Correlation functions of non-Markovian systems out of equilibrium: Analytical expressions beyond single-exponential memory

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Abstract. This paper is concerned with correlation functions of stochastic systems with memory, a prominent example being a molecule or colloid moving through a complex (e.g., viscoelastic) fluid environment. Analytical investigations of such systems based on non-Markovian stochastic equations are notoriously difficult. A common approximation is that of a single-exponential memory, corresponding to the introduction of one auxiliary variable coupled to the Markovian dynamics of the main variable. As a generalization, we here investigate a class of “toy” models with altogether three degrees of freedom, giving rise to more complex forms of memory. Specifically, we consider, mainly on an analytical basis, the under- and overdamped motion of a colloidal particle coupled linearly to two auxiliary variables, where the coupling between variables can be either reciprocal or non-reciprocal. Projecting out the auxiliary variables, we obtain non-Markovian Langevin equations with friction kernels and colored noise, whose structure is similar to that of a generalized Langevin equation. For the present systems, however, the non-Markovian equations may violate the fluctuation-dissipation relation as well as detailed balance, indicating that the systems are out of equilibrium. We then study systematically the connection between the coupling topology of the underlying Markovian system and various autocorrelation functions. We demonstrate that already two auxiliary variables can generate surprisingly complex (e.g., non-monotonic or oscillatory) memory and correlation functions. Finally, we show that a minimal overdamped model with two auxiliary variables and suitable non-reciprocal coupling yields correlation functions resembling those describing hydrodynamic backflow in an optical trap.

Keywords: Correlation functions, Memory effects, Friction
1. Introduction

In recent years, the investigation of non-Markovian ("memory") effects in physical systems has (re-)gained strong interest. "Non-Markovianity" implies that the dynamics of one (or several) "relevant" degree of freedom depends, to some extent, on its past. Such systems occur in many areas of physics, such as the physics of strongly correlated soft matter (e.g., particles in viscous suspensions [1, 2] or glass-forming liquids [3]), in active [4, 5, 6, 7, 8] and biological matter [9, 10], in reaction kinetics, protein dynamics [11], neurophysics, quantum optics [12], but also in systems subject to feedback control with time delay [13, 14, 15, 16]. Recent research on non-Markovian effects concerns, e.g., the complex behavior of dynamical correlation functions exhibiting multi-exponential [10] and oscillatory [2] decay, unusual transport properties such as (anomalous) diffusion [17, 18], mobility [19] and oscillating particle currents [20], spontaneous modes of motion in active matter [5], non-Markovian (quantum) phase transitions [21], and thermodynamic properties of stochastic non-Markovian systems [22, 23, 24, 25].

In theoretical approaches, non-Markovianity naturally arises as a result of a coarse-graining procedure, when the (typically "slow") variable of interest is coupled to other, less relevant (and typically "faster") ones. Unless the timescales of the slow and fast variables are completely separated, the dynamics of the slow variable will involve, to some extent, a history dependency, i.e. non-Markovianity. For classical systems, this is directly seen within the celebrated Mori-Zwanzig approach [26, 27] yielding a generalized Langevin equation (GLE) with a "friction" kernel and colored noise. In fact, both the kernel and the colored noise induce a history dependency. Further, GLEs are used to model the impact of complex environments, such as "particles" in the interior of a cell [18, 28] (as an alternative to other routes such as non-Gaussian diffusivity [29, 30, 31] or fractional Brownian motion [32, 33, 34]).

Clearly, non-Markovian dynamics renders any analytical (and numerical, see, e.g., [35]) treatment of a given model system more involved. For that reason, memory effects are often described on the basis of simple ansatzes, a popular one being GLEs with friction kernels composed of exponentials. In the spirit of the Markovian embedding method [36], the resulting GLEs can then be rewritten as a set of a (typically finite) number of Markovian equations involving \( n \) auxiliary variables. Many applications are based, in fact, on single-exponential kernels and thus, \( n = 1 \) auxiliary variables (see, e.g., [1]), but several recent studies consider \( n = 2 \) (see, e.g., [37]). For systems in thermal equilibrium with a bath, the corresponding colored noise correlations are typically assumed to be determined by the fluctuation dissipation relation (FDR) [38] (sometimes referred to as fluctuation-dissipation theorem of second kind), stating that the noise correlations and the friction kernel are proportional to one another. However, there are also pure non-equilibrium models with one auxiliary variable, such as the active Ornstein-Uhlenbeck process [39, 40, 41, 42] describing the motion of an active particle with fluctuating self-propulsion.

Most investigations so far were focused on specific, equilibrium or non-equilibrium,
systems. In contrast, the goal of the present paper is to systematically explore, on a more general level, the autocorrelation functions of the position (PACF) and velocity (VACF) of classical stochastic systems with friction kernels and colored noise generated by two auxiliary variables, i.e., $n = 2$. The VACF and PACF are particularly interesting quantities as they are experimentally (or numerically) accessible in a large variety of soft matter systems. For the sake of an analytical treatment, we focus on purely linear systems. Different from earlier studies, however, we do not assume that the couplings between the main variable and the auxiliary ones stem from an underlying Hamiltonian. This allows us to model both, equilibrium and non-equilibrium systems. In particular, we discuss both, reciprocal coupling schemes (which, in the case of position variables, are typical of conservative forces fulfilling Newton’s third law), and non-reciprocal coupling schemes, which are one possible ingredient for modelling non-equilibrium systems [23, 43]. In summary, we discuss a class of models whose (potential) non-equilibrium character is not induced by external forces or fields, but rather is of intrinsic character. Specifically, non-equilibrium in our models arises through non-reciprocal coupling and/or different bath temperatures in the Markovian description, which is then reflected by a broken FDR [38] in the non-Markovian description.

By considering different coupling topologies of the network and a wide range of coupling constants, we outline “maps” relating various behaviors of friction kernels in the non-Markovian picture and correlation functions. By this, we provide insight into the properties which a simple, analytically accessible model should have to capture specific features of measured correlation functions. Indeed, the case $n = 2$ introduces substantial additional complexity as compared to the single-exponential case, such as oscillatory or non-monotonic friction kernels and autocorrelation functions describing competing relaxational effects. For example, in case that the kernel has a maximum at a finite time, this can model a preferred “delay” time [23] (notice that the limit $n \to \infty$ corresponds to the case of a delta-distributed, i.e., discrete delay time often used in time-delayed feedback control [44]). Aside of modelling different friction kernels, our approach allows for identifying the impact of colored noise on the resulting correlation functions. As a concrete example, we show that a minimal overdamped model with two auxiliary variables and suitable coupling yields correlation functions resembling those describing hydrodynamic backflow in an optical trap [45].

The remainder of this paper is organized as follows. In Sec. 2.1 we introduce our models composed of small sets of linear (under- or overdamped) Langevin equations and the corresponding non-Markovian representations, focusing on the shape of the friction kernel depending on the coupling topology. Section 3 is devoted to the calculation of measurable dynamical quantities, particularly the VACF and PACF, and a discussion of exemplary analytical results. In Sec. 4 we discuss the FDR, and Sec. 5 describes an application. Our conclusions are summarized in Sec. 6. The paper includes several appendices comprising technical details.
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2. Theory

2.1. Markovian models

In this section we introduce sets of Langevin equations which are inspired by (yet not restricted to) the physical situation of a colloid moving in one dimension in a solvent characterized by the friction constant $\gamma_0$ and temperature $T_0$. The position and velocity of the colloid are given by $x$ and $v = \dot{x}$, respectively. Besides these physical variables, the equations of motion further contain couplings to auxiliary variables $y_i$, $i \in \{1, 2, \ldots, n\}$ whose significance will become apparent at a later point. Here we just assume that each auxiliary variable $y_i$ is exposed to its own thermal bath with temperature $T_i$. For the sake of a fully analytical treatment, we also assume that the coupling among all variables is linear.

We here restrict ourselves to systems involving two auxiliary variables, $n = 2$. Indeed, as we will show in the subsequent sections, already this case allows to describe non-Markovian correlations with features markedly different from the “standard” case of one auxiliary variable. Focusing first on underdamped motion (with mass $m = 1$), we specifically consider the equations

$$\dot{x} = v$$
$$\dot{v} = -\gamma_0 v - \kappa x + k_1 y_1 + k_2 y_2 + \xi_0$$
$$\dot{y}_i = -a_i y_i + b_i v + d_i y_j + \xi_i, \; i = 1, 2, \; j \neq i,$$

where $\xi_\alpha$ (with $\alpha = 0, 1, 2$) are zero-mean Gaussian white noises with correlations

$$\langle \xi_\alpha(t + \Delta t) \xi_\beta(t) \rangle = 2k_B T_\alpha \gamma_\alpha \delta_{\alpha\beta} \delta(\Delta t).$$

In Eq. (2), the brackets $\langle \cdots \rangle$ denote an ensemble average over different noise realizations and $k_B$ is the Boltzmann constant. In what follows, the constants $\gamma_1$ and $\gamma_2$ are set to one.

All coupling constants appearing in Eqs. (1) are real. The case $\kappa = 0$ leads to the absence of any conservative, $x$-dependent force, while $\kappa > 0$ describes the impact of a confining harmonic potential. In Eqs. (1c) we assume $a_i > 0$, corresponding to a confinement of the $y_i$-dynamics. The coupling constants $k_i$, $b_i$, and $d_i$ ($i = 1, 2$) connecting $v$ and the auxiliary variables $y_i$ can have arbitrary sign. Importantly, we do not impose any restrictions on these constants. Thus, the coupling can be reciprocal, corresponding to $k_i = b_i$ ($i = 1, 2$), and $d_1 = d_2$, or non-reciprocal, where these symmetries are not fulfilled. We note that the interpretation of the (non)reciprocity strongly depends on whether one considers the auxiliary variables as physical degrees of freedom. For example, if we consider in the underdamped model (1) the $y_i$ as velocities (of two additional particles), then all coupling terms between $v$ and $y_i$ are friction-like (i.e., non-conservative) and non-reciprocal coupling implies asymmetric frictional forces. As another example, if both $y_i$ are positions, then the choice $d_1 \neq d_2$ would correspond to harmonic “forces” which, however, do not fulfill Newton’s third law and are, in
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Figure 1. Schematic of the Markovian model system with $n = 2$ auxiliary variables in the underdamped case. Black arrows indicate the (linear) coupling between variables. The velocity ($v$) of the colloid couples to two auxiliary variables $y_i$ ($i \in \{1, 2\}$) with coupling strength $k_i$ and $b_i$, while the coupling between $y_i$ is determined by the constants $d_i$. Non-reciprocal coupling corresponds to $k_i \neq b_i$ and/or $d_1 \neq d_2$. All variables are subject to thermal baths with temperatures $T_0$ and $T_i$.

that sense, non-conservative. These issues are not relevant for the resulting correlation functions of the main variable (here $v$), which is why we leave the question of whether the $y_i$ have a physical meaning, at this point open. However, this question does become important in the context of equilibrium conditions, see Sec. 4.

An illustration of the “network” involving the three variables $v$, $y_1$ and $y_2$ [see Eqs. (1) with $\kappa = 0$] is given in Fig. 1. As we will demonstrate, the coupling topology of the network, i.e., the set of coupling parameters, crucially determines the resulting non-Markovian dynamics. The most general case is the “all-to-all” coupling topology (see Fig. 1), where all parameters $k_i$, $b_i$, and $d_i$, are non-zero. In addition, it is appropriate to introduce some special topologies (see insets in Fig. 2):

- “Ring” topology, defined by $k_1 = d_1 = b_2 = 0$. This corresponds to a unidirectional coupling of the form $v \rightarrow y_1 \rightarrow y_2 \rightarrow v$ which is, by construction, non-reciprocal in all variables. This topology naturally occurs when applying Markovian embedding to time-delayed feedback control [44].
- “Chain” topology, where $k_2 = b_2 = 0$, that is, $v$ couples only to $y_1$. The latter then provides the connection towards the second auxiliary variable ($y_2$). For this topology, one can still consider reciprocal and non-reciprocal cases depending on the remaining coupling constants.
- “Center” topology, defined by $d_1 = d_2 = 0$. Thus, there is no coupling between the auxiliary variables, while both of them couple to $v$ (and vice versa) either reciprocally or non-reciprocally.

Finally, Eqs. (1) can be easily rewritten to describe an overdamped system. To this end, we replace in Eqs. (1b) and (1c) the variable $v$ (velocity) by $x$ (position) and remove, at the same time, Eq. (1a). (Note that this is different from the usual overdamped limit of Eqs. (1) because we wish the auxiliary variables in our overdamped model to be coupled to $x$ and not to $\dot{x}$). Further, setting $\gamma_0 + \kappa = a_0$ yields our Markovian model...
for overdamped motion,

\[
\begin{align*}
\dot{x} &= -a_0 x + k_1 y_1 + k_2 y_2 + \xi_0 \quad (3a) \\
\dot{y}_i &= -a_i y_i + b_i x + d_i y_j + \xi_i, \quad (i = 1, 2, j \neq i). \quad (3b)
\end{align*}
\]

Equation (3a) corresponds to the overdamped equation of motion for the colloidal position in presence of a harmonic potential with stiffness \(a_0\) and a friction constant of one. Regarding the entire network of three variables, a particularly simple interpretation arises in the fully reciprocal case, that is, \(k_i = b_i, d_1 = d_2\). In this case, Eqs. (3b) describe a system of three colloidal particles with positions \(x, y_1, y_2\), which are mutually coupled by springs and (depending on the choice of \(a_0, a_i\)) are subject to additional harmonic traps. Thus, the coupling terms here relate to conservative forces. In contrast, non-reciprocal coupling implies (as in the underdamped case with position-like auxiliary variables) the presence of non-conservative forces which break Newton’s third law.

We close this section by a brief comparison of our models with some related (low-dimensional) models studied in the literature. Starting from the underdamped case Eq. (1) and setting the second auxiliary variable to zero \((y_2 = 0)\), we essentially arrive at the “Jeffrey model” of retarded friction, which has been introduced in the context of (macroscopic) rheology. More recently, Raikher and Rusakov [1] have used the resulting equations to fit data for a microrheological experiment, where a micron-sized colloid “trapped” in a harmonic potential (mimicking an optical trap) is moving through a viscoelastic solution. It is well established that the single auxiliary variable leads to a (single-)exponential memory, where the constant \(a_1\) plays the role of the inverse Maxwell (stress) relaxation time. Our model extends the ansatz in [1] by introducing a second auxiliary variable which may be coupled not only to \(v\), but also to the first one. Further, underdamped models with two or three auxiliary variables have been used by Kowalik et al. [46] for molecules moving in viscoelastic fluids. In these models, the auxiliary variables are typically not exposed to a heat bath. The most significant differences to our systems, however, is that the couplings in [46] are assumed to be reciprocal, as it is typical of systems derivable from a Hamiltonian. Finally, a common application of the overdamped case involving one auxiliary variable (i.e., \(y_2 = 0\)) is the “active Ornstein-Uhlenbeck model” [39, 40, 41], where \(x\) represents the particle position and \(y_1\) represents a fluctuating “self-propulsion” velocity. The coupling is unidirectional, with \(k_1 > 0\), \(b_1 = 0\), and \(a_0 > 0, a_1 > 0\). For a more detailed discussion of models of this type, see [23, 42].

2.2. Non-Markovian representation

In parallel to the sets of (Markovian) Langevin equations given in Eqs. (1) and (3), we consider the non-Markovian equation for \(v\) or \(x\) that result from “integrating out” (projecting) the auxiliary variables \(y_i\), Eqs. (1c) and (3b). To this end we use
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Laplace transformation techniques as outlined in Appendix A. We first consider the underdamped case. Starting from Eqs. (1), one obtains

\[ \dot{v} = -\int_0^t \Gamma(t-t')v(t')dt' - \kappa x + \xi_0 + \xi_c \]  

(4)

involving the friction kernel \( \Gamma(t) = 2\gamma_0\delta(t) + \gamma(t) \) and the colored noise, \( \xi_c = \xi_c(t) \) (see Eq. (A.12) for an explicit expression). The non-trivial contribution to the frictional kernel is given by

\[ \gamma(t) = \gamma^+(t) + \gamma^-(t), \]

(5)

where

\[ \gamma^\pm(t) = g^\pm \exp \left[ -(a_1 + a_2 \pm \omega) \frac{t}{2} \right] \]

(6)

with

\[ g^\pm = \mp \frac{(k_1b_1 - k_2b_2)(a_1 - a_2)}{2\omega} - \frac{k_1b_1 + k_2b_2}{2} \pm \frac{k_1d_1b_2 + k_2d_2b_1}{\omega} \]

(7)

and

\[ \omega = \sqrt{(a_1 - a_2)^2 + 4d_1d_2}. \]

(8)

It is worth to discuss some general features of the function \( \gamma(t) \) independent of a specific topology. First, the function \( \gamma(t) \) trivially vanishes when \( k_i = 0 \) or \( b_i = 0 \) \((i = 1, 2)\), that is, when \( v \) decouples from the auxiliary variables. Second, \( \gamma(t) \) does not depend on the noise terms (and thus, the temperatures \( T_i \)) of the auxiliary variables. This is why we can discuss the friction kernel separately from noise effects. The same holds for the constant \( \kappa \) in Eq. (1b), that is, the kernel is independent of the strength of confinement (if present). Third, the fact that \( \gamma(t) \) involves two exponential functions (resulting from the presence of two auxiliary variables) allows for the possibility of a non-monotonic friction kernel with a minimum or maximum (at \( t > 0 \)), if the prefactors have different signs. Clearly, such a non-monotonicity already represents a marked difference to the case of one auxiliary variable (i.e., single-exponential memory). Fourth, there are parameter ranges where \( \gamma(t) \) contains oscillatory contributions. This occurs when \( \omega \) defined in Eq. (8) becomes (purely) imaginary, that is,

\[ (a_1 - a_2)^2 < -4d_1d_2. \]

(9)

Since \( a_1 \) and \( a_2 \) are real, the left hand side is always positive (or zero). Thus, oscillations can not occur if either \( d_1 \) or \( d_2 \) is zero, that is, if there is a unidirectional coupling between the auxiliary variables, or if there is no coupling between \( y_i \) at all. Further, for oscillations to occur, \( d_1 \) and \( d_2 \) have to have different signs, i.e. the coupling between the
auxiliary variables has to be non-reciprocal. The fifth general statement regarding $\gamma(t)$ concerns its limit at time zero. Here, one finds from Eq. (6) $\lim_{t \to 0} \gamma(t) = -k_1 b_1 - k_2 b_2$; thus, the function $\gamma(t)$ can have an “offset”. The latter solely depends on the coupling between $v$ and the auxiliary variables, and is strictly negative for reciprocal cases.

Examples of the function $\gamma(t)$ are shown in Fig. 2. The most general case is the “all-to-all” topology (Fig. 2(a)) for which one may observe monotonic decay (via a sum of exponentials), oscillatory behavior, or non-monotonic behavior characterized by one minimum or maximum at a finite time. The other panels in Fig. 2 relate to the specific topologies introduced in Sec. 2.1. Their main features can be summarized as follows:

- For the “ring” topology (Fig. 2(b)): $\gamma(t)$ is always non-monotonic but never oscillatory (because of $d_1 = 0$). This is directly seen from the explicit expression

$$\gamma_{\text{ring}}(t) = -\frac{2k_2 b_1 d_2}{\omega} \exp \left[ -\frac{(a_1 + a_2) t}{2} \right] \sinh \left( \frac{\omega t}{2} \right),$$

revealing that $\gamma(t)$ starts from zero at $t = 0$ and then approaches a maximum or minimum at a finite time. We note that the nonmonotonic behavior remains upon introducing more auxiliary variables (i.e., $n > 2$) in the ring topology [23].

- For the “chain” topology (Fig. 2(c)), one may observe non-monotonicity,
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oscillations, and (by default) an offset at $t \to 0$. The explicit expression is given by

$$\gamma_{\text{chain}}(t) = k_1 b_1 \exp \left[ -(a_1 + a_2) \frac{t}{2} \right] \times \left( a_1 - a_2 \frac{\sinh \left( \frac{\omega t}{2} \right)}{\omega} - \cosh \left( \frac{\omega t}{2} \right) \right).$$

(11)

• In the “center” topology (Fig. 2(d)), oscillations are not possible because of $d_i = 0$. Still, non-monotonic behavior can occur, as seen from

$$\gamma_{\text{center}}(t) = - \sum_{i \in \{1, 2\}} k_i b_i \exp \left[ -a_i t \right].$$

(12)

Turning back to the non-Markovian Eq. (4), we now focus on the colored noise, $\xi_c$, whose explicit expression is given in Eq. (A.5). The colored noise involves a time integral, and thus, a history dependency. In this sense, $\xi_c$ may be seen as an additional source of memory. The corresponding noise correlation function in the stationary limit (for a derivation, see Appendix A.2), is given by

$$\lim_{t \to \infty} \langle \xi_c(t + \Delta t) \xi_c(t) \rangle = \Xi^+(\Delta t) + \Xi^-(\Delta t)$$

(13)

with

$$\Xi^\pm(\Delta t) = 2k_B \left( \frac{T_1 c_1^+ c_1^+}{a_1 + a_2 \pm \omega} + \frac{T_2 c_2^+ c_2^+}{a_1 + a_2 \pm \omega} + \frac{T_1 c_1^- c_1^+}{a_1 + a_2} + T_2 c_2^- c_2^+ \right) \exp \left[ -(a_1 + a_2 \pm \omega) \frac{\Delta t}{2} \right].$$

(14)

In Eq. (14), $c_i^\pm (i = 1, 2)$ are constants which are defined in Eq. (A.6). The appearance of the temperatures $T_i$ in Eq. (14) directly reflects that the colored noise and its correlations only appear when the auxiliary variables are coupled to heat baths. We also note that the noise correlations can be oscillatory in time. This occurs if $\omega$ defined in Eq. (8) becomes (purely) imaginary [see condition (9)] which, at the same time, implies that the (non-trivial) friction kernel, $\gamma(t)$, oscillates. A more detailed discussion of relations between friction kernel and noise correlations will be given in Sec. 4.

Finally, we briefly consider the overdamped case. Following the same steps of calculation as in the underdamped case, we obtain from Eqs. (3)

$$\dot{x} = - \int_0^t G(t - t') x(t') dt' + \xi_c(t) + \xi_0(t),$$

(15)

where the kernel $G(t - t')$ is, by construction, identical to the function $\Gamma(t)$ appearing in the underdamped case, see Eq. (4). Physically, the convolution integral in Eq. (15) describes a retarded harmonic force. When modelling colloidal motion, however, one is rather interested in the “friction kernel” where the convolution involves not $x$, but $\dot{x}$. Starting from Eq. (15), this can be achieved through an integration by parts (see Appendix A.3). Focusing on the long time limit one obtains

$$\int_0^t \tilde{\Gamma}(t - t') \dot{x}(t') = -a_0' x + \xi_0 + \xi_c,$$

(16)
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where \( \hat{\Gamma}(t) = 2\delta(t) + \gamma_o(t) \), \( \gamma_o(t) = \gamma^+(t) + \gamma^-(t) \), and

\[
\gamma^\pm(t) = \frac{-2\gamma^\pm(t)}{a_1 + a_2 \pm w},
\]

with \( \gamma^\pm(t) \) being defined in Eq. (6). Due to direct connection to the friction kernel in the underdamped model, many conclusions which we draw there also apply to the overdamped system. The main difference is the different sign. Further in Eq. (16), \( a'_0 = a_0 - \gamma^+(0)/(a_1 + a_2 + \omega) - \gamma^-(0)/(a_1 + a_2 - \omega) \), and the colored noise, \( \xi_c(t) \), is the same as that appearing in the underdamped case, see Eq. (A.5).

3. Correlation functions

While the memory kernels discussed in Sec. 2.2 determine the non-Markovian equations of motion (4) and (15) from a mathematical point of view, the quantities of prime physical interest (in terms of measurements) are rather the (auto-)correlation functions of the system. Here we discuss, in particular, the VACF and mean squared displacement (MSD) in the underdamped case, and briefly comment on the overdamped case.

3.1. Closed expressions

We start by considering the VACF in the long-time limit, defined by

\[
c_V(\Delta t) = \lim_{t \to \infty} \langle v(t)v(t + \Delta t) \rangle.
\]

(18)

Our analytical calculation of \( c_V \) relies on a Fourier transform of Eq. (4) (thus taking advantage of the convolution theorem) and subsequent back transformation, yielding

\[
v(t) = \int_{-\infty}^{\infty} ds \lambda(s) \left( \xi_0(t-s) + \xi_c(t-s) \right),
\]

(19)

where \( \lambda(s) \) is the Green’s Function in the time domain. Its Fourier transform, \( \hat{\lambda}(f) \) (with \( f \) being the frequency), follows from the transform of Eq. (4) as

\[
\hat{\lambda}(f) = -\frac{1}{if - \hat{\Gamma}(f) + i(\kappa/f)}.
\]

(20)

The explicit calculation of \( \lambda(s) \) thus involves the calculation of the Fourier transform of the full friction kernel, \( \hat{\Gamma}(f) \), as well as the inverse transformation of \( \hat{\lambda}(f) \). We show in Appendix C how this can be done using a partial fraction decomposition (for an alternative approach, see [47]). In what follows, we focus on the case \( \kappa = 0 \) (i.e., no confining potential). One obtains

\[
\lambda(t) = -\sum_{k=1}^{3} \epsilon_k e^{-F_k t},
\]

(21)
where the coefficients $\epsilon_k$ are given in Eq. (C.8) and $F_k$ denote the poles of $\hat{\lambda}$. In Eq. (21) we have assumed that all real parts are positive to ensure causality (i.e., $\lambda(t) = 0$ for $t < 0$) \cite{18}.

Combining Eqs. (18) and (19) we obtain with $\xi(t) = \xi_0(t) + \xi_o(t)$

$$c_V(\Delta t) = \int_{-\infty}^{t} ds \int_{-\infty}^{t+\Delta t} ds' \lambda(s)\lambda(s') \langle \xi(t-s)\xi(t+\Delta t-s') \rangle, \quad (22)$$

and, after noise averaging,

$$c_V(\Delta t) = \int_{-\infty}^{t} ds \lambda(s)\lambda(s+\Delta t)2\gamma_0 k_B T_0$$

$$+ \int_{-\infty}^{t} ds \int_{-\infty}^{t+\Delta t} ds' \lambda(s)\lambda(s') \langle \xi_o(t-s)\xi_o(t+\Delta t-s') \rangle. \quad (23)$$

On the right side of Eq. (23), we defined, first, the function $c_V^1(\Delta t)$ which is proportional to $T_0$ (and independent of $\xi_o$). Inserting the Green’s function Eq. (21) and performing the integral we obtain (for $t \to \infty$)

$$c_V^1(\Delta t) = 2\gamma_0 k_B T_0 \sum_{k=1}^{3} \frac{\epsilon_k \epsilon_l}{F_k + F_l} \left( e^{-F_k \Delta t} + e^{-F_l \Delta t} \right). \quad (24)$$

The second function defined in Eq. (23), $c_V^II(\Delta t)$, involves the correlations of the colored noise [see Eq. (13)] and is thus linear in $T_1$ and $T_2$. The remaining integral is quite cumbersome, it can be performed using a computer algebra program (Mathematica 10.1 \cite{14}).

Having obtained the VACF, the MSD can be calculated from the relation \cite{49}

$$\langle (\Delta x(t))^2 \rangle \equiv \langle [x(t) - x(0)]^2 \rangle = 2t \int_{0}^{t} dt' \left( 1 - \frac{t'}{t} \right) c_V(t'). \quad (25)$$

The calculation becomes most convenient in the case that the auxiliary variables are not coupled to a heat bath, that is, $T_1 = T_2 = 0$, corresponding to $\xi_o(t) = 0$, and thus, $c_V(t) = c_V^1(t)$ [see Eq. (23)]. In this case we obtain from Eqs. (24) and (25),

$$\langle (\Delta x(t))^2 \rangle = 4\gamma_0 k_B T_0 \sum_{k \leq l \in \{1, \ldots, 3\}} \frac{\epsilon_k \epsilon_l}{F_k + F_l} \left( \frac{e^{-F_k t} - 1 + F_k t}{F_k^2} + \frac{e^{-F_l t} - 1 + F_l t}{F_l^2} \right). \quad (26)$$

From Eq. (26), we can readily see that the MSD grows linear in the long time limit, corresponding to normal diffusion, i.e. $\lim_{t \to \infty} \langle (\Delta x(t))^2 \rangle \propto t$.

Finally, for the overdamped system, the expression for the PACF follows directly from the expression for $c_V(t)$ by just changing the dynamic variable from $v$ to $x$. This is since the projected equations \cite{4} for $\dot{y}$ and (15) for $\dot{x}$, respectively, are formally equivalent.

\‡ Script available from the authors upon request
3.2. Results

We now discuss results for the correlation functions of an underdamped system. Clearly, one is faced with a rather large parameter space spanned by the coupling parameters between the network variables, the constants $\gamma_0$ and $a_i$, and the temperatures $T_\alpha$ ($\alpha = 0, 1, 2$). After scanning broad ranges of these parameters, we here focus on a few, particularly interesting situations. We first consider systems without colored noise, where the history dependency arises only through the friction kernels. Indeed, we will see that this type of memory dominates the behavior of the correlation functions as compared to the effect of colored noise studied subsequently.

3.2.1. Systems with white noise

We start by considering a system with “center” topology and $T_1 = T_2 = 0$. The VACF is then given by $c_V(t) = c_V^I(t)$ [see Eqs. (23) and (24)]. We recall that the center topology implies a (non-trivial) friction kernel $\gamma(t)$, which is either monotonic or non-monotonic with one maximum or minimum at a finite time, see Eq. (12). The latter equation also indicates that all dynamical functions (memory kernel, VACF, MSD) only depend on the products $k_i b_i$ rather than on each coupling constant individually [this is explicitly seen in Eq. (12)]. For that reason, we can discuss the results in the plane spanned by $k_1 b_1$ and $k_2 b_2$ (for fixed $\gamma_0$, $a_i$). For each of these products we consider a range of positive and negative values. Notice that $k_i b_i < 0$ corresponds to different signs of $k_i$ and $b_i$, which necessarily implies non-reciprocal coupling.

In Fig. 3 we present a “map” illustrating the various behaviors of the VACF, MSD and friction kernel in the parameter plane spanned by $k_1 b_1$ and $k_2 b_2$. We can identify several regions. In the grey region, the system is linearly unstable in the sense that the coefficient matrix of the deterministic part of the Markovian equations (1) for $v$ and $y_i$ has (at least) one eigenvalue, whose real part is positive. Outside the grey region, all eigenvalues have negative real parts. In the presence of (white) noise acting on $v$, the variance of $v$, that is, the correlation function $\langle v(t)v(t) \rangle$ in its stationary limit, diverges when one approaches the stability border (of the deterministic system) from the left. This, again, signals the instability.

The remaining part of the plane can be divided according to different criteria. Focusing first on the VACF we find that the simplest behavior occurs within the striped region, where the VACF decays monotonically from its initial value at $\Delta t = 0$ to its long-time limit, $\lim_{\Delta t \to \infty} c_V(\Delta t) = 0$. Outside the striped, but still within the orange region, the VACF remains to be non-negative everywhere, but exhibits a minimum and a local maximum at finite $\Delta t > 0$, before eventually decaying to zero (see middle right panel for an example). Within the violet region, the VACF shows damped oscillatory behavior characterized by, at least, three roots. We note that throughout this range, one of the products $k_i b_i$ is negative, implying that the coupling between the variables in the underlying Markovian network is non-reciprocal. Finally, outside the violet and orange regions, the VACF has one minimum at negative values, but does not oscillate.
Correlation functions of non-Markovian systems out of equilibrium

Figure 3. Overview of the various behaviors of the VACF and the MSD for underdamped systems with center topology in the absence of colored noise ($T_1 = T_2 = 0$). The remaining constants are set to $T_0 = 0.5$, $\gamma_0 = 1$, $a_1 = 1/2$ and $a_2 = 3/2$. Also shown are the corresponding friction kernels. The correlation functions related to several exemplary parameter combinations (indicated by crosses) are shown in the left and right panel. To enhance overall visibility, all VACFs and MSDs are multiplied by scaling factors given in Table B2. The various colored areas are explained in the main text.

in the sense that it has less than three roots.

Traditionally, minima in the VACF are often discussed in the context of strongly correlated liquids, where each particle (or molecule) is surrounded by several neighbours (see, e.g., [49]). These neighbours form a “cage” around the particle considered, leading to backscattering and thus, negative values of the VACF at intermediate times. In the present, single-particle system, the minima rather result from the non-Markovian friction induced by the auxiliary variables. To better understand the occurrence and location of the minima we note that, for the case of white noise considered here, there is an exact relationship between the time derivative of the VACF and the function $\gamma(t)$. This relation, well known from the theory of liquids [49, 50], is derived by multiplying Eq. (4) by $v(0)$ and taking the average on both sides. Using that $\langle v(0) \xi_0 \rangle = 0$ and $\xi_c = 0$, we obtain

$$\dot{c}_V(t) = -\int_0^t \Gamma(t - t')c_V(t')dt' = -\gamma_0 c_V(t) - \int_0^t \gamma(t - t')c_V(t')dt', \quad (27)$$
where \( \dot{c}_V(t) = \langle \dot{v}(t)v(0) \rangle \) and we have implicitly assumed that the system at \( t = 0 \) is already in the steady state. According to Eq. (27), a minimum of the VACF (i.e., \( \dot{c}_V(t) = 0 \) at a finite time \( t_{\text{min}} \)) requires that the function \( \gamma(t) \) is non-local in time (which is trivially fulfilled in all cases considered here). Let us focus here on cases where \( \gamma(t) \) has a maximum at a finite time and is entirely positive. This case is particularly interesting, e.g., in the context of time-delayed feedback control [23]; the maximum in \( \gamma(t) \) then corresponds to a preferred “delay” time. As a major trend we observe an increase of \( t_{\text{min}} \) with the time related to the maximum of the kernel (not shown here). This may be understood such that the larger the delay, the later the VACF “feels” the effect of the memory and changes its decay.

A further interesting relationship emerges when we differentiate Eq. (27) with respect to time and set \( t = 0 \). This yields

\[
\frac{\ddot{c}_V(0)}{c_V(0)} = -\gamma_0 \frac{\dot{c}_V(0)}{c_V(0)} - \gamma(0).
\]

(28)

We here focus on the case \( \gamma_0 = 0 \), for which Eq. (28) implies that the value \( \gamma(0) \) alone controls the initial curvature of the VACF (note that \( c_V(0) > 0 \)). In particular, for positive \( \gamma(0) \) the curvature is negative, and it becomes more and more negative with increasing \( \gamma(0) \). This suggests, as a trend, that the change of sign of the VACF and the minimum \( t_{\text{min}} \) occur the earlier, the larger \( \gamma(0) \) is. Physically speaking, large (positive) values of \( \gamma(0) \) lead to strong “braking” of the motion, yielding a quick change of sign of the VACF. That this is indeed a major trend can be seen in Fig. 4 where we plot the location of the first minimum as function of \( \gamma(0) \) for a large set of coupling parameters. Importantly, the corresponding network topologies include cases beyond the center topology (considered in Fig. 3), thereby enabling additional, particularly oscillating, shapes of \( \gamma(t) \). Indeed, oscillatory kernels are absent for the center topology but emerge in the chain (or fully coupled) topology, see Eq. (11). Despite the large variety of coupling parameters considered in Fig. 4 we see that the general trend described above remains valid. It is most pronounced for monotonous kernels, but oscillating kernels yield similar behavior. However, the observed trend breaks down for negative values of \( \gamma(0) \), where the initial curvature of the VACF is positive, and the direct connection to the minimum is lost.

A further question in this context is whether non-centered coupling topologies also yield other behaviors of the VACF not seen in Fig. 3. This question concerns, in particular, oscillatory kernels emerging for the chain topology, see Eq. (11), or for all-to-all coupling. Figure 4 shows three examples of corresponding VACFs with different oscillation frequencies of \( \gamma(t) \) i.e., different imaginary parts of the quantity \( \omega \) defined in Eq. (8). In all cases, \( T_1 = T_2 = 0 \). Several observations can be made. For small frequencies \( \text{Im}(\omega) \), the VACF displays oscillatory behavior, similar to the cases discussed for the center topology (where, by definition, \( \text{Im}(\omega) = 0 \)). On the other hand, for high frequencies, the VACF decays essentially monotonically and converges to the VACF of a (Markovian) system with delta-distributed friction kernel. In between these cases, one
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Figure 4.  (a) Position of the first minimum of the VACF, $t_{\text{min}}$, as function of the initial value of the friction kernel. The data pertain to $\gamma_0 = 0$ and $T_0 = 1$. Further, the constants $a_1$ and $a_2$ are randomly chosen from an uniform distribution between 0...5, and all coupling parameters are randomly chosen from an uniform distribution from $-5...5$. Therefore, the plot contains data for different coupling topologies. The different colours of data points correspond to different functional shapes of $\gamma(t)$. (b) Examplary VACFs of underdamped systems with oscillatory friction kernels characterized by different oscillation frequencies (chain topology, $T_1 = T_2 = 0$). The parameters are $a_0 = 1, a_1 = 0.5, a_2 = 1.5, k_1 = -5, b_1 = 2, k_2 = b_2 = 0, d_2 = 1$, and different values of $d_1$.

may observe VACFs with a “plateau” at intermediate times. Similar behavior occurs in the presence of colored noise (see next paragraph).

We finally consider the MSDs in the underdamped (white-noise-)systems with center topology, which are indicated in Fig. 3 by dash-dotted green lines. At very short times $\Delta t$, we observe ballistic behavior ($\propto (\Delta t)^2$) in all cases considered, consistent with the appearance of the inertial term in Eq. (1b). Further, the long-time behavior of the MSD is always diffusive, (i.e., $\propto \Delta t$). In contrast, at intermediate times, the MSD may display changes in the curvature (white region) and even non-monotonicity, as the plot at largest $k_2$ (see top left) reveals. Inspecting Fig. 3 we find that such complex behavior of the MSD occurs together with oscillations in the VACF.

3.2.2. Systems with colored noise  So far we have focused on the white-noise case, $T_1 = T_2 = 0$. To illustrate the impact of colored noise, $\xi_c$ (which represents an additional type of memory), we show in Fig. 5 the analog of the map presented in Fig. 3, yet with $T_1 = T_2 = T_0$. We recall that the VACF now involves both, $c_V^I(\Delta t)$, and $c_V^II(\Delta t)$ stemming from the correlations of the colored noise [see Eq. (23)], while the friction kernels remain unchanged. Interestingly, the differences regarding the VACFs are rather subtle (apart from different magnitudes), as a comparison with Fig. 3 reveals. Closer inspection shows that there are slight shifts of the boundaries separating different regions of the maps. More prominently, the MSDs in the case $\xi_c \neq 0$ exhibit a smoother behavior at the coupling parameters, where changes of the curvature occur at $\xi_c = 0$. 
Correlation functions of non-Markovian systems out of equilibrium

Figure 5. Same as Fig. 3 but with colored noise ($T_1 = T_2 = T_0$). To enhance visibility, the VACFs and MSDs are scaled (with factors given in Table B2 in the Appendix).

Figure 6. Examplary friction kernels [(a), (c), (e)] and corresponding VACFs [(b), (d), (f)] for underdamped systems with colored noise that fulfill the FDR. The parameters of the underlying (fully coupled) Markovian system are given in Table B3.

(compare, e.g., left bottom panels of Fig. 3 and Fig. 5). We may conclude, however, that the main trends observed already in the white-noise system, where memory arises solely through the friction kernel, remain unchanged.

To close this section, we consider in Fig. 6 examples of correlation functions in systems with all-to-all coupling of the variables and colored noise. The results do not indicate any profound changes in the VACF relative to the VACFs already discussed for simpler topologies or in the absence of colored noise. A special feature of the cases considered in Fig. 6, however, is that the friction kernel and the colored noise are related. This will be discussed in more detail in the next section.
4. Fluctuation-Dissipation relation

The non-Markovian equations derived in Sec. 2.2 formally resemble the so-called generalized Langevin equations (GLE) resulting from Mori-Zwanzig projection \[26, 27\] of, e.g., the Hamilton equations of a many-particle system onto a slow variable (such as the velocity of a tagged particle). For systems in thermal equilibrium, the frictional and stochastic forces that result from integrating out irrelevant variables balance each other, as expressed via the fluctuation-dissipation relation (FDR) \[38\] (sometimes referred to as fluctuation-dissipation theorem of second kind) between the friction kernel and the (colored) noise correlations. Here we explore the presence of a FDR for both, the under- and overdamped version of our model. However, the validity of FDR alone does not guarantee thermal equilibrium in a strict sense, different from the detailed balance (DB) condition \[51, 52\] which acts on the level of the underlying Markovian equations. For the (simpler) case of overdamped systems, we therefore study both measures (for a recent discussion of the FDR and DB in underdamped models, see \[43, 23\]).

4.1. Underdamped case

In the underdamped case, the relation of interest is given by

\[
\langle \xi(t)\xi(t+\Delta t) \rangle \overset{?}{=} \Gamma(\Delta t)\langle v^2 \rangle ,
\]

where the left hand side represents the correlations of the total noise, \( \xi = \xi_0 + \xi_c \), and \( \Gamma \) is the full friction kernel including the term involving \( \gamma_0 \) (compare Eq. (4)). Using (5), (6), (14) and (13), and noting the decoupling between white and colored noise, i.e., \( \langle \xi_0 \xi_c \rangle = 0 \) (which follows from the statistical independency of \( \xi_0 \) and \( \xi_i \)), Eq. (29) can be written as

\[
2\gamma_0 k_B T_0 \delta(\Delta t) + \langle \xi_c(t)\xi_c(t+\Delta t) \rangle \overset{?}{=} \langle v^2 \rangle \left[ 2\gamma_0 \delta(\Delta t) + \gamma^+(\Delta t) + \gamma^-(\Delta t) \right] .
\]

A valid FDR implies that Eq. (30) is fulfilled at all times \( \Delta t \). As the structure of Eq. (30) reveals, this hangs essentially on two aspects.

First, the prefactors of the delta distributions appearing on both sides of Eq. (30) must be identical (a difference can not be compensated by the remaining functions, which are finite sums of exponentials). In an equilibrium underdamped system, the equipartition theorem (with mass \( m = 1 \)) dictates \( \langle v^2 \rangle = c_V(t=0) = k_B T_0 \), such that the equality is trivially fulfilled. However, equipartition is not automatically fulfilled in the underdamped systems at hand. We note in passing that we only consider the equipartition theorem for the variable \( v \) here, and neglected the variables \( y_1, y_2 \) involved in the underlying Markovian model Eq. (1). The argument is that \( y_1, y_2 \) are considered as auxiliary variables which do not necessarily have a physical meaning [see the discussion below Eqs. (1)].
Using Eq. (23) for the VACF, the condition that the equipartition theorem for the velocity $v$ holds can be expressed as

$$\langle v^2 \rangle = c_V(0) = c_V^1 k_B T_0 \gamma_0 + c_V^{H1} k_B T_1 + c_V^{H2} k_B T_2$$

$$= k_B T_0 .$$

(31)

where $c_V^I \equiv c_V^I(0)/\gamma_0 k_B T_0$ and $c_V^{H,i} \equiv c_V^{H,i}(0)/k_B T_i$ ($i = 1, 2$). The definition of $c_V^{H,i}(0)$ follows directly from Eq. (23) when one notes that the noise correlations entering the integral separate into contributions proportional to $T_1$ and $T_2$, respectively.

The second condition for the FDR (30) to hold is the equality of the contribution from the remaining colored noise and friction kernel in Eq. (30) at any time. Clearly, for (time-)non-local friction kernels $\gamma^\pm$, the FDR at finite $\Delta t$ can only hold if the correlations of the colored noise are non-zero. Therefore, systems with $T_i = 0$ (such as considered in Fig. 3) automatically violate the FDR. There is a further, rather general observation which can be made: the colored-noise correlations have their maximum at $\Delta = 0$ [as can be seen explicitly from Eq. (14)]. Therefore, the FDR can only be fulfilled if the non-trivial part of the friction kernel has its maximum at $\Delta t = 0$ as well. This immediately implies that the systems with ring topology break the FDR.

To check the FDR at finite times, we recall from Eqs. (13) and (14) and (6) that both functions depend on time through the exponentials $\exp(-(a_1 + a_2 \pm \omega)t/2)$. The FDR can thus only be fulfilled if the coefficients of these two exponentials match. This leads to a two-dimensional matrix equation for the vector $(T_1, T_2)$

$$\left( \begin{array}{cc} \eta_1^+ - c_V^{H1} g^+ & \eta_2^+ - c_V^{H2} g^+ \\ \eta_2^- - c_V^{H1} g^- & \eta_2^- - c_V^{H2} g^- \end{array} \right) \left( \begin{array}{c} T_1 \\ T_2 \end{array} \right) = c_V^1 \gamma_0 T_0 \left( \begin{array}{c} g^+ \\ g^- \end{array} \right).$$

(32)

where [from Eq. (13)], $\eta_i^{\pm} = c_i^+ c_i^- / (a_1 + a_2 \pm \omega) + c_i^+ c_i^- / (a_1 + a_2)$, $i = 1, 2$, $g^\pm$ is defined according to Eq. (7), and we have replaced $\langle v^2 \rangle$ by Eq. (31).

From Eq. (32) it is seen that the validity of the FDR depends on both, the coupling parameters (determining the entries of the matrices), and on the temperatures of the auxiliary variables, $T_1$ and $T_2$. To test the FDR for fixed coupling parameters and fixed $T_0$, we solve Eq. (32) with respect to the vector $(T_1, T_2)$ (thereby inverting the matrix on the left hand side). If the resulting products $T_1$ and $T_2$ are real and positive, then the FDR can be satisfied. These values automatically also satisfy the equipartition condition, Eq. (31).

Due to the large parameter space, it is essentially impossible to test the validity of the FDR for every combination of coupling constant and friction parameters in the underlying Markovian model. However, some observations can be made. For $d_1 = d_2 = 0$ (center topology), closer analysis of Eq. (32) reveals that positive temperatures $T_1, T_2$ can only be found if $k_i b_i < 0$. For all-to-all coupled systems, we moreover find (from a numerical analysis) as a major trend that the “back-and-forth” coupling constants must have opposite signs and a similar magnitude, i.e., $k_i \approx -b_i$, $d_1 \approx -d_2$ (for an illustration, see Fig. 7). This signals that non-reciprocal coupling is a necessary ingredient for the
FDR to hold (along with different bath temperatures). At first sight, this finding may seem somewhat surprising, since one may suspect a violation of Newton’s third (action-reaction) law. However, one has to keep in mind that the auxiliary variables do not necessarily have a physical interpretation; moreover, if one assigns them a physical character, the latter may be velocity-like rather than position-like. Therefore, “non-reciprocal” here does not necessarily imply unbalanced mechanical forces. We also note that a similar observation, i.e., non-reciprocal coupling as a condition for a valid FDR, has been made in a (micro-)rheological model with one auxiliary variable \( n = 1 \) proposed in [1], as well as in the \( n = 1 \)-case of the linear underdamped model studied in [43] (see Appendix F of that paper).

Finally, we note that the question of whether the FDR is fulfilled is not easily inferred from inspection of the VACF and the MSD. To give some examples, we show in the right part of Fig. 6 three friction kernels with corresponding VACFs, where the FDR is satisfied. Further, in parts (a) and (b), the underlying Markovian network is all-to-all coupled, yielding the possibility of oscillatory friction kernels. It is seen that the corresponding VACF displays a plateau or oscillations. Part (c) is an example from a network with center topology, where the friction kernel decays monotonically and the VACF displays a minimum. This case is similar to the behavior in the white region in Fig. 6.

4.2. Overdamped case

In an overdamped system, it is natural to assume that at the times considered, the velocities have relaxed to their equilibrium values. Thus, the equipartition theorem for
the velocity $\langle v^2 \rangle = k_B T_0$ (with $m = 1$) is fulfilled automatically, and the FDR related to the non-Markovian equation (16) is given by

$$\langle \xi(t)\xi(t+\Delta t) \rangle = \Gammak_B T_0$$

(33)
or (using the cancellation of delta-like terms)

$$\langle \xi_c(t)\xi_c(t+\Delta t) \rangle = k_B T_0 \left[ \gamma^+ (\Delta t) + \gamma^- (\Delta t) \right]$$

(34)

where the functions on the right side are defined in Eq. (17). Equation (34) can again be written as a matrix equation for the temperatures $T_1, T_2$, which can be solved numerically.

A result of such a calculation is presented in Fig. 8 where we have fixed all coupling constants except $k_1, b_1$ which relate the main variable (here $x$) and the first auxiliary variable, $y_1$. In the green, shaded areas of the $k_1-b_1$-plane, the calculated temperatures $T_1$ and $T_2$ are real and positive and thus, the FDR holds. Interestingly, these areas include large regions characterized by non-reciprocal coupling ($k_1 \neq b_1$) and even (small) regions where $k_1$ and $b_1$ have opposite signs. Moreover, we find (numerically) that in the areas where the FDR holds, the potential energy in the harmonic trap fulfills equipartition, i.e., $1/2 \langle x^2 \rangle = 1/2 k_B T_0$.

A special situation occurs on the diagonal, i.e., for the reciprocal choice $k_1=b_1$ (note that the other coupling constants are reciprocally chosen as well). Here, the resulting temperatures are all equal, i.e., $T_1 = T_2 = T_0$. Moreover, this fully reciprocal situation satisfies not only the FDR, but also the more severe detailed balance (DB) condition [51]. The latter can be checked by considering the probability currents (related to the three variables) in the corresponding Fokker-Planck equation, see [23, 51, 43]. In this context it is important to note that, under certain conditions, the DB condition for the linear system at hand can also be fulfilled with non-reciprocal coupling or different temperatures [23]. In the special case considered in Fig. 8 however, DB only holds on the diagonal. Combining this with our findings regarding the FDR, we see that there are indeed large parameter regions (with non-reciprocal coupling, see green areas), where DB is violated, but the FDR is satisfied.

The regions in Fig. 8 can be analysed on the Markovian level of our model, as well. Along the diagonal $k_i = b_i$, the Markovian model corresponds to overdamped Brownian particles coupled to each other with springs (see top panel on the right). For negative $k_i = b_i$, the force resulting from the spring has the opposite direction, as for positive $k_i = b_i$, which corresponds to the use of a deflection pulley (see bottom panel). For $k_i \neq b_i$, the coupling is non-reciprocal and does not correspond to any type of mechanical coupling (see middle panel).

5. Application

In this final section, we discuss an example illustrating that the rather generic models and corresponding correlation functions introduced before can be used to provide a simple description (fitting) of correlation functions in a real system.
Figure 8. Illustration of the ranges of the coupling constants $k_1$, $b_1$ in which the FDR can be fulfilled in the overdamped case (green areas). The corresponding (positive) temperatures $T_1$, $T_2$ depend on the combination $(k_1, b_1)$ considered, while the remaining parameters are fixed ($T_0 = 1$, $k_2 = b_2 = 1$, $d_1 = d_2 = 1$, and $a_0 = 3.6$, $a_1 = 3$, $a_2 = 2$). Along the diagonal line (reciprocal coupling), detailed balance (DB) holds. For $k_1 = b_1 > 0$ (violet part of the diagonal), the parameters correspond to a Brownian particle coupled to other Brownian particles and a fixed point via springs, see top panel on the right. For $k_1 = b_1 < 0$ (blue part of the diagonal), the system can still fulfill DB (mechanically, $y_1$ may be viewed as a deflection pulley), see bottom panel on the right. The middle panel on the right illustrates the case of non-reciprocal coupling between $x$ and $y_1$, where however, the FDR is still fulfilled.

Specifically, inspired by the combined experimental-theoretical study presented in Ref. [45], we consider correlation functions of a micron-sized colloidal particle suspended in a viscous solvent. The colloidal particle is optically “trapped”, i.e., exposed to a confining potential. The focus of Ref. [45] was the measurement and theoretical description of colored noise related to “anticorrelations” in the position autocorrelation function (PACF), that is, regions of negative values of the PACF at intermediate times, as visible from the dotted line in Fig. 9.

Physically, the anticorrelations are induced by hydrodynamic backflow: the particle transfers momentum to the surrounding medium [45], which generates vortices at the sphere’s surface. These vortices then diffuse over one particle radius on a timescale $\tau_f$. 
Correlation functions of non-Markovian systems out of equilibrium

Figure 9. Positional autocorrelation function (PACF) of a colloidal bead in a static optical trap. Black dots denote normalized experimental data [45]. The negative overshoot arises due to hydrodynamic backflow at the timescale $\tau_f$ of vortices generated at the surface of the bead. We have fitted the PACF (red line) using a model with two auxiliary variables, as schematically shown in the same inset.

which eventually leads to a backward force acting on the particle at later times [53].

Clearly, the simple models introduced in the present paper cannot provide a full hydrodynamic description of this effect (as it was done, e.g., in [51, 55]), in particular, our models can not describe the detailed time-dependency of the PACF ($\propto t^{-3/2}$) in the long-time limit. Still, by a systematic fit of the experimental data for the PACF in [45] we found that the general shape of the PACF, particularly the emergence of anticorrelations, can be mimicked by our simple linear model with two auxiliary variables. Since the effects we are mainly interested in take place well-above the ballistic timescale, we employ, for the sake of simplicity, the overdamped model (3). Note that the parameter $a_0$ (coupling linearly to the position) then corresponds to the harmonic trap.

Our fitting strategy was guided by the following considerations. In the first place, we attempted to fit the data with a reduced version of Eq. (3) involving only one auxiliary variable, $y_1$ (subject to a heat bath), yielding single-exponential memory and colored noise. It turns out that with this ansatz, one can either mimic the initial decay or the decay of the anticorrelations, but not the full PACF. This shows that (at least) two auxiliary variables are required. In this context we note that the definition of a Markovian “model” corresponding to given data is not unique, and we here aim for a most simple one. To keep the number of fitting parameters as small as possible, we fixed $a_0$ to $a_0^{-1} = \tau_K = 42.7 \mu s$, which is the timescale corresponding to the harmonic force given in the experiment. The auxiliary variables were incorporated using a special, non-reciprocal, version of the center topology (where $y_2$ is coupled only unidirectionally to $x$, i.e., $b_2 = 0$) with positive temperatures $T_i$. With $a_2 > 0$ and $T_2 > 0$, the variable $y_2$ is then governed by an Ornstein-Uhlenbeck process. The resulting non-Markovian
model involves a (single-) exponentially decaying kernel [see Eq. (12)], with decay time \( \tau_1 = 1/a_1 \); \( y_2 \) does not contribute to the friction kernel but to the colored noise. The actual parameter values resulting from the fitting procedure (carried out with a Nelder Mead algorithm [56]) are given in Table B4 in Appendix B.

The resulting PACF is shown as a red line in Fig. 9. One can see that it describes the measured data quite well. It is interesting to look in more detail at the timescales (marked at the top of Fig. 9). The smallest timescale is \( \tau_f \), which was determined in [45] and measures the vortex diffusion. The other three timescales correspond to the three variables of our model. We recall that \( \tau_K \) was used to fix \( a_0 \). Further, \( \tau_2 = 1/a_2 \), which is much smaller than \( \tau_K \), is located within the region of initial decay. This conforms with the idea that the Ornstein-Uhlenbeck process \( y_2 \) provides a “kick” into the system affecting the first decay. Indeed, due to the unidirectional coupling between \( x \) and \( y_2 \) our model has purely non-equilibrium character in the sense that it does not satisfy the FDR, nor DB [23]. This is in contrast to the (underdamped) Langevin equation used in Ref. [45] where the FDR is assumed to hold from the outset. The largest timescale \( \tau_1 = 1/a_1 \), which is related to \( y_1 \), is larger by several orders of magnitude than \( \tau_K \). It falls in the region where anti-correlations occur. Thus, in this sense, the coupling with the auxiliary variable \( y_1 \) mimics the effect of the hydrodynamic backflow.

6. Conclusions and outlook

In this paper we have provided a comprehensive study of autocorrelation functions of non-Markovian systems which can be mapped to linear Markovian systems with two embedded (auxiliary) variables. The two levels of description can be connected by a projection procedure, very similar to Mori-Zwanzig-like coarse-graining approaches. In the resulting equation for the variable of interest, the non-Markovianity then appears through (time-nonlocal) friction kernels and colored noise. Contrary to the standard GLE, however, here we do not assume that the coupling terms involved in the Markovian equations are reciprocal, i.e., derivable from an underlying Hamiltonian. In other words, the resulting “forces” (related to position-dependent terms) can violate Newton’s third law. Our analysis pertains to linear systems with few variables, which enables us to perform all calculations analytically. This includes, in particular, the calculation of autocorrelation functions of the velocity (underdamped systems) or position (overdamped systems), which are experimentally accessible quantities in a large variety of soft matter systems.

As a first step, we have explored in detail the interplay between the coupling topology of the underlying Markovian equations and the resulting friction kernel. In particular, already with two auxiliary variables one can describe highly non-trivial kernels including oscillations, finite values at zero time, and non-monotonicity with maxima or minima at finite times. For the linear systems at hand, these kernels are independent of the heat baths to which the auxiliary variables are coupled. Second, already the relatively simple center topology with (white) noise only in the main variable...
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allows to describe a range of behaviors of time-dependent autocorrelation functions of the velocity (underdamped case) or position (overdamped) case, including, in particular, oscillatory behavior (see Fig. 3). The first minimum of the autocorrelation function can be related to the instantaneous value of the friction kernel.

In calculating the correlation functions, the case of non-zero auxiliary temperatures ($T_1 \neq 0, T_2 \neq 0$) and thus, colored noise, turned out to be doable, yet quite cumbersome. Therefore it was interesting to see that including this colored noise did not introduce truly new features in the correlation functions. Thus, when modelling friction kernels by simple ansatzes, starting from deterministic auxiliary equations seems to be the most plausible choice. However, colored noise becomes crucial when one requires that the non-Markovian model satisfies the FDR (or even DB). Clearly, this is well established for standard GLEs, but not in the present systems, where the existence of equilibrium is not guaranteed. We have separately investigated the FDR in the underdamped and overdamped systems, thereby deriving explicit conditions which were then checked numerically. In the actual underdamped systems considered, the FDR can only be satisfied for non-reciprocal coupling. This is different in the overdamped case where, for the topology considered, the coupling (corresponding to mechanical forces) had to be reciprocal for the FDR to be fulfilled. In the overdamped case, we have additionally checked the DB condition. Interestingly, we found parameter regions (characterized by non-reciprocal coupling) where FDR is fulfilled but not DB. We note that for the class of systems studied here (no additional external forces), situations where FDR is fulfilled but DB is violated do not occur if only one auxiliary variable is involved [23]. This confirms (along with our results for the correlation functions) that the choice $n = 2$ introduces indeed novel aspects of the system’s properties.

The results of the present paper may be of interest in several contexts. This concerns, first, the modelling of actual experimental data. A classical example is passive or active microrheology, where one measures the diffusive (or active) motion of a micro-sized object through a viscous fluid. An example of such a modeling was discussed in Sec. 5 where we demonstrated that our model with two auxiliary variables provides indeed a good description of the experimentally measured PACF data. Furthermore, the simple ansatzes suggested here may also be used to fit numerical data (e.g., from Molecular dynamics or Brownian Dynamics simulations) for autocorrelation functions, where the corresponding kernels then follow from the fitted coupling constants. For example, a two-exponential kernel (with a maximum) has recently found to be sufficient to explain oscillatory PACF in a colloidal system [2]. Our results for the appearance of oscillations are consistent with [2], and by exploring a broader parameter space (i.e., topologies of the underlying Markovian network), we provide a complete picture of the achievable behaviors. Moreover, the simple models may also be used as an inspiration to introduce, at a relatively low computational cost, memory effects in numerical simulations of complex many-particle systems by adding few degrees of freedom to each true particle (for a recent discussion of the use of embedding techniques in numerical simulations, see [35]).
From a more fundamental point of view, the present study contributes to the understanding of non-Markovian systems regarding their non-equilibrium character and, connected with that, the impact on measurable quantities. Here we have focused on the FDR and DB as measures of equilibrium (for a discussion of further thermodynamic notions in related linear systems, see, e.g., [13, 23]). Interestingly, we have found that the autocorrelation functions do not really reflect whether or not these equilibrium conditions are fulfilled. Finally, while the present work was mostly devoted to the non-Markovian dynamics of a single particle, it seems interesting to explore an extension towards coupled systems. Work in this direction is on the way.

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Appendix A. Projection

In this Appendix we provide the details of the derivation of the non-Markovian equations in Sec. 2.2.

Appendix A.1. Derivation of kernel and colored noise

To project the Markovian Langevin equations (1) and (3) onto equations for the main dynamical variables, we utilize the Laplace transform [57] defined by \( \mathcal{L}\{g(t)\}(s) = \int_0^\infty g(t)e^{-st}dt \equiv \hat{g}(s) \). In the underdamped case, we obtain from Eq. (1)

\[
\begin{align*}
sv - v_0 &= -\gamma_0 \hat{v} + k_1 \hat{v} + k_2 \hat{y}_2 + \hat{\xi}_0(t) \\
\hat{y}_1 &= -a_1 \hat{y}_1 + b_1 \hat{v} + d_1 \hat{y}_2 + \hat{\xi}_1(t) \\
\hat{y}_2 &= -a_2 \hat{y}_2 + b_2 \hat{v} + d_2 \hat{y}_1 + \hat{\xi}_2(t)
\end{align*}
\]

Here, \( v_0 \) is the initial velocity, and we have set the initial values of \( y_1 \) and \( y_2 \) to zero. This is since we are mainly interested in the long-time behavior, where the system has achieved a steady state, where the initial conditions become irrelevant. Rearranging and inserting the equations into one another we find

\[
\begin{align*}
sv - v_0 &= -\gamma_0 \hat{v} \\
&+ \left[ \frac{b_1(s + a_2)}{(s + a_1)(s + a_2) - d_1d_2} + \frac{d_1b_2}{(s + a_1)(s + a_2) - d_1d_2} \right] k_1 \hat{v} \\
&+ \left[ \frac{b_2(s + a_1)}{(s + a_2)(s + a_1) - d_1d_2} + \frac{d_2b_1}{(s + a_1)(s + a_2) - d_1d_2} \right] k_2 \hat{v} \\
&+ \left[ \frac{k_1(s + a_2)}{(s + a_1)(s + a_2) - d_1d_2} \hat{\xi}_1 + \frac{k_1d_1}{(s + a_1)(s + a_2) - d_1d_2} \hat{\xi}_2 \right] \\
&+ \left[ \frac{k_2(s + a_1)}{(s + a_2)(s + a_1) - d_1d_2} \hat{\xi}_2 + \frac{k_2d_2}{(s + a_1)(s + a_2) - d_1d_2} \hat{\xi}_1 \right].
\end{align*}
\]
To transform Eq. (A.3) back into the time domain we use the convolution theorem
\[ \mathcal{L}^{-1}\{\hat{f}(s) \cdot \hat{g}(s)\} = \int_0^t f(t-u)g(u)du \] and the inverse Laplace transforms
\[ \mathcal{L}^{-1}\{\frac{1}{(s + a_1)(s + a_2) - d_1d_2}\} = \frac{1}{\omega}e^{-(a_1+a_2)t/2}\text{Sinh}(\omega t/2) \]
\[ \mathcal{L}^{-1}\{\frac{s + a_2}{(s + a_1)(s + a_2) - d_1d_2}\} = e^{-(a_1+a_2)t/2}[\text{Cosh}(\omega t/2) + (a_2 - a_1)\text{Sinh}(\omega t/2)/\omega], \tag{A.4} \]
where \(\omega\) is given in Eq. (8). Applying the relations (A.4) to the terms on the right side of Eq. (A.3) and sorting with respect to \(v\) finally brings us to Eq. (4), which involves the colored noise
\[ \xi_c(t) = \int_0^t dt' \exp[-\omega^+ t'] \left( c_1^+ \xi_1(t') + c_2^+ \xi_2(t') \right) \]
\[ + \int_0^t dt' \exp[-\omega^- t'] \left( c_1^- \xi_1(t') + c_2^- \xi_2(t') \right) \tag{A.5} \]
with the constants
\[ c_1^\pm = \frac{k_1}{2} \mp \frac{a_2k_1 - a_1k_1 + 2d_2k_2}{2\omega} \]
\[ c_2^\pm = \frac{k_2}{2} \mp \frac{a_1k_2 - a_2k_2 + 2d_1k_1}{2\omega}, \tag{A.6} \]
and
\[ \omega^\pm = \frac{a_1 + a_2 \pm \omega}{2}. \tag{A.7} \]

Appendix A.2. Correlations of the colored noise

To derive Eq. (13) in the main text, we multiply the instantaneous values of the colored noise, \(\xi_c\) [see Eq. (A.5)] at two times \(t, t + \Delta t\) and then perform the noise average. Taking into account that the noise terms related to different auxiliary variables are uncorrelated, i.e., \(\langle \xi_1(t)\xi_2(t') \rangle = 0 \ \forall t, t'\), it is clear that the final correlation function is a sum of contributions involving \(\xi_1\) and \(\xi_2\), respectively. Here we focus on the terms
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related to $\xi_1$. Assuming $\Delta t > 0$, one finds

$$
\langle \xi_c(t + \Delta t) \xi_c(t) \rangle_1 = \int_0^t dt' \int_0^{t+\Delta t} du \left( c_1^+ c_1^- e^{-(\omega_+ + \omega_-) t'} + c_1^+ c_1^- e^{-(\omega_+ - \omega_-) u} \right) \langle \xi_1(t - t') \xi_1(t + \Delta t - u) \rangle
$$

(A.8)

$$
= 2k_B T_1 \int_0^t dt' c_1^+ c_1^- e^{-(\omega_+ + \omega_-) t'} + c_1^+ c_1^- e^{-(\omega_+ - \omega_-) t'}
$$

(A.9)

$$
= -2k_B T_1 \left[ \frac{c_1^+ c_1^-}{\omega_+ + \omega_-} e^{-(\omega_+ + \omega_-) t'} + \frac{c_1^- c_1^+}{2\omega_-} e^{-(\omega_+ + \omega_-) t'} \right] \bigg|_{t' = 0}^{t = t + \Delta t}
$$

(A.10)

$$
= 2k_B T_1 \left( -\frac{c_1^+ c_1^-}{2\omega_+} e^{-(\omega_+ + \omega_-) t'} - \frac{c_1^- c_1^+}{\omega_+ + \omega_-} e^{-(\omega_+ + \omega_-) t'} - \frac{c_1^- c_1^+}{2\omega_-} e^{-(\omega_+ + \omega_-) t'} \right)
$$

(A.11)

$$
= 2k_B T_1 \left[ \frac{c_1^+ c_1^-}{2\omega_+} e^{-\omega_+ \Delta t} \left( 1 - e^{-w_+ 2t} \right) + \frac{c_1^- c_1^+}{\omega_+ + \omega_-} e^{-\omega_- \Delta t} \left( 1 - e^{-(\omega_+ + \omega_-) t} \right) \right]
$$

(A.12)

By the same steps, one obtains the contribution involving $\xi_2$, yielding the same result but with changed indices $1 \leftrightarrow 2$. The sum of the two contributions then yields the full correlation function of the colored noise, Eq. (13).

Appendix A.3. Friction kernel in the overdamped case

For the overdamped case, the derivation of the projected equation (15) is identical to that of Eq. (4). In order to find the friction kernel for the velocity $\dot{x}$, we use integration by parts

$$
\int_0^t G(t - t') x(t') dt'
$$

$$
= -2g \frac{e^{-(a_1 + a_2 + \omega) t/2} x(0) - x(t)}{a_1 + a_2 + \omega}
$$

$$
- 2g \frac{e^{-(a_1 + a_2 - \omega) t/2} x(0) - x(t)}{a_1 + a_2 - \omega} + \int_0^t \tilde{\Gamma}(t - t') v(t') dt',
$$

(A.13)
Table B1. Parameters for the functions $\gamma(t)$ plotted in Fig. 2. The abbreviations are “dec” for monotonically decaying (grey lines), “max” (“min”) for non-monotonic with a maximum (minimum) at a finite time (blue solid (dashed) lines), and “osc” for oscillating (red lines).

|      | $a_1$ | $a_2$ | $k_1$ | $k_2$ | $b_1$ | $b_2$ | $d_1$ | $d_2$ |
|------|-------|-------|-------|-------|-------|-------|-------|-------|
| Fig. 2(a) |       |       |       |       |       |       |       |       |
| dec  | 2     | 2     | -1    | -1    | 1     | 1     | 1     | 1     |
| max  | 5.37  | 0.79  | -2    | -3.35 | -1.01 | 0.29  | 0.04  | 0.61  |
| osc  | 0.85  | 0.29  | -0.069| 0.58  | -2.03 | 0.84  | -1.54 | 2.61  |
| Fig. 2(b) |       |       |       |       |       |       |       |       |
| min  | 2.18  | 2.13  | 0     | -1.34 | -0.82 | 0     | 0     | 2.05  |
| max  | 3.64  | 0.79  | 0     | 0.05  | 32.17 | 0     | 0     | -3.25 |
| Fig. 2(c) |       |       |       |       |       |       |       |       |
| dec  | 1     | 1     | -1    | 0     | 1     | 0     | 1     | 0.10  |
| osc  | 0.10  | 0.20  | -0.67 | 0     | 1     | 0     | -1    | 1     |
| min  | 2     | 0.20  | -1.0  | 0     | 1     | 0     | -0.68 | 1     |
| Fig. 2(d) |       |       |       |       |       |       |       |       |
| dec  | 1     | 2     | -0.5  | -0.50 | 1     | 1     | 0     | 0     |
| min  | 0.50  | 1.50  | 0.95  | -1.90 | 1     | 1     | 0     | 0     |
| max  | 0.50  | 1.50  | -1.44 | 1.44  | 1     | 1     | 0     | 0     |

where $\tilde{\Gamma}(t)$ is the desired friction kernel defined below Eq. (16) in the main text, and $g^\pm$ has been defined in Eq. (7). In the long time limit, the exponential functions in the first lines of (A.13) vanish. What remains from these terms is a term proportional to the position, which we name $-(a'_0 - a_0)x(t)$. This finally leads to Eq. (16).

Appendix B. Parameters und data extraction

In this Appendix we provide numerical values characterizing various parameter sets used in this study. Table B1 contains parameters for the non-trivial parts of the friction kernel, $\gamma(t)$, plotted in Fig. 2. Table B2 provides the scaling factors of the VACFs and MSDs in Fig. 3 and Fig. 5 which have been introduced to enhance visibility. Table B3 contains the parameters for the systems considered in Fig. 6. Finally, Table B4 contains the parameter values used for the fitting of the (experimentally obtained) PACF in Fig. 9. The experimental data of the log scaled PACF have been extracted from the PDF file of [45]. To this end, we have manually extracted the data points in the time regimes of interest using the tool WebPlotDigitizer [58].

Appendix C. Green’s function in the time domain

In this Appendix we present the derivation of Eq. (21), starting from the Fourier transform of the Green’s function given in Eq. (20). We focus on the case $\kappa = 0$,
Table B2. Factors by which the VACFs and MSDs plotted in Fig. 3 and Fig. 5 are scaled:

| Figure panel | VACF | MSD |
|--------------|------|-----|
| upper left   | 1.58 | 0.74 |
| middle left  | 2.64 | 0.56 |
| lower left   | 12.25 | 11.80 |
| upper right  | 0.64 | 0.06 |
| middle right | 3.76 | 0.49 |
| lower right  | 5.35 | 1.21 |

| Figure panel | VACF | MSD |
|--------------|------|-----|
| upper left   | 0.48 | 0.09 |
| middle left  | 2.28 | 0.41 |
| lower left   | 5.19 | 1.36 |
| upper right  | 0.57 | 0.05 |
| middle right | 1.68 | 0.13 |
| lower right  | 3.03 | 0.44 |

Table B3. Parameters for the functions $\gamma(t)$ and corresponding VACFs plotted in Fig. 6.

| $T_0$ | $T_1$ | $T_2$ | $\gamma_0$ | $a_1$ | $a_2$ | $k_1$ | $k_2$ | $b_1$ | $b_2$ | $d_1$ | $d_2$ |
|-------|-------|-------|-------------|------|------|------|------|------|------|------|------|
| a)    | 3.72  | 2.80  | 1.10        | 4    | 1    | 2    | -0.83| -1.22| 1    | 1    | 3    | -2.50|
| b)    | 3.72  | 3.06  | 0.44        | 4    | 1    | 2    | -1.22| -2.00| 1    | 1    | 2    | -2.00|
| c)    | 3.72  | 0.58  | 0.93        | 4    | 1    | 2    | -1.60| -2.00| 1    | 1    | 0    | 0    |

Table B4. Fit parameters from fit in Fig. 9 with $C_i = \sqrt{2k_BT_i/\gamma_i}$. We set $b_2 = 0$. To translate to real time, the constants $a_0, a_1, a_2$ have to be multiplied with 45823s$^{-1}$.

| $a_0$ | $a_1$ | $a_2$ | $k_1 b_1$ | $C_0$ | $C_1$ | $k_2 C_2$ |
|-------|------|------|----------|------|------|----------|
| 0.511 | 0.172| 1.472 | -0.0402  | 0.65 | 4.9619| 1.3451   |

but briefly comment on the case $\kappa > 0$ after Eq. (C.9). As a first step, we calculate the Fourier transform of the full friction kernel, $\hat{\Gamma}(t)$. Using $\hat{h} = \mathcal{F}[h(t)](f) = \int_{-\infty}^{\infty} dt h(t) \exp[ift]$ and inserting Eq. (5) we find

$$
\hat{\Gamma}(f) = \int_0^\infty dt \left[ 2\gamma_0 \delta(t) + g^+ \exp \left( -(a_1 + a_2 + \omega) \frac{t}{2} \right) + g^- \exp \left( -(a_1 + a_2 - \omega) \frac{t}{2} \right) \right] \times \exp[ift] 
$$

(C.1)

where we have omitted the negative part of the integral because $\Gamma(t) = 0$, $t < 0$ (due to causality), and $g^+$ and $\omega$ are defined in Eqs. (7) and (8), respectively. Carrying out the integrals yields

$$
\hat{\Gamma}(f) = \gamma_0 + \frac{g^+}{\frac{1}{2}(a_1 + a_2 + \omega) - if} + \frac{g^-}{\frac{1}{2}(a_1 + a_2 - \omega) - if} .
$$

(C.2)

Inserting Eq. (C.2) into Eq. (20) and using Eq. (A.7), we obtain

$$
\hat{\lambda}(f) = - \left[ if - \gamma_0 - \frac{g^+}{\omega^+ - if} - \frac{g^-}{\omega^- - if} \right]^{-1} 
$$

(C.3)
To perform the back transformation we perform a partial fraction decomposition. To this end we find the common denominator of the fraction appearing in the brackets \[ \ldots \] in Eq. (C.3) and substitute \( \tilde{f} = if \). This yields
\[
\hat{\lambda}(-if) = \frac{-(\omega^+ - \tilde{f})(\omega^- - \tilde{f})}{(a_0 + \tilde{f})(\omega^+ - \tilde{f})(\omega^- - \tilde{f}) + g^+ (\omega^- - \tilde{f}) + g^- (\omega^+ - \tilde{f})} . \tag{C.4}
\]

The denominator is a polynomial of third order, which therefore has three complex roots \( F_1, F_2 \) and \( F_3 \). These can be expressed explicitly in terms of the parameters \( a_i, k_i \) and \( b_i \). The most convenient way to find these (quite cumbersome) expressions is to use computer algebra programs, for example Mathematica.

Having obtained the roots, Eq. (C.4) can be rewritten as
\[
\hat{\lambda}(f) = -\frac{(\omega^+ - if)(\omega^- - if)}{(if - F_1)(if - F_2)(if - F_3)} , \tag{C.5}
\]
which we now aim to express as
\[
\hat{\lambda}(f) = \frac{\epsilon_1}{if - F_1} + \frac{\epsilon_2}{if - F_2} + \frac{\epsilon_3}{if - F_3} . \tag{C.6}
\]
The remaining task is to determine the constants \( \epsilon_1, \epsilon_2 \) and \( \epsilon_3 \). To this end we obtain the common denominator in Eq. (C.6) and compare the resulting numerator with the one in Eq. (C.5), yielding
\[
-(\omega^+ - if)(\omega^- - if) \overset{1}{=} \epsilon_1(if - F_2)(if - F_3) + \epsilon_2(if - F_1)(if - F_3) + \epsilon_3(if - F_1)(if - F_2) . \tag{C.7}
\]
The left and right hand sides of Eq. (C.7) are polynomials of degree two in \( f \). In order to fulfil (C.7) for all values of \( f \), the coefficients of the polynomials on both sides have to be identical. This yields the following explicit expressions for \( \epsilon_1, \epsilon_2, \) and \( \epsilon_3 \) in terms of the roots,
\[
\epsilon_1 = \frac{(\omega^+ - F_1)(F_1 - \omega^-)}{(F_1 - F_2)(F_1 - F_3)} ; \quad \epsilon_2 = \frac{(\omega^+ - F_2)(\omega^- - F_2)}{(F_1 - F_2)(F_2 - F_3)} ; \\
\epsilon_3 = \frac{(\omega^+ - F_3)(\omega^- - F_3)}{(F_1 - F_3)(-F_2 + F_3)} . \tag{C.8}
\]
The last step of the calculation is the back transform of Eq. (C.6) into the time domain,
\[
\lambda(t) = \sum_{k=1}^{3} \mathcal{F}^{-1} \left[ \frac{\epsilon_k}{if - F_k} \right] \\
= -\sum_{k=1}^{3} \epsilon_k \exp[-F_k t] \theta(t) \tag{C.9}
\]
In Eq. (C.9), the Heaviside step function ensures causality. This function arises if we assume that the real parts of \( F_k \) are positive, which we (numerically) find to be satisfied for all parameters where the Markovian system is stable (see discussion of Fig. 3). This finally leads to Eq. (21) in the main text.

In the case \( \kappa > 0 \) [corresponding to a finite confining potential in Eq. (1b)], the denominator’s degree of Eq. (C.5) is increased by one (yielding four roots), and we end up with an expression for \( \lambda(t) \) identical to Eq. (C.9), except that the sum contains four (instead of three) terms. We have used this approach to calculate the VACF for \( \kappa > 0 \) for systems with center topology.

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