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Communication: Universal Markovian reduction of Brownian particle dynamics

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Non-Markovian processes can often be turned Markovian by enlarging the set of variables. Here we show, by an explicit construction, how this can be done for the dynamics of a Brownian particle obeying the generalized Langevin equation. Given an arbitrary bath spectral density J_0, we introduce an orthogonal transformation of the bath variables into effective modes, leading stepwise to a semi-infinite chain with nearest-neighbor interactions. The transformation is uniquely determined by J_0 and defines a sequence $\{J_n\}_{n\in\mathbb{N}}$ of residual spectral densities describing the interaction of the terminal chain mode, at each step, with the remaining bath. We derive a simple one-term recurrence relation for this sequence and show that its limit is the quasi-Ohmic expression provided by the Rubin model of dissipation. Numerical calculations show that, irrespective of the details of J_0, convergence is fast enough to be useful in practice for an effective Ohmic reduction of the dissipative dynamics. © *2011 American Institute of Physics*. [doi:10.1063/1.3532408]

I. INTRODUCTION

The study of open systems, in both the classical and the quantum case, is a subject of major interest in physics, chemistry, and various other disciplines. In many applications and fundamental experiments, one is faced with the reduced dynamics of a relatively simple subsystem which can be manipulated and measured, while the environment is only partially under control. A thorough understanding of the ensuing dynamics has been obtained for the Markovian case, in which feedback from the environment to the system can be neglected, and general analytical results are available together with efficient numerical algorithms.[1] The situation is much more involved in the non-Markovian regime, which typically arises due to strong coupling and similar time scales of system and bath evolution. Although general non-Markovian strategies are, to some extent, available,[1] they typically lack simple results of general validity which lead to numerically feasible approaches. A bridge between the two situations can be built relying on a suitable embedding of a non-Markovian dynamics in a Markovian one, as recently addressed in Refs. 2 and 3. Indeed, while it is common wisdom that a non-Markovian process can be embedded in a Markovian one by a suitable enlargement of the number of relevant variables already at a classical level, there is no universal recipe for how this can be done and which class of non-Markovian processes can be reached.

In the present communication, we demonstrate how such a Markovian reduction can be achieved for the ubiquitous model of dissipation provided by a Brownian particle, or a two-level system, linearly coupled to a bath of harmonic oscillators characterized by an arbitrary spectral density (SD).[4] The procedure is physically transparent, in that it focuses exclusively on the SD, and all relevant quantities can be constructed in terms of the SD. As will be shown below, the system dynamics can equivalently be described including, besides the Brownian particle degree of freedom, a set of effective environmental modes coupled in a linear-chain fashion. The terminal mode of the chain couples to a residual bath and undergoes a Brownian-like dynamics, which rapidly approaches an Ohmic behavior over the whole interval of relevant frequencies as the length of the chain increases. The model as such is closely related to Mori's theory[5] and its generalizations.[6] While previous work by two of us[2] has focused on the implications of a truncation of such effective mode chains with a strictly Ohmic reservoir, the present analysis proves the convergence toward Ohmic behavior, and therefore the general validity of the procedure.

II. EFFECTIVE-MODE TRANSFORMATION

Our starting point is the Caldeira–Leggett Hamiltonian,[4] here written in mass-weighted bath coordinates x_k,

$$H = \frac{p^2}{2m} + V(s) + \frac{1}{2}\sum_{k=1}^{N}\left[p_k^2 + \omega_k^2\left(x_k - \frac{c_k}{\omega_k^2}s\right)^2\right], \qquad (1)$$

which is known to lead, in the continuum limit, to a generalized Langevin dynamics for the system described by the s degree of freedom. The reduced system dynamics is entirely determined by the system potential $V(s)$ and the SD of the

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environmental coupling, $J_0(\omega)$, which reads[1]

$$J_0(\omega) = \frac{\pi}{2}\sum_{k=1}^{N}\frac{c_k^2}{\omega_k}\delta(\omega-\omega_k). \tag{2}$$

In general, $J_0(\omega)$ is a real odd parity function defined by the real part of the frequency-dependent memory kernel $\gamma(\omega)$ entering the generalized Langevin equation (GLE), namely, $J_0(\omega) = m\omega \mathrm{Re}\gamma(\omega)$ and $J_0(\omega) \geq 0$ for $\omega > 0$. It fully determines $\gamma(\omega)$ by virtue of the Kramers–Kronig relations, as well as the correlation function of the GLE random force by virtue of the fluctuation-dissipation theorem. In the following, we assume, as a typical situation, that $J_0(\omega)$ is strictly positive and continuous in the interval $(0, \omega_R)$, with ω_R a high-frequency cutoff, and zero elsewhere.

Given a GLE and its SD J_0, a microscopic model for the dissipative dynamics of the s degree of freedom can be defined from Eq. (2), e.g., by introducing a bath of harmonic oscillators with evenly spaced frequencies $\omega_k = k\Delta\omega$ $(k = 1, \ldots N)$ and setting the coupling coefficients of Eq. (1) to $c_k = \sqrt{2\omega_k \Delta\omega J_0(\omega_k)/\pi}$. The system-bath interaction term in Eq. (1)

$$H^{\mathrm{int}} = -\sum_{k=1}^{N} c_k x_k s = -D_0 X_1 s \tag{3}$$

naturally introduces an effective mode $X_1 = \sum_{k=1}^{N} c_k x_k / D_0$, where D_0 is a normalization constant, $D_0^2 = \sum_{k=1}^{N} c_k^2$. This defines the first column of an otherwise arbitrary, orthogonal matrix $\boldsymbol{T}$ transforming the bath coordinates $\boldsymbol{x}^t = (x_1, \ldots, x_N)$ into $\boldsymbol{X}^t = (X_1, X_2', \ldots, X_N')$, $\boldsymbol{X} = \boldsymbol{T}^t\boldsymbol{x}$. The transformation can be fixed by requiring that the "residual" bath composed of coordinates $X_2', X_3', \ldots, X_N'$ is in normal form, with eigenfrequencies $\bar{\Omega}_i, i = 2, \ldots N$. The SD $J_0(\omega)$ *alone*, on the other hand, directly fixes the frequency Ω_1 of the effective mode and its coupling coefficient D_0, as indicated below, Eq. (5). The couplings $C_k = -(\boldsymbol{T}^t\boldsymbol{\omega}^2\boldsymbol{T})_{1,k}$ $(k = 2, \ldots N)$ between the normal modes of the residual bath and X_1 allow one to rewrite Eq. (1) as a Caldeira–Leggett-like Hamiltonian for the X_1 degree of freedom, thereby defining the SD $J_1(\omega)$ "felt" by the effective mode X_1, which is the only bath mode directly coupled to the s degree of freedom. Clearly, in the continuum limit, the procedure can be indefinitely iterated and used to define a sequence of effective modes $X_1, X_2, \ldots, X_M, \ldots$ coupled in a linear-chain fashion, *and* a corresponding sequence of SDs, $J_1, J_2, \ldots, J_M, \ldots$, characterizing the residual bath "felt" by each mode. In this way, one introduces an orthogonal coordinate transformation which converts the continuum version of Eq. (1) into the form

$$H = \frac{p^2}{2m} + V(s) + \Delta V(s) - D_0 s X_1 + -\sum_{n=1}^{\infty} D_n X_n X_{n+1} + \frac{1}{2}\sum_{n=1}^{\infty}\left[P_n^2 + \Omega_n^2 X_n^2\right], \tag{4}$$

where, for $n \geq 0$,

$$D_n^2 = \frac{2}{\pi}\int_0^\infty d\omega J_n(\omega)\omega, \quad \Omega_{n+1}^2 = \frac{2}{\pi D_n^2}\int_0^\infty d\omega J_n(\omega)\omega^3. \tag{5}$$

In the above expression, $\Delta V(s) = \delta\Omega_0^2 s^2/2$ is a counter term involving the renormalization frequency $\delta\Omega_0^2 = (2/\pi)\int_0^\infty d\omega J_0(\omega)/\omega$ and $\{X_n, P_n\}_{n\in\mathbb{N}}$ are entirely determined by $J_0(\omega)$. As shown below, this canonical transformation allows one to write an explicit expression for $\{J_n\}_{n\in\mathbb{N}}$ *without* knowing the eigenfrequencies of the residual bath at each step. Other transformations to linear-chain models have been suggested,[7,8] which, however, do not define the couplings in pure coordinate form.

III. SEQUENCE OF SPECTRAL DENSITIES

As observed by Leggett,[9,10] the SD acting on the system degree of freedom can be obtained from the analytically continued Fourier-transformed equations of motion as the imaginary part of a propagator[11]

$$J_0(\omega) = -\lim_{\epsilon\to 0^+} \mathrm{Im}\, L_0(\omega + \mathrm{i}\epsilon) \equiv -\mathrm{Im}\, L_0^+(\omega).$$

This procedure has recently been used by two of us to obtain a continued-fraction expression for the SD generated by a linear chain with Markovian closure, which, in turn, formed the basis for approximating a given SD.[2] Employing a similar strategy, we now focus on the properties of the residual spectral densities J_M closing the chain after M effective modes have been extracted as outlined above. For the Hamiltonian of Eq. (1), after introducing the first effective mode X_1, we obtain

$$L_0(z) = -z^2 - \frac{D_0^2}{\Omega_1^2 - z^2 - \sum_k \frac{C_k^2}{\bar{\Omega}_k^2 - z^2}},$$

where $\bar{\Omega}_k$ and C_k have been defined above. In the continuum limit, with the help of Eq. (2), the sum in the denominator can be replaced by the function

$$W_1(z) = \sum_{k=2}^{N}\frac{C_k^2}{\bar{\Omega}_k^2 - z^2} \approx \frac{2}{\pi}\int_0^\infty d\omega \frac{J_1(\omega)\omega}{\omega^2 - z^2},$$

or, equivalently,

$$W_1(z) = \frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega \frac{J_1(\omega)}{\omega - z}. \tag{6}$$

The procedure is legitimate since the eigenfrequencies $\bar{\Omega}_k$ satisfy $\omega_1 \leq \bar{\Omega}_2 \leq \omega_2 \ldots \leq \bar{\Omega}_N \leq \omega_N$, thereby covering uniformly the interval $(0, \omega_R)$ as $\Delta\omega \to 0$. In this form, W_1 is given as an integral of its limiting imaginary part, $J_1(\omega) = \mathrm{Im}W_1^+(\omega)$. In the following, a function W_1 defined by Eq. (6) will be referred to as the *Cauchy transform*[12] of J_1; it is an analytic function in the whole complex plane except for the support of J_1 on the real axis, which vanishes as z^{-2} for $|z| \to \infty$. We *define*

$$W_0(z) = \frac{D_0^2}{\Omega_1^2 - z^2 - W_1(z)}, \tag{7}$$

which, analogously to $L_0(z) = -z^2 - W_0(z)$, gives $J_0(\omega) = \mathrm{Im}W_0^+(\omega)$. It follows that J_1 can be written in terms of J_0 as $J_1(\omega) = D_0^2 J_0(\omega)/|W_0^+(\omega)|^2$, where W_0 is the Cauchy transform of J_0. In order to prove this, we notice that according

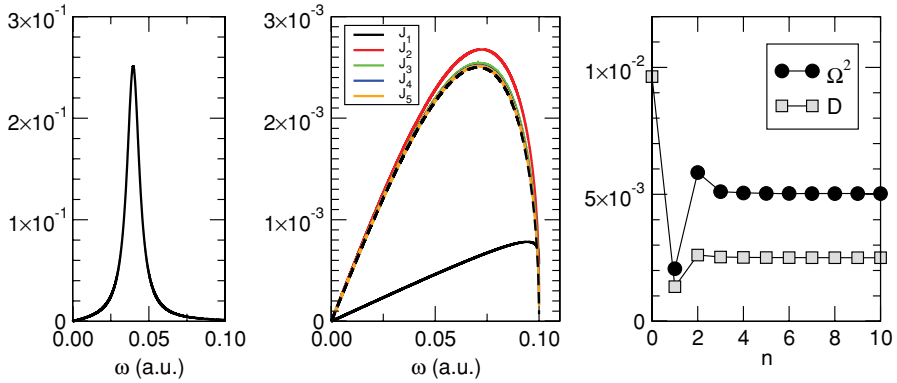

FIG. 1. Left: the SD J_0 defined in Eq. (13) for $\omega_0 = 0.04$ a.u., $d_0 = 0.01$ a.u., and $\gamma = 0.01$ a.u. Middle: results of the deconvolution of J_0 for the first five modes, obtained when setting the high-frequency cutoff ω_R to 0.1 a.u. The Rubin SD of Eq. (12) with the same ω_R is shown as dashed line. Right: Effective modes parameters (Ω_n^2 and D_n) up to $n = 10$.

to its definition, Eq. (7), W_0 is indeed analytic in the upper and lower half planes *and* vanishes as z^{-2} for $|z| \to \infty$. Note in this context that the denominator vanishes on the real axis only, since $\Omega_1^2 - z^2 - W_1(z) = 0$ is the eigenvalue equation solved by the frequencies ω_k appearing in Eq. (1). Writing $W_0(z)$ as a Cauchy integral on a large semicircle in the upper half plane, we can add a term $\pm(\omega - z^*)^{-1}$ to the integrand and obtain the desired result from the real and imaginary parts of the resulting expression. In general, then

$$J_{n+1}(\omega) = \frac{D_n^2 J_n(\omega)}{|W_n^+(\omega)|^2} \tag{8}$$

defines a recurrence relation for the SD $J_{n+1}(\omega)$ felt by the $(n+1)$th effective mode, given the SD $J_n(\omega)$ of the nth mode. According to Eq. (8), the Cauchy transform of J_{n+1} must be of the form $W_{n+1}(z) = g_{n+1}(z) - (D_n^2/W_n(z))$, where $g_{n+1}(z)$ is an analytic function with vanishing imaginary part on the real axis, uniquely fixed by asking that it offsets the behavior of $W_n^{-1}(z)$ as $|z| \to \infty$, $W_n(z) \approx -(D_n^2/z^2)(1 + (\Omega_{n+1}^2/z^2) + \ldots)$. One therefore equivalently has

$$W_{n+1}(z) = \Omega_{n+1}^2 - z^2 - \frac{D_n^2}{W_n(z)}. \tag{9}$$

This is a recurrence relation for the Cauchy transforms which only requires the first Cauchy transform $W_0(z)$ as input and easily provides the sequence $J_n(\omega) = \mathrm{ImW}_n^+(\omega)$.

Equation (9) represents the main result of this communication. It is a simple recurrence relation between the Cauchy transforms of the SDs, which allows us to write the limiting condition as

$$W(z) = \Omega^2 - z^2 - \frac{D^2}{W(z)}, \tag{10}$$

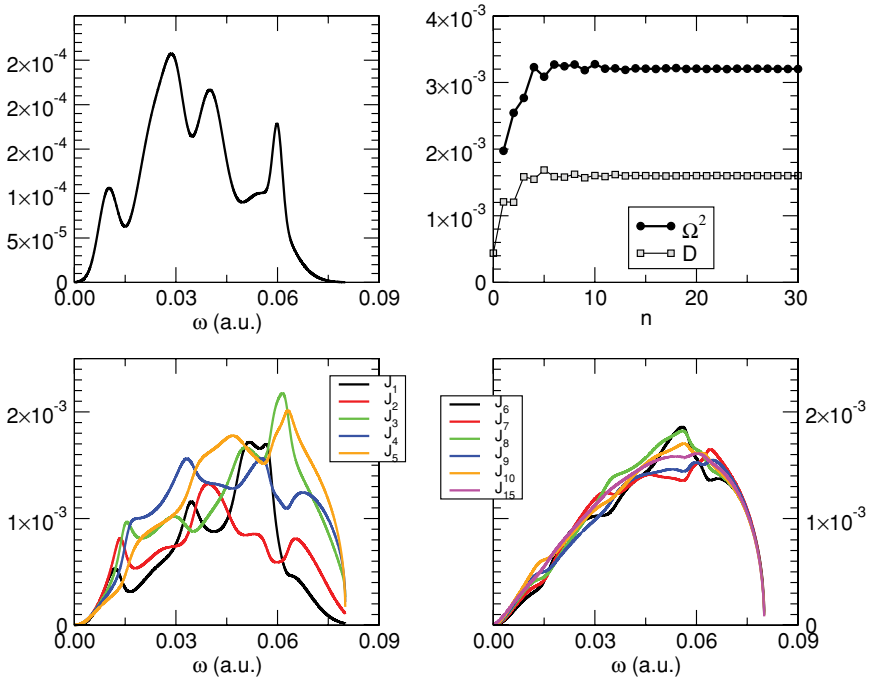

FIG. 2. Deconvolution of the highly structured SD J_0 shown in the upper left panel, with $\omega_R = 0.08$ a.u. Top right: effective mode parameters up to $n = 30$. Bottom: the sequence J_n for $n = 1, \ldots, 15$.

provided that $\Omega = \lim_n \Omega_n$ and $D = \lim_n D_n$ exist. The physical solution ($\mathrm{Im}W^+ \geq 0$) provides the SD which terminates the chain and which has a nonvanishing value for $\omega^2 \in [\Omega^2 - 2D, \Omega^2 + 2D]$ only. In other words, the limiting SD reads as

$$J(\omega) = \frac{1}{2}\sqrt{(\omega^2 - \omega_L^2)(\omega_R^2 - \omega^2)} \quad \omega_L \leq \omega \leq \omega_R, \tag{11}$$

where $\omega_R^2 = \Omega^2 + 2D$ and $\omega_L^2 = Max\{\Omega^2 - 2D, 0\}$. The requirement $J_0(\omega) > 0$ for $\omega > 0$ fixes $\Omega^2 = 2D$, since the condition $\Omega^2 > 2D$ (though physically admissible) would correspond to a SD J_0 with a low-frequency cutoff $\omega_L = \sqrt{\Omega^2 - 2D}$. Thus, Eq. (11) reduces to the quasi-Ohmic SD, provided by the Rubin model of dissipation,[1,13]

$$J_{\mathrm{Rubin}}(\omega) = \frac{\omega\omega_R}{2}\sqrt{1 - \frac{\omega^2}{\omega_R^2}}\Theta(\omega_R - \omega). \tag{12}$$

This means that *provided a sufficient number of effective modes is included in the definition of the system, the resulting dynamics is Markovian*. In practice, as we show numerically below, this number is rather small, since convergence is quite fast even for structured spectral densities. Notice, though, that when $J_0(\omega)$ has a low-frequency cutoff ω_L but is otherwise positive on the interval (ω_L, ω_R), Eq. (11) shows that no Markovian reduction is possible, no matter how many effective modes are included in the system.

A comment is in order regarding the designation of the dynamics as Markovian. The Ohmic limiting spectral density still represents colored noise in a quantum-mechanical setting, and an *exact* Markovian embedding can indeed only be achieved in the classical case. Quantum Ohmic friction can be taken as the closest situation to classical Markovian behavior, and is the most natural limit that can be achieved by the present procedure. It is to be stressed in this context that, contrary to the classical case, the proper identification of a non-Markovian dynamics in the quantum case is still to be clarified, see, e.g., Ref. 14 for recent proposals in this direction.

We also stress that the above procedure generally fails to converge for SD with *gaps*, e.g., those occurring in photonic crystals. This can be traced back to the fact that $\mathrm{Re}W_n^+(\omega)$ necessarily has a zero at some point $\bar{\omega} \in (0, \omega_R)$. If $\bar{\omega}$ falls in the gap of the SD, one has $W_n^+(\bar{\omega}) = 0$ and by virtue of Eq. (9), this introduces an isolated pole in $W_{n+1}(z)$ which precludes the use of Eq. (6). Even in this case, however, an orthogonal transformation of bath variables into linear-chain modes can still be introduced to define a number of chains of effective modes, one for each interval where $J_0(\omega) > 0$.

IV. NUMERICAL RESULTS

The above procedure for the determination of the sequence $\{J_n\}_{n\in\mathbb{N}}$ of effective SDs can be easily implemented numerically, relying on the recurrence relation Eq. (9) for the SD Cauchy transforms. To demonstrate the rapidity of convergence, we show results obtained for several representative SDs, starting from the Lorentzian shaped case

$$J_0(\omega) = \frac{d_0^2\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}. \tag{13}$$

This is the effective SD felt by a Brownian particle coupled to a harmonic oscillator of frequency ω_0 which, in turn, interacts with an Ohmic bath.[10] This coupling scheme is evident in the middle panel of Fig. 1: J_1 is a truncated Ohmic SD and J_n, for $n > 2$, is indistinguishable from the Rubin SD given by Eq. (12) for the chosen cutoff ω_R. Such convergence can also be checked by computing the ratio $\Omega_n^2/D_n \to 2$. As a second example, we consider a highly structured and multipeaked SD as plotted in Fig. 2. It is clear from the figure that also in this case, convergence is quite fast, and the limiting Rubin SD is obtained after few (say 10–15) iterations.

The effectiveness of the method has already been demonstrated in Ref. 2, where the same effective mode chain was closed with a strictly Ohmic SD and the reduced dynamics of the enlarged system was compared with exact wave packet calculations employing the original Hamiltonian of Eq. (1). Notice that the closure necessarily modifies the quantum dynamics of the complete system, but approximations introduced at this point do not affect the short-time dynamics, which is entirely determined by the first members of the chain.[2,7] Here, we have proven that the procedure indeed converges, and we have explicitly derived its universal limit, given by the quasi-Ohmic Rubin SD.

V. CONCLUSIONS

We have presented a recursive procedure to recast the non-Markovian dynamics of a Brownian particle, interacting with a bath characterized by an arbitrary SD, into the dynamics of an enlarged set of variables including effective modes of the reservoir coupled to a quasi-Ohmic residual SD. The approach provides an explicit analytic relationship among successive residual SDs, which can be easily evaluated numerically starting from an arbitrary (gapless) initial SD. These results pave the way for an efficient general treatment of dissipation in the presence of arbitrarily complex environments.

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