therefore did not assume a definite form of the distribution from the outset. However, in their investigation they calculated the linear response solely for $\mu=1$ and $\gamma=0$, as already noted in Sec. II. Later on, Sollich [20] and Ritort [19] treated the FDR in trap models quite generally. Again, both authors considered randomizing variables only. Their treatments were aimed at discussing analogies and differences between the MB model [30] and the entropic Barrat-Mezard model [34].

In the present paper, I will consider the MB model and compare results for a randomizing and uncorrelated variable. In the discrete formulation of the preceding chapters, the transition rates for this model read

$$W_{kl} = \rho_k \kappa_l \text{ with } \rho_k = \beta_0 e^{-\beta_0 \epsilon_k} \text{ and } \kappa_l = \kappa_\infty e^{-\beta \epsilon_l} \tag{29}$$

with $\beta_0=T_0^{-1}$ the inverse of the transition temperature and κ_∞ a constant to be set to unity in the following. The lack of a stable equilibrium population below the transition is expressed by the fact that the quantity $Z=\Sigma_n(\rho_n/\kappa_n)$ diverges. As in the preceding section, the system is assumed to be quenched from infinite temperature to $T<T_0$ in the beginning of the experimental protocol. In the present treatment for simplicity only symmetric distributions $\sigma_k(M_k)=\sigma_k(-M_k)$ will be used, although this restriction is by no means necessary. Additionally, I will not consider a dependence of the variables M on the energies and only the case $M_k=M$ will be considered with zero mean and unit variance, $\langle M\rangle=0$, $\langle M^2\rangle=1$. In this case the general expressions given above simplify somewhat. The numerical approach used to solve the ME is outlined in Appendix C.

Before discussing the case of uncorrelated variables, I will briefly recall the known results for randomizing variables [19,20].

A. Randomizing variables

For the case considered here, the correlation function, Eq. (27), reads as

$$\Pi(t,t_w) = \sum_k e^{-\kappa_k(t-t_w)} p_k(t_w) \tag{30}$$

and the response is given by $R(t,t_w)=\beta[\gamma\partial_{t_w}\Pi(t,t_w)-\mu\partial_t\Pi(t,t_w)]$, cf. Eqs. (16) and (28). This is identical to the expression given by Ritort [19]. For long times, the correlation function obeys the scaling relations [30]

$$\Pi(t_w + t, t_w) \simeq p(x)(t/t_w)^{-x} \text{ with } x = T/T_0 < 1, \tag{31}$$

with the amplitude $p(x)=\sin(\pi x)/(\pi x)$. This scaling is found to be obeyed with an excellent accuracy from numerical calculations. Fits of $\Pi(t_w+t,t_w)$ to $p(x)(t/t_w)^{-\lambda_\Pi}$ in the scaling region (roughly $t\geq 10^2$) yield $\lambda_\Pi=x$ with an error of the order of $10^{-2}\%$ and $p(x)\simeq \mathrm{sync}(\pi x)$ with slight deviations for higher temperatures (on the order of 10% for $x=0.85$).

If the FDR, $X(t,t_w)$, according to Eq. (1) is considered, one finds in the scaling regime, cf. Ref. [19],

$$X(t,t_w) \simeq \gamma + \mu(t_w/t) \tag{32}$$

the long-time limit of which is given by $X^\infty=\gamma$. The FDR and its implications for the shape of FD plots have been discussed in detail by Ritort, to which I refer here [19]. In particular, only for $\mu=0$ one finds a unique slope in the FD plot, reminiscent of 1SB behavior. For $\gamma=0$, the slope of the integrated response in such a plot changes continuously until for small correlation it vanishes [20].

B. Uncorrelated variables

Now I consider the case of variables that are uncorrelated from the dynamics of the traps. For symmetric distributions $\sigma_k(M_k)$ and ϵ_k-independent values of the variables $M_k=M$, the correlation depends on $G_{kk}(t)$, the probability of finding the system in state k at t provided it was in this state at $t=0$. According to Eq. (C8), this probability can be written as $G_{kk}(t)=e^{-\kappa_k t}+\kappa_k\int_0^t d\tau e^{-\kappa_k(t-\tau)}p_k(\tau)$. The first term gives the probability that no jump has taken place in the time t. The second term accounts for all jumps that have taken place out of state k at a time $\tau\leq t$ and the process then started anew. Using Eq. (20), the correlation function $C(t,t_w)$ reads

$$C(t,t_w) = \sum_k G_{kk}(t-t_w)p_k(t_w) = \Pi(t,t_w) + \Delta C(t,t_w) \tag{33}$$

where $\Pi(t,t_w)$ is given in Eq. (30) and the second term

$$\Delta C(t,t_w) = \sum_k \kappa_k \int_0^{(t-t_w)} d\tau e^{-\kappa_k(t-t_w-\tau)} p_k(\tau)p_k(t_w) \tag{34}$$

stems from the second term in the expression for $G_{kk}(t)$, as discussed above. Accordingly, Eq. (33) can be interpreted as follows. The Greens function $G_{kk}(t-t_w)$ gives the probability to find the system in the same trap at times t_w and $(t-t_w)$. While Π gives the probability that no transition has taken place during the interval $(t-t_w)$, $\Delta C(t,t_w)$ is a measure of the probability that a back-jump to the original trap has taken place during $(t-t_w)$. This means that the system was in trap k at t_w, has jumped out of that trap, and still is found in the same trap at (t_w+t). Therefore it will be denoted as back-jump probability in the following. This term has been neglected in a previous study of the aging phenomena in the random energy model [33], which, however, is not justified, as will soon become clear.

In Fig. 1(a), I show two examples of $C(t_w+t,t_w)$ for various t_w and $x=0.6$ (upper panel) and $x=0.3$ (lower panel). The curves for different t_w are undistinguishable for $t_w\geq 10^2$, meaning that a (t/t_w) scaling is perfectly obeyed. The slopes of the scaling functions, however, are different. Whereas C follows a $(t/t_w)^{x-1}$ scaling for $x=0.6$, this changes to $(t/t_w)^{-x}$ for $x=0.3$ (dotted lines). It should be kept in mind that Π

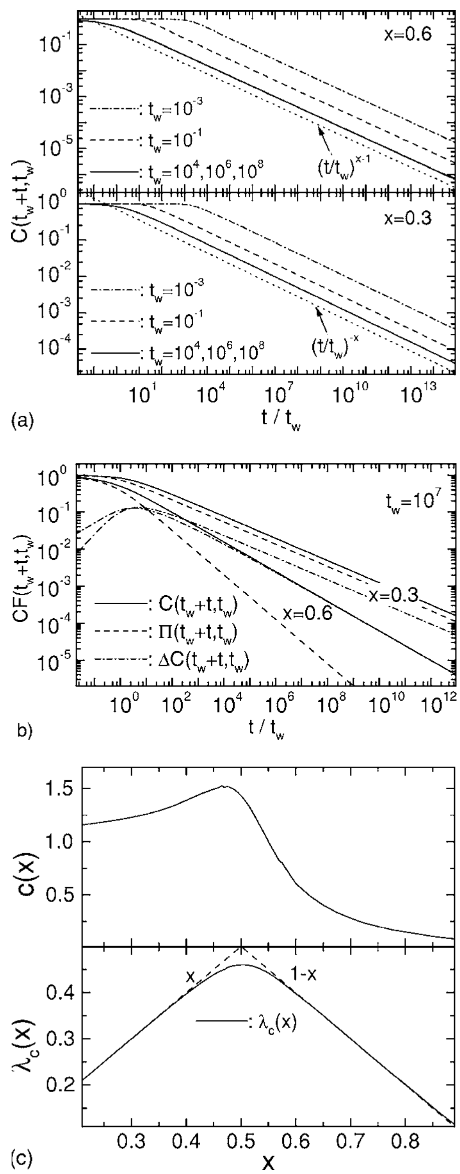

FIG. 1. (a) $C(t_w+t,t_w)$ vs (t/t_w), for $x=0.6$ (upper panel) and $x=0.3$ (lower panel) for various waiting times t_w for the MB model with an uncorrelated variable. Additionally shown as dotted lines are the scaling forms for both temperatures. (b) $C(t_w+t,t_w)$, $\Pi(tw+t,tw)$, and $\Delta C(t_w+t,t_w)$ vs (t/t_w), for $x=0.6$ and $x=0.3$ for the MB model with an uncorrelated variable for $t_w=10^7$. (c) Fitting parameters $c(x)$ and $\lambda_c(x)$ vs temperature x obtained from least-squares fits to Eq. (35).

scales like $(t/t_w)^{-x}$ in the whole low-temperature phase of the model. In order to see why the scaling of C is different, Fig. 1(b) shows plots of C, Π, and ΔC for $x=0.6$ and $x=0.3$. For $x=0.3$ the slope of all quantities is the same. This is quite different for $x>1/2$, as can be seen from the shown example for $x=0.6$. Here, $\Delta C\sim(t/t_w)^{x-1}$ while $\Pi\sim(t/t_w)^{-x}$. Thus at long times C is dominated by ΔC in this case. This can be understood as follows. For $x>1/2$, frequent jumps take place because many barriers can be overcome thermally. Therefore Π decays quickly. For the same reason the back-jump probability is quite large and ΔC dominates the correlation function. Also the short-time behavior of ΔC is easily understood from the above considerations. At short times, no back-jumps to the starting trap have yet taken place and therefore ΔC vanishes. It only starts from zero in a linear way with a slope given by $\Sigma_k\kappa_k\rho_k p_k(t_w)$, as can be shown from Eq. (34).

In a next step, I have calculated $C(t_w+t,t_w)$ for various temperatures in the scaling regime (typically, $t_w=10^5$ and 10^7) and fitted the results to a power-law, $C(t_w+t,t_w)=c(x)\times(t/t_w)^{-\lambda_c(x)}$ for $t\geq 10^3$. The fitting parameters $c(x)$ and $\lambda_c(x)$ were averaged afterwards. The absolute errors of the fits were smaller than $10^{-3}\%$ in all cases. The results of this procedure are shown in Fig. 1(c) and can be summarized as

$$C(t_w+t,t_w)=c(x)(t/t_w)^{-\lambda_c(x)} \text{ with } \lambda_c(x)\simeq\begin{cases}1-x & \text{for } x>1/2,\\ x & \text{for } x<1/2.\end{cases} \quad (35)$$

It is obvious from Fig. 1(c) that this equation holds with high accuracy for $x>0.6$ and $x<0.4$. Therefore, for $x>1/2$, the scaling behavior of the correlation of an uncorrelated variable is quite different from that of a randomizing variable, while for $x<1/2$ the qualitative behavior is similar [correlation $\sim(t/t_w)^{-x}$].

An important difference to the case of a randomizing variable is the fact that the asymmetry does not vanish if an uncorrelated variable is considered. Instead, it is explicitly given by, cf. Eq. (21),

$$A(t,t_w)=\sum_{k,l}G_{kl}(t)[\rho_k\kappa_l p_l(t_w)-\rho_l\kappa_k p_k(t_w)]. \quad (36)$$

In the calculation of A only the off-diagonal term in the expression for $G_{kl}(t)$ is relevant, since the "diagonal" term with $k=l$ in Eq. (36) vanishes. As a technical aside I mention that in the actual numerical calculation, both expressions for $G_{kl}(t)$, Eq. (C8) as well as Eq. (C9), have been compared to the direct integration technique and all three methods yield identical results. In Fig. 2(a) $A(t_w+t,t_w)$ is shown for $x=0.6$ and several values of the waiting time t_w. In the upper panel a linear scale is chosen in order to show that the sign of A changes as a function of time for t_w roughly larger than 10^2. The lower panel shows A on a logarithmic scale. For short t_w it is seen that $A\sim(t/t_w)$ for short times and that there is a scaling regime in the long-time limit, $(t/t_w)>10^2$, where the asymmetry behaves as $A\sim t_w^{-1}(t/t_w)^{x-1}$. For long times, scaling plots for the asymmetry can be obtained from either scaling A to its maximum value $A_{\max}$ or from considering A/t_w. The latter way will be used in the following. For $(t/t_w)>10^3$, I have fitted the asymmetry to a power-law ($t_w=10^8$) with the results

$$A(t_w+t,t_w)=a(x)t_w^{-1}(t/t_w)^{-\lambda_A(x)} \text{ with } \lambda_A(x)\simeq\begin{cases}1-x & \text{for } x>1/2,\\ x & \text{for } x<1/2,\end{cases} \quad (37)$$

cf. Fig. 2(b). As for $C(t_w+t,t_w)$, a crossover in the exponent from $\lambda_A(x)\simeq(1-x)$ to $\lambda_A(x)\simeq x$ near $x=1/2$ is found.

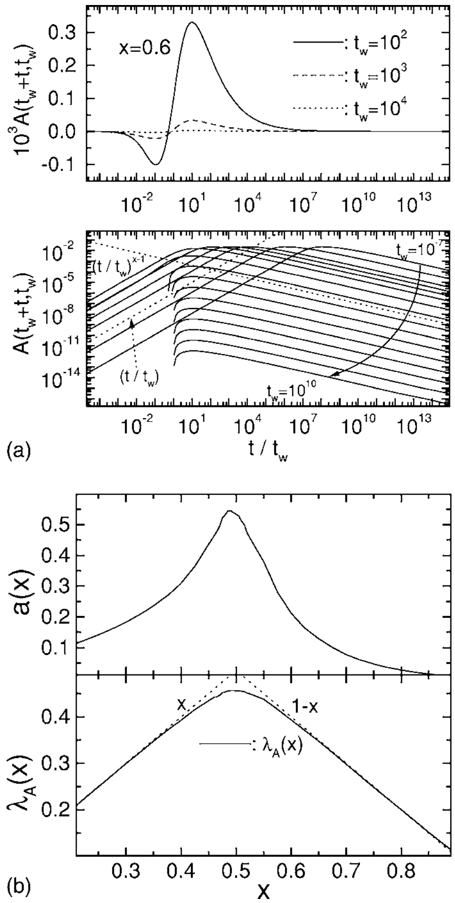

FIG. 2. (a) The asymmetry $A(t_w+t,t_w)$ vs (t/t_w), for $x=0.6$ for various waiting times t_w for the MB model with an uncorrelated variable. Upper panel: linear scale, lower panel: logarithmic scale. In the lower panel the dotted lines are proportional to (t/t_w) and $(t/t_w)^{x-1}$. (b) Fitting parameters $a(x)$ and $\lambda_A(x)$ vs temperature x obtained from least-squares fits to Eq. (37).

The additional diminishing of $A \propto t_w^{-1}$ can be understood qualitatively from the following argument. As stated in Sec. II, the asymmetry vanishes for populations that are equilibrated with respect to the states k and only parametrically depend on time. For the MB model, the populations obey the scaling form $p_k(t) \simeq t^{x-1}(\rho_k/\kappa_k)$ for long times [2]. If this expression is used in Eq. (36), one finds that A vanishes. However, for larger ϵ_k it takes a longer time until $p_k(t)$ follows the scaling-law, as can be seen from Fig. 3. In that figure, I have plotted $(\kappa_k/\rho_k)p_k(t)$ versus time for $x=0.3$ (upper panel) and $x=0.6$ (lower panel) for different ϵ_k. It is obvious that the t^{x-1} scaling is followed only for times much longer than the lifetime of trap k, $t \gg (1/\kappa_k)$. This means that with increasing t_w the fraction of the populations in the scaling regime increases and therefore A diminishes. However, even for very long t_w, A still remains finite, a fact that will prove to be very important for the FDR. This also means that the assumption of a vanishing asymmetry is not justified in the present case.

Next, I will consider the FDR, which always can be decomposed into two separate contributions, cf. Eqs. (1) and (16),

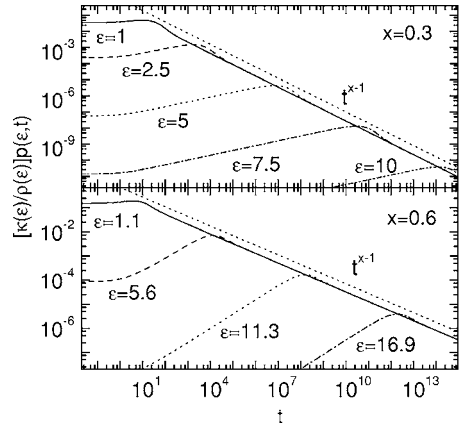

FIG. 3. The reduced populations $[\kappa(\epsilon)/\rho(\epsilon)]p(\epsilon,t)$ vs time for some values of the energy-variable ϵ for the MB model. Upper panel: $x=0.3$, lower panel: $x=0.6$. For comparison the scaling behavior t^{x-1} is shown additionally. For larger ϵ it takes a longer time to reach the scaling regime.

$$X(t,t_w) = X_\gamma(t,t_w) + X_\mu(t,t_w) \tag{38}$$

with obvious definitions of the summands. Therefore the two functions can be discussed seperately. For a discussion of the FDR, the scaling behavior of the time-derivatives of the correlation are needed in addition to those of the correlation and the asymmetry.

Using the scaling-law for the correlation, Eq. (35), and $\partial_t C(t,t_w) = -(t_w/t)\partial_{t_w} C(t,t_w)$ [19], one finds for X_μ:

$$X_\mu(t,t_w) = -\mu \frac{\partial_t C(t,t_w)}{\partial_{t_w} C(t,t_w)} \simeq \mu\left(\frac{t_w}{t}\right). \tag{39}$$

This behavior is identical to the case of randomizing variables and X_μ tends to zero for long times.

For X_γ, on the other hand, from the general expression

$$X_\gamma(t,t_w) = \gamma\left[1 - \frac{A(t,t_w)}{\partial_{t_w} C(t,t_w)}\right] \tag{40}$$

and the scaling of A and $\partial_{t_w} C(t,t_w)$ *one would assume* $X_\gamma(t,t_w)$ in the scaling regime to be given by

$$X_\gamma(t,t_w)_{\text{expected}} \simeq \gamma\left[1 - \frac{a(x)}{\lambda_c(x)c(x)}\left(\frac{t-t_w}{t}\right)\right] \tag{41}$$

with the long-time limit $X_\gamma^\infty(x) = \gamma(1-[a(x)/\lambda_c(x)c(x)])$. This expectation is, however, *not* found numerically.

In Fig. 4(a) the results of calculations of X_γ and X_μ according to Eqs. (39) and (40) are shown for a long waiting time $t_w=10^8$ and several temperatures. For X_μ only a single curve (dashed line) for $x=0.2$ is shown because it is temperature-independent. The dotted line shows the (t_w/t) behavior. For X_γ, the lines are for $x=0.8, 0.6$ (full lines) and $x=0.4, 0.2$ (dotted-dashed lines) from bottom to top. It is evident that only for $x=0.2$ and 0.4 there is a finite long-time limit, $X_\gamma^\infty \neq 0$, which is reached for approximately $(t/t_w) \geq 10^3$. For $x > 1/2$, the long-time limit vanishes. The dotted lines have slopes $(t/t_w)^{-(2x-1)}$. Thus only for $x < 1/2$, the expected behavior according to Eq. (41) is found. The inset

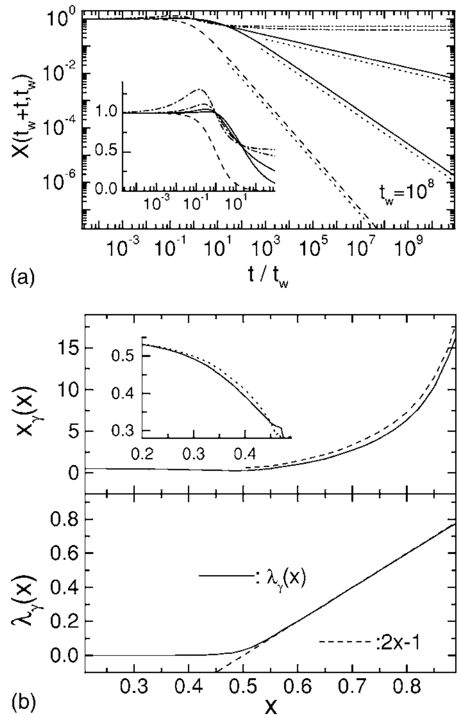

FIG. 4. (a) $X_\gamma(t_w+t,t_w)$ and $X_\mu(t_w+t,t_w)$ vs (t/t_w) for $t_w=10^8$ and several temperatures x. Dashed line: X_μ for $x=0.2$. X_μ is temperature-independent. Full lines: X_γ for $x=0.8$ (lower line) and 0.6 (upper line). Dotted-dashed lines: X_γ for $x=0.4$ (lower line) and 0.2 (upper line). The dotted lines have slopes -1, -0.6, and -0.2 from bottom to top. Inset: The short-time behavior of the same curves on a linear scale. (b) Fitting parameters $x_\gamma(x)$ and $\lambda_\gamma(x)$ vs temperature x obtained from least-squares fits to Eq. (42). Additionally shown in the upper panel is $[xp(x)/a(x)]$ for $x>1/2$ as the dashed line. The inset shows $x_\gamma(x)$ (full line) and $\{1-a(x)/[xc(x)]\}$ (dotted line) for $x<1/2$.

shows the short-time behavior on a linear scale. It is evident that both X_μ and X_γ start from unity for short times, i.e.,

$$X(t_w+t,t_w)=\gamma+\mu \text{ for } t \ll t_w$$

which is the same behavior as for randomizing variables. This is because in this limit both A and ΔC vanish. Also the fact that X_γ exceeds unity in some time regime is easily understood because the asymmetry A becomes negative for short times, cf. Fig. 2(a). For X_γ, one finds a power-law behavior according to $X_\gamma(t_w+t,t_w)=\gamma x_\gamma(x)(t/t_w)^{-\lambda_\gamma(x)}$ in the scaling regime ($t_w \gg 10^4$). Fitting the data to such a law yields the following result:

$$X_\gamma(t_w+t,t_w)=\gamma x_\gamma(x)(t/t_w)^{-\lambda_\gamma(x)} \text{ with}$$
$$\lambda_\gamma(x)\simeq\begin{cases}2x-1 & \text{for } x>1/2,\\ 0 & \text{for } x<1/2.\end{cases} \qquad (42)$$

The fitting parameters $x_\gamma(x)$ and $\lambda_\gamma(x)$ are plotted in Fig. 4(b) as a function of temperature, x. It is obvious that the above relations for $\lambda_\gamma(x)$ are perfectly obeyed apart from some small temperature range around $x=1/2$. Thus, only for $x<1/2$, the expected behavior according to Eq. (41) is found numerically. In Fig. 4(b), I have additionally plotted $[1-a(x)/(xc(x))]$ as the dotted line for $x<1/2$ in the inset in the upper panel. The deviations to $x_\gamma(x)$ are less than 10% for $x<0.45$.

In order to understand the discrepancy between the behavior naively expected, Eq. (41), and the one found numerically, Eq. (42), for $x>1/2$ one has to take a somewhat closer look at the correlation again. As mentioned already above, $C(t,t_w)$ consists of two terms with different scaling behavior, cf. Eq. (33). While Π always scales like $(t/t_w)^{-x}$, ΔC behaves like $(t/t_w)^{(x-1)}$ for $x>1/2$. Explicitly, one has for the leading behavior in this case $\partial_{t_w}C(t,t_w)\simeq(1-x)\Delta c(x)t_w^{-1}(t/t_w)^{x-1}+xp(x)t_w^{-1}(t/t_w)^{-x}$ with the second term being much smaller than the first one, cf. Fig. 1(b). The scaling behavior of $X_\gamma(t,t_w)$ found numerically for $x>1/2$, Eq. (42), can be understood in the following way. One considers the term $A/\partial_{t_w}C$ and uses $\partial_{t_w}\Delta C \gg \partial_{t_w}\Pi$, yielding $A/\partial_{t_w}C \simeq (A/\partial_{t_w}\Delta C)[1-(\partial_{t_w}\Pi/\partial_{t_w}\Delta C)]$. In order to proceed, one compares A to $\partial_{t_w}\Delta C$. Numerically, it is found that

$$A(t,t_w)=\partial_{t_w}\Delta C(t,t_w); \quad x>1/2 \qquad (43)$$

holds with high accuracy (deviations less than $10^{-3}\%$) for long times. One therefore finds

$$X_\gamma(t,t_w)\simeq\gamma\frac{\partial_{t_w}\Pi(t,t_w)}{\partial_{t_w}\Delta C(t,t_w)}=\gamma\frac{\partial_{t_w}\Pi(t,t_w)}{A(t,t_w)}; \quad x>1/2. \qquad (44)$$

Now, using $\partial_{t_w}\Pi(t_w+t,t_w)\simeq xp(x)t_w^{-1}(t/t_w)^{-x}$ and Eq. (37) for $x>1/2$ one recovers Eq. (42) with $x_\gamma(x)\simeq xp(x)/a(x)$. This behavior is additionally shown as the dashed line in the upper panel of Fig. 4(b). The deviations of $x_\gamma(x)\simeq xp(x)/a(x)$ from the fitted values are on the order of 10%. Given the fact that the values stem from completely different fits, and only the leading behavior of $\partial_{t_w}\Pi(t_w+t,t_w)$ has been used this confirms the consistency of the data.

The finding that $A=\partial_{t_w}\Delta C$ for $x>1/2$, Eq. (43), explicitly shows that the asymmetry cannot be expressed as a time-derivative of the correlation function. Instead, A is related to ΔC and this accounts for the correlation decay only partly.

Summarizing the results for the FDR, it is seen that only for $x<1/2$ there is a finite long-time limit X_γ^∞=const, while for $x>1/2$ one has $X_\gamma^\infty=0$, i.e.,

$$X^\infty(x)\simeq\begin{cases}0 & \text{for } x>1/2,\\ X_\gamma^\infty(x) & \text{for } x<1/2.\end{cases} \qquad (45)$$

As a consequence, for $x<1/2$, the FDR behaves similarly to the case of randomizing variables with the only difference that in the case of uncorrelated variables X^∞ is temperature-dependent. For $x>1/2$, however, one has $X^\infty=0$. In particular, this means that different variables do not even give rise to a well-defined long-time limit, which one would like to use for the definition of an effective temperature. It should be noted that the prominent difference regarding the FDR is given by the nonvanishing asymmtery in the case of uncorrelated variables. If one simply would have assumed the asymmetry to vanish in the scaling regime, the FDR for uncorrelated variables would be identical to the corresponding

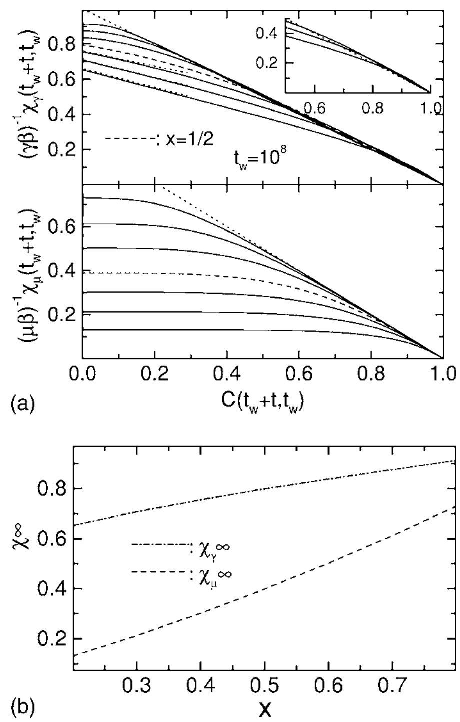

FIG. 5. (a) FD plots, integrated response vs correlation, for the MB model with an uncorrelated variable for different temperatures x. Upper panel: $(\gamma\beta)^{-1}\chi_\gamma(t_w+t,t_w)$ vs $C(t_w+t,t_w)$, lower panel: $(\mu\beta)^{-1}\chi_\mu(t_w+t,t_w)$ vs $C(t_w+t,t_w)$. In both cases the temperatures are x=0.2, 0.3, 0.4, 0.5, 0.6, 0.7, and 0.8 from bottom to top. The inset in the upper panel shows $(\gamma\beta)^{-1}\chi_\gamma(t_w+t,t_w)$ vs $C(t_w+t,t_w)$ for x=0.2, 0.3, and 0.4 from bottom to top. Note the change in slope. (b) The long-time limits χ_γ^∞ and χ_μ^∞ for $t_w=10^8$ as a function of temperature.

one for randomizing variables, as is obvious from a comparison of Eqs. (39) and (40) for $A(t,t_w)=0$ with Eq. (32).

The integrated response also can be decomposed into two independent functions

$$\chi(t,t_w) = \chi_\gamma(t,t_w) + \chi_\mu(t,t_w) \qquad (46)$$

and consequently the same holds for the FD plots, i.e., plots of $\chi(t,t_w)$ versus the correlation $C(t,t_w)$. Figure 5(a) shows FD plots for several temperatures x for a long waiting time $t_w=10^8$ with x increasing from bottom to top. No t_w dependence of the integrated response and the correlation are observed for $t_w=10^8$ for any temperature. In the scaling regime, the FDR gives the slope in the FD plot [1], $X=-\beta(\partial\chi/\partial C)$ and this is nicely confirmed in the plots. Note that for this expression to be valid it is sufficient that all quantities exhibit a (t/t_w) scaling. It is thus not necessarily required that X is a function of the correlation alone. The dotted lines in the upper panel for $x<1/2$ have slopes $X^\infty(x)$. Thus from the above discussion of the FDR, one expects that the limiting slope of the FD plots for $x>1/2$ vanishes. For $x<1/2$, on the other hand, for finite γ a nonzero limiting slope in the FD plots is expected, cf. Eq. (45). However, also for $x<1/2$, there are no straight lines in the FD plot, as can be seen in the inset of the upper panel of Fig. 5(a), where χ_γ is shown for x=0.2, 0.3. and 0.4 for large C.

In summary, one can state that in the case of uncorrelated variables the situation is similar to the case of randomizing variables as discussed in detail by Ritort [19]. A prominent difference, however, is given by the fact that one does not find straight lines as expected for 1SB-like FD plots for uncorrelated variables. Instead, the slope varies until the limiting slope X_γ^∞ is reached. For $x>1/2$ the situation changes completely. Here, the limiting value of the FDR vanishes, $X^\infty=0$. This is another important difference to the case of randomizing variables. Still another difference is given by the limiting value of the integrated response itself. Whereas one can show that $\chi\to(\beta\gamma+\beta_0\mu)$ for $C\to 0$ [19] for randomizing variables, in the present case such a universal behavior is not observed. Instead, both functions are increasing functions of temperature, as is obvious from Fig. 5(b), where I plotted the long-time limits χ_μ^∞ and χ_γ^∞ as a function of temperature, x. Finally, it should be noted that I solely consider variables with no dependence on the trap-energy. From a discussion of various randomizing but energy-dependent variables it has been shown that in some cases not even a limiting FD plot exists [2]. In that work it has been found that the limiting FDR is $X^\infty=0$ in all cases in which a limiting FD plot exists and therefore one might expect $T_{\rm eff}=\infty$ in the trap model for $\gamma=0$. It is not clear at this point whether a similar situation occurs if uncorrelated variables with an energy dependence are considered. However, the present calculations clearly show that for $\gamma\neq 0$ X^∞ behaves different for randomizing and uncorrelated variables. More importantly, both types of variables considered here are so-called neutral variables. It thus appears that the definition of an effective temperature in a trap model is not unique even if only neutral variables are considered.

IV. CONCLUSIONS

In the present paper I have considered the fluctuation-dissipation relation for a general class of stochastic models obeying a master equation. I have chosen transition rates which in the presence of a field are perturbed in a multiplicative way. For a nonstationary Markov process, in general no simple relation between the response and the correlation exists. If the process considered is stationary, the situation simplifies somewhat. The main result of the present paper is given in Eq. (16) and it shows that also for stationary Markov processes the response cannot be related to time-derivatives of the correlation function alone. Instead, the asymmetry $A(t,t_w)$ occurs additionally in the expression for the response, which is not related to any physical quantity in an obvious way. It is only in equilibrium that $A(t,t_w)$ vanishes, the system becomes time-translational invariant, and the FDT holds, if the dependence on the field of the transition rates is chosen in a symmetric way $(\gamma+\mu=1)$. To the best of my knowledge, Hoffmann and Sibani [15,16] were the first who considered the asymmetry $A(t,t_w)$. Their expression for the FDR coincides with Eq. (16) for the special case $\gamma=1$. However, they did not further discuss the meaning of this function apart from the fact that it vanishes if the relaxation is determined by probability distributions that are homogeneous with respect to the states of the stochastic process under consideration.

Motivated by the fact that in several treatments of the FDR for trap models the asymmtery does not occur, I considered different classes of dynamical variables. In the case of variables that randomize with a single transition among the states of the system the asymmetry vanishes under very mild conditions, cf. Eq. (28). On the contrary, for variables that are completely uncorrelated from the underlying dynamics, the asymmetry is finite. As both types of variables can be chosen to be neutral, these considerations already show that the use of the FDR for the definition of an effective temperature might be problematic in some cases.

As an example, I considered the trap model with transition rates chosen according to the version of the model given by MB [30]. For randomizing variables the known results derived by Ritort are recovered [19]. For uncorrelated variables, the situation is very different. First, the asymmetry is finite and shows a similar scaling behavior as the correlation function, which is different from that of the correlation for randomizing variables for $x>1/2$. For randomizing variables the correlation shows a $(t/t_w)^{-x}$ scaling, whereas for uncorrelated variables this is found only for $x<1/2$. For $x>1/2$, one finds a $(t/t_w)^{x-1}$ scaling instead, which is the same as for the populations. In contrast to the case of a randomizing variable, the correlation function contains two terms, one of which gives the probability that the value of the variable has not changed at all in the time-interval considered. This term coincides with the correlation function for a randomizing variable. However, there is another term which gives the probability of back-jumps to the original trap and thus accounts for the correlation among different traps. For $x>1/2$, this term dominates the correlation function for long times. It is found that the asymmetry equals this term for $x>1/2$. As discussed above, the asymmetry diminishes due to the scaling behavior of the populations, but this is not enough to allow one to neglect it. The fact that the asymmetry does not vanish implies a behavior of the FDR that is qualitatively different from the case of randomizing variables. In particular, the time-dependence of $X(t,t_w)$ changes with temperature in a different way. The same holds for the long-time limit of the FDR, X^∞. Also this limit is different for randomizing and uncorrelated variables. Only if one would assume the asymmetry to vanish for uncorrelated variables, the results regarding the FDR would be identical to the case of randomizing variables even though the correlation functions would still behave differently.

Regarding the possible definition of an effective temperature using $X(t,t_w)$, one faces the same problems that have already been discussed earlier [2]. The model only has a single time scale. Therefore, in order to have a sensible definition of T_{eff}, one should have a straight line in a FD plot. Otherwise, T_{eff} defined via $X(t,t_w)$ would change within a single time-sector, which makes X inappropriate for a meaningful definition of T_{eff} [3]. If a randomizing variable and $\mu=0$ is chosen, one obtains straight lines in a FD plot, but not for $\mu\neq 0$ [19]. For uncorrelated variables, one never obtains straight lines. Also the idea to use the long-time limit X^∞ for the definition of T_{eff} is hampered by the fact that it behaves differently for randomizing and uncorrelated variables. Apparently, the fact that both types of variables are neutral is not enough for such a definition. At present, it appears not clear which additional properties of a variable are required in order to allow a unique definition of T_{eff}. It also is not clear how the FDR changes in the case of uncorrelated variables, if an additional energy-dependence is considered, as has been done by Fielding and Sollich for randomizing variables [2].

Finally, it should be mentioned that the asymmetry can be shown to be finite also for some models in which equilibrium can be reached for long times. An example is provided by the MB model with a Gaussian density of states [30]. In these kinds of models all aging effects are of a transient nature. It can be shown that at least for some models the same holds for the asymmetry, as will be shown in a forthcoming publication [36].

To conclude, I have shown that for some general class of models the fluctuation dissipation relation is determined by time-derivatives of the correlation function and an additional function, the asymmetry $A(t,t_w)$. In general, the asymmetry can be shown to vanish for randomizing variables under the conditions considered usually. For the models considered in this paper, $A(t,t_w)$ has a strong impact on the behavior of the FDR and complicates the definition of an effective temperature.

ACKNOWLEDGMENT

Part of this work was supported by the DFG under Contract No. Di693/1-2.

APPENDIX A: CALCULATION OF THE LINEAR RESPONSE

In this Appendix the calculation of the response for a system obeying the ME, Eq. (2), using time-dependent perturbation theory is described. For the calculations it is preferable to use a matrix notation for the $G_{kl}(t,t_0)$, $\mathcal{G}(t,t_0)_{kl}=G_{kl}(t,t_0)$. Using Eq. (4) for the master-operator, the ME reads

$$\partial_t \mathcal{G}(t,t_0) = \mathcal{W}(t)\mathcal{G}(t,t_0). \tag{A1}$$

In the following, it is assumed that the solution of the ME in the absence of the field is known. In general, it can be written in the form

$$\mathcal{G}(t,t_0) = \mathcal{T}\exp\left(\int_{t_0}^{t} d\tau \mathcal{W}(\tau)\right)\mathcal{G}(t_0,t_0), \tag{A2}$$

where $\mathcal{T}$ denotes the time-ordering operator and $\mathcal{G}(t_0,t_0)_{kl}=\delta_{kl}$. In the presence of the field the transition rates are given by Eq. (8) and the corresponding master-operator accordingly reads as $\mathcal{W}^{(H)}(t)_{kl}=W_{kl}^{(H)}(t)-\delta_{kl}\Sigma_n W_{nl}^{(H)}(t)$. The ME is written as $\partial_t\mathcal{G}^{(H)}(t,t_0)=\mathcal{W}^{(H)}(t)\mathcal{G}^{(H)}(t,t_0)$.

In order to calculate the response of the system to an external field applied at time $t=t_w$, the ME in the presence of the field is solved using time-dependent perturbation theory. A solution of the problem in terms of a series, $\mathcal{G}^{(H)}(t,t_0)$

$=\mathcal{G}^{(0)}(t,t_0)+\mathcal{G}^{(1)}(t,t_0)+\cdots$ can be used to calculate the expectation value $\langle M(t)\rangle_{(H)}=\Sigma_{kl}M_k G_{kl}^{(H)}(t,0)p_k^0$ in linear order with respect to the field. According to Eq. (7) the response can be obtained via $R(t,t_w)=\delta(\Sigma_{kl}M_k G_{kl}^{(1)}(t,0)p_k^0)/\delta H(t_w)|_{H=0}$. In order to perform the calculation, one proceeds in the following way. First, one writes $\mathcal{G}^{(H)}(t,t_0)=\mathcal{G}(t,t_0)\mathcal{G}^{(I)}(t,t_0)$, $[\mathcal{G}(t,t_0)\equiv\mathcal{G}^{(0)}(t,t_0)]$, thus defining an "interaction representation" I. This yields

$$\partial_t\mathcal{G}^{(I)}(t,t_0)=[\mathcal{G}(t,t_0)^{-1}\mathcal{V}(t)\mathcal{G}(t,t_0)]\mathcal{G}^{(I)}(t,t_0). \tag{A3}$$

The matrix elements of the perturbation, $\mathcal{V}(t)_{kl}$, follow from a first-order expansion of the transition probabilities $W_{kl}^{(H)}(t)$. Thus any form of the $W_{kl}^{(H)}(t)$ allowing for a Taylor expansion can be used in the calculation. Here, I use the form given in Eq. (8) which explictly gives

$$\mathcal{V}(t)_{kl}=\beta H(t)\left(W_{kl}(t)X_{kl}-\delta_{kl}\sum_n W_{nl}(t)X_{nl}\right). \tag{A4}$$

Using this expression and the first-order approximation to the solution of Eq. (A3),

$$\mathcal{G}^{(1)}(t,t_0)=\int_{t_0}^{t}dt'\,\mathcal{G}(t,t')\mathcal{V}(t')\mathcal{G}(t',t_0),$$

one finds for $H(t)=H\delta(t-t_w)$:

$$G_{kl}^{(1)}(t,t_0)=\Theta(t-t_w)\beta H\sum_{m,n}[G_{km}(t,t_w)-G_{kn}(t,t_w)]W_{mn}(t_w)X_{mn}G_{nl}(t_w,t_0) \tag{A5}$$

and therefore for $t>t_w$

$$R(t,t_w)=\beta\sum_{k,l,n}M_k[G_{kn}(t,t_w)-G_{kl}(t,t_w)]W_{nl}(t_w)X_{nl}p_l(t_w).$$

Insertion of $X_{kl}=\gamma M_k-\mu M_l$ yields Eqs. (9) and (10) given in the text.

APPENDIX B: A SIMPLE NONSTATIONARY MARKOV PROCESS

Here, I will consider the following simple model. All transition rates are chosen to depend solely on the destination state,

$$W_{kl}(t)=g(t)a_k=Zp_k^{eq}g(t) \tag{B1}$$

where I defined $Z=\Sigma_k a_k$ and $p_k^{eq}=Z^{-1}a_k$. In this case, the solution of the ME is trivial [25]. Defining $\mathcal{E}(t,t_0)=\exp(-Z\int_{t_0}^{t}d\tau g(\tau))$ one finds for the Greens function:

$$G_{kl}(t,t_0)=p_k^{eq}[1-\mathcal{E}(t,t_0)]+\delta_{kl}\mathcal{E}(t,t_0). \tag{B2}$$

The system reaches an equilibrium state for long times if

$$\lim_{t\to\infty}\mathcal{E}(t,t_0)=0$$

resulting in $G_{kl}(t,t_0)\to p_k^{eq}$.

Using Eqs. (6), (10), and (12) allows one to calculate all quantities of interest explicitly. With the definitions

$$\langle M^n\rangle=\sum_k M_k^n p_k^{eq};\quad \langle\Delta M^2\rangle=\langle(M-\langle M\rangle)^2\rangle,$$

$$\langle M^n\rangle_0=\sum_k M_k^n p_k^0;\quad \langle\delta M^n\rangle=\langle M^n\rangle-\langle M^n\rangle_0 \tag{B3}$$

one finds

$$C(t,t_w)=\{\langle M^2\rangle+\langle\Delta M^2\rangle\mathcal{E}(t,t_w)\}+\langle M\rangle\langle\delta M\rangle[\mathcal{E}(t,0)-\mathcal{E}(t_w,0)]-\langle\delta M^2\rangle\mathcal{E}(t,0),$$

$$\begin{aligned}R_\gamma(t,t_w)&=\beta\gamma Zg(t_w)[\langle\Delta M^2\rangle\mathcal{E}(t,t_w)+\langle M\rangle\langle\delta M\rangle\mathcal{E}(t,0)],\\ R_\mu(t,t_w)&=\beta\mu Zg(t_w)[\langle\Delta M^2\rangle\mathcal{E}(t,t_w)+(\langle M\rangle\langle\delta M\rangle-\langle\delta M^2\rangle)\mathcal{E}(t,0)],\end{aligned} \tag{B4}$$

$$A_{\text{n.s.}}(t,t_w)=Zg(t_w)\langle M\rangle\langle\delta M\rangle[\mathcal{E}(t_w,0)-\mathcal{E}(t,0)].$$

While it is easy to see that $R_\gamma(t,t_w)=\partial_{t_w}C(t,t_w)-A_{\text{n.s.}}(t,t_w)$, one finds

$$R_\mu(t,t_w)=-\beta\mu\frac{g(t_w)}{g(t)}\partial_t C(t,t_w). \tag{B5}$$

If the system is prepared in an equilibrium state initially, $p_k^0=p_k^{eq}$, one has $\langle\delta M^n\rangle=0$ and the asymmetry vanishes, $A_{\text{n.s.}}(t,t_w)=0$. If the function $g(t)$ is of a form with finite values $g(0)$ and $g(\infty)$, e.g., $g(t)=1+\Gamma e^{-\Gamma t}$ with some rate Γ, it is evident from Eq. (B5) that for long times $[g(t_w)/g(t)]\to 1$ and the FDT holds if $\gamma+\mu=1$.

APPENDIX C: NUMERICAL SOLUTION OF THE ME FOR THE TRAP MODEL

For the trap model with the transition rates given in Eq. (29) and an exponential density of states,

$$\rho(\epsilon)=\beta_0 e^{-\beta_0\epsilon}\text{ with }\beta_0=T_0^{-1};\quad \epsilon\in[0,\infty] \tag{C1}$$

the ME,

$$\dot{p}(\epsilon,t)=-\kappa(\epsilon)p(\epsilon,t)+\rho(\epsilon)\int_0^\infty d\epsilon'\,\kappa(\epsilon')p(\epsilon',t), \tag{C2}$$

can be solved numerically using various techniques. One technique that can be used for direct integration has been proposed in Ref. [35] and allows one to calculate $p(\epsilon,t)$ for long time intervals. However, due to the special form of the transition rates, $W(\epsilon|\epsilon')=\rho(\epsilon)\kappa(\epsilon')$, it is also possible to symmetrize the matrix of transition rates using the symmetry relation:

$$W(\epsilon|\epsilon')\times[\rho(\epsilon')/\kappa(\epsilon')]=W(\epsilon'|\epsilon)\times[\rho(\epsilon)/\kappa(\epsilon)]. \tag{C3}$$

Thus one can consider the symmetric matrix with elements

$$W(\epsilon|\epsilon')^{(s)}=[W(\epsilon|\epsilon')W(\epsilon'|\epsilon)]^{1/2}\text{ and }W(\epsilon|\epsilon)=-\kappa(\epsilon), \tag{C4}$$

which is obtained from $W(\epsilon|\epsilon')$ via $W(\epsilon|\epsilon')^{(s)}=[\rho(\epsilon)/\kappa(\epsilon)]^{-1/2}W(\epsilon|\epsilon')[\rho(\epsilon')/\kappa(\epsilon')]^{1/2}$. The symmetry of this matrix ensures that all eigenvalues are real.

In order to proceed with the numerical diagonalization of the matrix of transition rates and thus the calculation of the time-dependent populations $p(\epsilon,t)$, one uses a discrete version of the model. The values of ϵ are given on a grid with values ϵ_k, $k=1,2,\ldots,N$ with typical values for N being $N \sim 200-1000$. Then, using the abbreviations $\kappa_k=\kappa(\epsilon_k)$, $\rho_k=\rho(\epsilon_k)$, $p_k(t)=p(\epsilon_k,t)$, and $G_{kl}(t)=G(\epsilon_k,\epsilon_l;t)$, one only has to replace all integrals by the appropriate sums and proceeds with the numerical analysis.

The populations are given in terms of the eigenvectors S_{km} and the eigenvalues λ_m:

$$p_k(t)=[\rho_k/\kappa_k]^{1/2}\sum_l p_l(0)[\kappa_l/\rho_l]^{1/2}\sum_m S_{lm}S_{km}e^{\lambda_m t}. \quad \text{(C5)}$$

In order to calculate the $G_{kl}(t)$, one writes the backward equation in the form

$$\dot{G}_{kl}(t)=-\kappa_l G_{kl}(t)+\kappa_l\sum_n G_{kn}(t)\rho_n \quad \text{(C6)}$$

and uses $p_k(t)=\Sigma_n G_{kn}(t)p_n^0=\Sigma_n G_{kn}(t)\rho_n$. Remember that at $t=0$, the system is quenched from infinite temperature and therefore one has $p_n^0=\rho_n$. This way, one finds

$$\dot{G}_{kl}(t)=-\kappa_l G_{kl}(t)+\kappa_l p_k(t) \quad \text{(C7)}$$

with the formal solution

$$G_{kl}(t)=\delta_{kl}e^{-\kappa_l t}+\kappa_l\int_0^t d\tau e^{-\kappa_l(t-\tau)}p_k(\tau). \quad \text{(C8)}$$

Thus, in order to calculate $G_{kl}(t)$, it is sufficient to solve the ME for the populations $p_k(t)$. For the off-diagonal contributions, one can furthermore avoid the explicit calculation of the time-integral on the right-hand side of Eq. (C7), if one uses the formal solution of the ME for the populations, $p_l(t)=\rho_l e^{-\kappa_l t}+\rho_l\int_0^t d\tau e^{-\kappa_l(t-\tau)}\Sigma_n\kappa_n p_n(\tau)$ yielding

$$\int_0^t d\tau e^{-\kappa_l(t-\tau)}p_k(\tau)=[p_k(t)-(\rho_k/\rho_l)p_l(t)]/(\kappa_l-\kappa_k)$$

for $k\neq l$. This allows one to write

$$G_{kl}(t)=\frac{\kappa_l}{\kappa_l-\kappa_k}[p_k(t)-(\rho_k/\rho_l)p_l(t)], \quad k\neq l. \quad \text{(C9)}$$

For the calculation of the diagonal elements $G_{kk}(t)$, Eq. (C8) together with Eq. (C5) is used.

Summarizing, the numerical treatment of the ME is in complete analogy to the case of an ME which fulfills detailed balance [14]. It is important to point out that for large values of ϵ_k, the prefactor in Eq. (C5), $[\rho_k/\kappa_k]^{1/2}\propto e^{-(1/2)(\beta_0-\beta)\epsilon_k}$, becomes quite large for $T<T_0$. This, however, poses no problem in the numerical work. In order to assure that this is so, I have compared the solutions of the ME obtained by diagonalization with the direct integration in the time domain and found identical results for many values of β. Additionally, the results obtained for the time-dependent populations, $p_k(t)$ and the correlation function $\Pi(t,t_w)$, cf. Eq. (27), coincide with the analytical expressions in the scaling regime [30]. The numerical treatment via the diagonalization of the matrix of transition rates has the advantage that it is much faster than the integration in the time domain, in particular for the long time scales considered in the present context.

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