Quantum-Classical Decomposition of Gaussian Quantum Environments: A Stochastic Pseudomode Model

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We show that the effect of a Gaussian bosonic environment linearly coupled to a quantum system can be simulated by a stochastic Lindblad master equation characterized by a set of ancillary bosonic modes initially at zero temperature and classical stochastic fields. We test the method for Ohmic environments with exponential and polynomial cut-offs against, respectively, the hierarchical equations of motion and the deterministic pseudomode model, with respect to which the number of ancillary quantum degrees of freedom is reduced. For a subset of rational spectral densities, all parameters are explicitly specified without the need for any fitting procedure, thereby simplifying the modeling strategy. Interestingly, the classical fields in this decomposition must sometimes be imaginary valued, which can have counterintuitive effects on the system properties, which we demonstrate by showing that they can decrease the entropy of the system, in contrast to real-valued fields.

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Most quantum systems are inherently open $[1,2]$ $[1,2]$, i.e., their dynamics depends on the interaction with an external environment. A typical example is when the system is in contact with a continuum of degrees of freedom constituting a thermal bath. The system dynamics can take qualitatively different forms depending on the characteristics of the bath and on the system-bath interaction. For example, under the Born-Markov approximation, the reduced system dynamics can be described by a Lindblad equation [\[3,](#page-38-2)[4\]](#page-38-3) or by a more general nonsecular Redfield equation [\[5\]](#page-38-4), depending on the presence of near-degeneracies (compared with the broadening) in the system's spectrum [\[6](#page-38-5)[–9\]](#page-39-0). In regimes where a coherent exchange of information with the bath occurs, more general master equations (possibly nonlocal in time) are required to correctly account for these memory effects $[1,10,11]$ $[1,10,11]$ $[1,10,11]$.

Within this general landscape, a wide range of physical environments can be represented by Gaussian baths (such as those made out of bosonic and fermionic degrees of freedom at thermal equilibrium) linearly interacting with the system. In this case, the effects of the bath on the

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system are fully characterized by the properties of correlation functions involving the bath operators that mediate the interaction. As a consequence, the regimes mentioned above can now all be described by properties of these correlation functions, which also bear information about the nonclassicality of the system dynamics [\[12](#page-39-3)[,13\]](#page-39-4).

Intuitively, when the correlations decay faster than the characteristic time associated with the system, the regime is Markovian and the effects of the bath on the system can be modeled by master equations local in time and written in Lindblad form. In the opposite case, the bath response time is slow enough to allow the system and the bath to coherently exchange energy before its eventual dissipation into the continuum. Several approaches have been developed to analyze this non-Markovian regime [\[1,](#page-38-0) [2,](#page-38-1)[14\]](#page-39-5), such as generalized master equations derived from the Feynmann-Vernon influence functional formalism [\[15–](#page-39-6)[23\]](#page-39-7), the hierarchical equations of motion (HEOM) $[24–34]$ $[24–34]$, the reaction coordinate method $[35–40]$ $[35–40]$, the polaron transformation [\[41–](#page-39-12)[56\]](#page-40-0), collisional methods [\[57–](#page-40-1) [60\]](#page-40-2), cascaded networks [\[61–](#page-40-3)[69\]](#page-40-4), and the pseudomode model [\[70–](#page-40-5)[84\]](#page-41-0). These methods are also nonperturbative in the interaction strength, thereby allowing one to model the correct system-bath hybridization properties of the steady state.

Among the methods listed above, the pseudomode model consists in replacing the continuum of environmental degrees of freedom with a discrete set of effective dissipative quantum harmonic modes. These modes

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FIG. 1. The stochastic pseudomode model. (a) A system *S* interacts with a physical bath made out of a continuum of environmental modes. (b) The continuum can be approximated by a discrete set of leaky quantum pseudomodes; see Eq. [\(4\).](#page-2-0) (c) The subset of the quantum pseudomodes that generate classical correlations can be replaced [see Eq. (16)] by the stochastic classical field defined in Eq. [\(14\).](#page-4-1)

are designed to approximate the original bath correlation function as a discrete sum of decaying exponentials, similarly to the HEOM method. As shown in Refs. [\[80](#page-41-1)[,84\]](#page-41-0), the domain of this ansatz can be further enlarged by allowing some of the model parameters to take unphysical values. Depending on the correlation function, different regimes might allow a more efficient representation in terms of pseudomodes. For example, in certain bath models at zero temperature [\[80\]](#page-41-1), the continuum of Matsubara frequencies implies correlations decaying polynomially in time, thereby posing a possible challenge from a simulation standpoint $[10,85,86]$ $[10,85,86]$ $[10,85,86]$ as the number of pseudomodes required necessarily ends up scaling with the simulation time. While this issue is often not evident in practical applications, it emerges when vanishing spectral properties of the system need to be resolved, such as in the low-temperature Kondo regime.

Alongside these fully deterministic methods, stochastic techniques have also been used to describe the effects of a quantum environment by driving the dynamics with classical noise. This was originally implemented in the context of Markovian [\[87](#page-41-4)[–93\]](#page-41-5) and non-Markovian [\[94](#page-41-6)[–97\]](#page-41-7) quantum state diffusion. To deepen the analysis of memory kernels, this formalism was adapted to Liouville space [\[98](#page-41-8)[–102\]](#page-41-9), and later further generalized to also include fermionic baths $[103-105]$ $[103-105]$. The difficulty of averaging over correlated stochastic processes led to the development of hybrid techniques involving the HEOM [\[33](#page-39-13)[,106](#page-41-12)[–110\]](#page-41-13), classical and semiclassical optimizations [\[111](#page-41-14)[–113\]](#page-41-15), and piecewise ensemble averaging [\[114\]](#page-41-16).

Here we introduce a hybrid approach to reproduce non-Markovian effects in open quantum systems in the context of the pseudomode model, i.e., using ancillary quantum harmonic modes alongside a single stochastic classical drive, see Fig. [1.](#page-1-0) The system reduced dynamics can be computed by solving a Lindblad-like master equation that does not involve memory kernels (as in pure quantum state diffusion) and it does not require multiple cross-correlated stochastic processes (as in the purely stochastic Liouville space approaches).

In contrast to the mathematical auxiliary degrees of freedom present in HEOM-related studies, this effective master equation provides a rather intuitive interpretation where the system is directly coupled to one or more leaky modes and to a classical stochastic field. The effective nature of this model does not grant a physical meaning for this interpretation and, depending on the decomposition, either the leaky modes or the classical field can be unphysical in the sense they depend on imaginary-valued non-Hermitian parameters. However, at the same time, it allows us explore wider (unphysical) regimes for the ancillary degrees of freedom that can improve the optimization of the model,

We show that this hybrid approach can be introduced as a consequence of a classical-quantum decomposition of the environmental *effects on the system* (i.e., not directly as a physical description of the properties of the bath), which, in the Gaussian case, translates into defining the corresponding (classical or quantum) contributions to the bath correlation function. Interestingly, this decomposition is not unique but it can be chosen to optimize the model. For example, this feature leads to the possibility to initialize the ancillary harmonic quantum degrees of freedom in their vacuum state, *for any temperature of the original bath*. This directly allows a further, practical, optimization of the Hilbert space dimension due to a smaller Fock space construction.

In addition, in the case where the environment can be described as a sum of underdamped spectral densities, the corresponding stochastic pseudomode model requires only a single, physical, zero-temperature quantum degree of freedom per spectral density. This is in stark contrast with the fully deterministic pseudomode model, where further quantum degrees of freedom are needed to fit the Matsubara part of the correlation. This leads to advantages in modeling certain open quantum systems, such as when the system is coupled to multiple baths at different temperatures. In this case, we show that the possibility to encode all collective temperature effects into a single field substantially optimizes the simulation resources with respect to the fully deterministic pseudomode model. We demonstrate this with a practical example where a system is coupled to multiple baths at different temperatures.

Importantly, for the general case we analytically determine an expression for the number of pseudomodes for rational spectral densities for which the model is defined without free parameters *(i.e., without requiring any fitting)* for all temperatures. For nonrational spectral densities, a fitting procedure is still required to optimize the number of pseudomodes.

Finally, we also demonstrate the unusual feature that, for a zero-temperature bath, the imaginary nature of the classical fields can increase the order in the system, as described by its von Neumann entropy (which can be understood as the system-environment entanglement entropy at zero temperature). This is contrast to real-valued classical fields, which are expected to increase the disorder of the system state.

This article is organized as follows. In Sec. [I](#page-2-1) we introduce the pseudomode model in its fully quantized, deterministic version. In Sec. [II](#page-3-0) we introduce a quantumclassical decomposition of the environmental correlation function, which we then use in Sec. [III](#page-4-2) to define a stochastic version of the pseudomode model. In Sec. [III A](#page-5-0) we further analyze the bias and stochastic sources of errors in the model, and in Sec. [III B](#page-6-0) we present a variant of the model with the advantage of allowing all quantum modes to be initially at zero temperature. In Sec. [IV](#page-7-0) we show that all parameters of the model can be computed analytically for spectral densities that can be written as a specific class of rational functions. In Sec. [V](#page-8-0) we consider two specific examples of spectral densities. In Sec. VA we test the stochastic method against the fully quantized, deterministic pseudomode model for the case of underdamped Brownian spectral densities. In Sec. [V B](#page-10-0) we consider Ohmic spectral densities with an exponential cut-off that are outside the rational domain, thereby not allowing a full analytical analysis. In Sec. [VI](#page-11-0) we apply the hybrid formalism to describe a system coupled to multiple baths at different initial temperatures. In Sec. [VII](#page-11-1) we analyze the effects of unphysical stochastic fields on the von Neumann entropy of the system. Each section in the main text is accompanied by a corresponding one in the appendixes, where we describe all technical details.

I. PSEUDOMODE MODEL

In this section, we review the pseudomode model and introduce the main notation used throughout this article. We consider a system *S* coupled to a bosonic environment *B* as described by the Hamiltonian ($\hbar = 1$)

$$
H = HS + HI + HB, \t\t(1)
$$

where H_S is the system Hamiltonian and $H_B = \sum_k \omega_k b_k^{\dagger} b_k$ characterizes the energy ω_k of each environmental mode b_k . We suppose the system-environment coupling to be in the form $H_I = sX$, where *s* is a system operator and $X =$ $\sum_{k} g_{k}(b_{k} + b_{k}^{\dagger})$ is a linear interaction operator (in terms of the real coupling strengths $g_k \in \mathbb{R}$). When the environment is initially in thermal equilibrium at inverse temperature β , the dynamics of the reduced system density matrix $\rho_S(t)$

can be written as

$$
\rho_S(t) = T e^{-\mathcal{F}(t,s,C(t))} \rho_S(0). \tag{2}
$$

Here the superoperator $\mathcal{F}(t, s, C(t))$, whose explicit form is shown in Appendix [A,](#page-13-0) depends only on the system coupling operator *s* and the free correlation function of the environmental interaction operator

$$
C(t) = \langle X(t_2)X(t_1) \rangle
$$

=
$$
\int_0^\infty d\omega \frac{J(\omega)}{\pi} \left[\coth(\beta \omega/2) \cos(\omega t) - i \sin(\omega t) \right],
$$
 (3)

where $t = t_2 - t_1$, and where we introduced the spectral density $J(\omega) = \pi \sum_k g_k^2 \delta(\omega - \omega_k)$. Here $X(t) =$ $U_B^{\dagger}(t)XU_B(t)$ is the bath coupling operator in the Heisenberg picture of the free bath [in terms of $U_B(t) = e^{-iH_Bt}$], and the expectation value is taken with respect to a thermal state $\rho_B = \exp[-\beta \sum_k \omega_k b_k^{\dagger} b_k]/Z_\beta$ at inverse temperature β , with Z_{β} enforcing unit trace.

The formal expression in Eq. [\(2\)](#page-2-2) is not easily evaluated as it includes environmental memory effects encoded in the time ordering of the double time integral in the exponential. However, the expression for the superoperator $F(t, s, C(t))$ suggests the possibility to define approximation schemes in which the environment is replaced by a fictitious one whose two-point free correlation function and system coupling operator match the original ones. In particular, the pseudomode model introduces an environment made out of lossy harmonic modes that are purely mathematical entities as they have no direct relation to the original environmental modes. Even more, as noted in Ref. [\[80\]](#page-41-1), since we focus only on the reduced system dynamics, the domain of the parameters in the model can be further enlarged to unphysical values, thereby allowing more flexibility in optimizing the approximation.

Specifically, the pseudomode model consists in approximating the reduced system dynamics of the original open quantum system in Eq. (1) as

$$
\rho_S(t) \simeq \mathrm{Tr}_{\mathrm{PM}} \rho(t), \tag{4}
$$

where $\rho(t)$ is the density matrix in an enlarged Hilbert space $\mathcal{H} = \mathcal{H}_{S} \otimes \mathcal{H}_{PM}$, where \mathcal{H}_{S} and $\mathcal{H}_{PM} = \otimes_{j=1}^{N_{PM}} \mathcal{H}_{j}$ represent the Hilbert spaces of the system and the pseudomodes, respectively (in which H_i is the space of the *j* th pseudomode). The dynamics in this enlarged space is computed through the Lindblad equation

$$
\dot{\rho}(t) = -i[H_{\rm PM}, \rho(t)] + \sum_{j=1}^{N_{\rm PM}} D_j[\rho(t)],\tag{5}
$$

where

$$
H_{\rm PM} = H_S + \sum_{j=1}^{N_{\rm PM}} \left(\lambda_j X_j s + \Omega_j a_j^{\dagger} a_j \right), \tag{6}
$$

with $X_j = a_j + a_j^{\dagger}$ in terms of the bosonic pseudomode a_j and where $\lambda_i, \Omega_i \in \mathbb{C}$ are formal interaction strengths and energies. We note that when these parameters are allowed to be complex, the original Lindblad equation does not acquire any complex conjugation as one would expect in non-Hermitian systems [\[115](#page-41-17)[–118\]](#page-42-0). For this reason, this equation was dubbed the "pseudo-Schrödinger equation" in Ref. [\[80\]](#page-41-1). Each pseudomode undergoes nonunitary dynamics as described by the dissipators

$$
D_j[\cdot] = \Gamma_j[(1 + n_j)(2a_j \cdot a_j^{\dagger} - a_j^{\dagger} a_j \cdot \cdot \cdot a_j^{\dagger} a_j) + n_j(2a_j^{\dagger} \cdot a_j - a_j a_j^{\dagger} \cdot \cdot \cdot a_j a_j^{\dagger})].
$$
 (7)

The initial condition for Eq. [\(5\)](#page-2-4) is given by $\rho(0) =$ $\rho_S(0) \prod_j \exp \left[-\beta_j \Omega_j a_j^{\dagger} a_j\right] / Z_j$, where $Z_j = 1/(1 - \exp j)$ $[-\beta_i \Omega_i]$) in terms of the temperaturelike parameters $\beta_i \in$ C. Importantly, the nonunitary dynamics in the systempseudomode (S-PM) space described in Eq. [\(5\)](#page-2-4) is equivalent to that of an open quantum system in which each pseudomode interacts with quantum white noise residual environments; see Appendix [B.](#page-17-0) The Gaussianity of this formal open quantum system implies that the quality of the approximation in Eq. [\(4\)](#page-2-0) depends on the accuracy to which the correlation of the pseudomodes' coupling operators matches the original one. More specifically, the pseudomode model parameters are optimized to minimize the following approximation:

$$
C(t) \simeq \sum_{j=1}^{N_{\text{PM}}} \lambda_j^2 \langle X_j(t)X_j(0) \rangle
$$

=
$$
\sum_{j=0}^{N_{\text{PM}}} \lambda_j^2 e^{-\Gamma_j |t|} [(1 + n_j) e^{-i\Omega_j t} + n_j e^{i\Omega_j t}]
$$
 (8)

for all $t \in \mathbb{R}$ [\[119\]](#page-42-1) and where $n_i = 1/(\exp[\beta \Omega_i] - 1)$. In general, physical correlations of the original model include nonexponential decay at long times, which implies the above approximation can become an exact equality only in the limit $N_{\text{PM}} \rightarrow \infty$.

In summary, the pseudomode model allows one to replace the original continuum of environmental modes with a discrete set of unphysical modes. This allows one to compute the reduced system dynamics nonperturbatively in the system-environment coupling by solving a Lindbladlike differential equation. We stress that while Lindblad master equations are usually derived under some perturbative approximation, Eq. (5) does not rely on such an assumption. As shown in Appenidix [B](#page-17-0) (see also Refs. [\[79,](#page-41-18)[80\]](#page-41-1)), Lindblad dissipation exactly corresponds to an open quantum system whose correlation function is a sum of decaying exponentials, i.e., to the ansatz on the right-hand side of Eq. [\(8\).](#page-3-1) As a consequence, the only approximation made by the pseudomode model is in the bias error between this ansatz and the original correlation [left-hand side of Eq. [\(8\)\]](#page-3-1).

In this context, we now introduce a hybrid model in which classical stochastic fields are used alongside quantum pseudomodes. This allows to lift the constraint on the ansatz given in Eq. (8) to further reduce, on average, the bias error. For spectral densities that can be written as a rational function, this error becomes negligible. This comes at the cost of introducing stochastic errors whose magnitude scale inversely with the square root of the number of realizations used in the averaging. This highlights a qualitative difference in the requirements of the computational resources. By our replacing some of the original quantum modes with classical fields, the dimension of the Hilbert space of the effective model is reduced at the cost of the additional time required for the averaging.

II. QUANTUM-CLASSICAL DECOMPOSITION OF THE CORRELATION FUNCTION

In this section, we introduce a nonunique decomposition of the bath correlation function in terms of a quantum part and a classical part. By using a spectral expansion, we can reproduce the latter contribution using classical stochastic noise.

We start by noting that the correlation in Eq. (3) can be decomposed into two contributions with different symmetries under time reversal, i.e.,

$$
C(t) = Cs(t) + Cas(t),
$$
\n(9)

where

$$
C_s(t) = \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \coth(\beta \omega/2) \cos(\omega t)),
$$

\n
$$
C_{\rm as}(t) = -\frac{i}{\pi} \int_0^\infty d\omega J(\omega) \sin(\omega t) \tag{10}
$$

are the symmetric and antisymmetric contributions, respectively. To provide a more general setup, we consider the slightly different decomposition

$$
C(t) = C_{\text{class}}(t) + C_Q(t),\tag{11}
$$

in terms of a "classical" component and a "quantum" component defined as $C_{\text{class}}(t) = C_s(t) + f_s(t)$ and $C_O(t) =$ $C_{as}(t) - f_s(t)$, respectively. Here $f_s(t)$ is a generic symmetric function that makes this decomposition nonunique. As we will show, it is possible to take advantage of this feature so as to simplify the description of the quantum degrees of freedom of the pseudomode model. Importantly, the quantum component of the correlation does not have, in general, any particular symmetry under time reversal (i.e., it can be any linear combination of symmetric and antisymmetric functions), while the classical part is symmetric. This feature allows us to interpret the classical contribution to the correlation as originating from stochastic noise. This can be seen by explicitly writing the following spectral representation of the classical correlation *(*interpreted as a function in $\mathcal{L}^2([-T, T])$, with $T \in \mathbb{R}$):

$$
C_{\text{class}}(t) = c_0 + 2 \sum_{n=1}^{\infty} c_n \cos[n\pi t/T],
$$
 (12)

where

$$
c_n = \frac{1}{2T} \int_{-T}^{T} d\tau \cos(n\pi \tau/T) C_{\text{class}}(t), \qquad (13)
$$

which denotes the inner product between the classical correlation and the sinusoidal functional basis in $\mathcal{L}^2([-T, T])$. Given this expansion, we can further define a stochastic field as

$$
\xi(t) = \sqrt{c_0} \xi_0 + \sum_{n=1}^{N_{\xi}} \sqrt{2c_n} [\xi_n \cos(n\pi t/T) + \xi_{-n} \sin(n\pi t/T)],
$$
\n(14)

where $N_{\xi} \in \mathbb{N}$ is a truncation parameter and ξ_n , $n =$ $-N_{\xi}, \ldots, N_{\xi}$, are independent Gaussian random variables with zero mean and unit variance. This spectral representation is designed to allow the correlation of the stochastic field to be equivalent to the classical contribution $C_{\text{class}}(t)$, i.e.,

$$
C_{\text{class}}^{\mathbb{E}}(t) \equiv \mathbb{E}[\xi(t_2)\xi(t_1)] = c_0 + 2\sum_{n=1}^{N_{\xi}} c_n \cos[n\pi t/T]
$$

$$
\rightarrow C_{\text{class}}(t), \qquad (15)
$$

in the limit $N_{\xi} \rightarrow \infty$; here $\mathbb{E}[\cdot]$ denotes the average over the Gaussian random variables ξ_n . It is interesting to note that the presence of the (antisymmetric) sine function in the expression for $\xi(t)$ is essential to reproduce a stationary correlation; see Appendix C_2 for more details.

In summary, the procedure to define the stochastic process can be outlined as follows:

(1) We decompose the classical part of the correlation function into Fourier components as described in Eq. [\(12\).](#page-4-3) This involves the computation of N_{ξ} + 1 coefficients given explicitly in Eq. [\(13\).](#page-4-4)

- (2) We then extract $2N_{\xi} + 1$ Gaussian random numbers ξ*n*, which can be, together with the coefficients computed as described above, directly used in Eq. [\(14\)](#page-4-1) to compute the stochastic field.
- (3) The field in Eq. (14) can then be used to solve the stochastic Schrödinger equation in Eq. [\(16\)](#page-4-0) presented in Sec. [III.](#page-4-2)

Equation [\(16\)](#page-4-0) defines a stochastic pseudomode model in which classical stochastic noise is used alongside quantum pseudomodes to reduce both the dimension of the effective Hilbert space and the bias errors in the approximation of the original correlation function. Furthermore, it is possible to take advantage of the nonuniqueness of the representation in Eq. [\(11\)](#page-3-2) to allow all quantum degrees of freedom to be initially at zero temperature. We show this in the following section.

III. A STOCHASTIC PSEUDOMODE MODEL

In this section, we introduce a hybrid pseudomode model in which classical stochastic fields and quantum pseudomodes are used together to simulate different contributions to the original bath, see Fig. [1.](#page-1-0)

We define the following stochastic pseudomode model:

$$
\dot{\rho}^{\xi}(t) = -i[H_{\text{PM}}^{\xi}, \rho^{\xi}(t)] + \sum_{j=0}^{N_{\text{PM}}} D_j[\rho^{\xi}(t)]\rho(t), \qquad (16)
$$

defined for times $t \in [0, T_{\text{dynamics}}]$, with $T_{\text{dynamics}} \leq T$ and where the Hamiltonian

$$
H_{\text{PM}}^{\xi} = H_S + \sum_{j=1}^{N_{\text{PM}}} \left(\lambda_j X_j s + \Omega_j a_j^{\dagger} a_j \right) + s \xi(t) \tag{17}
$$

depends on N_{PM} pseudomodes a_j [having frequency Ω_j and interaction operator $\lambda_j X_j = \lambda_j (a_j + a_j^{\dagger})$ and an extra classical Gaussian stationary stochastic field ξ(*t*) defined by Eq. [\(14\).](#page-4-1) Both the pseudomodes and the classical field interact with the system through the system operator *s*. The pseudomodes are initially in a "thermal" state, so that $\rho(0) = \rho_S(0) \exp[-\sum_j \beta_j \Omega_j a_j^{\dagger} a_j]/Z_j$, where $Z_j =$ $1/(1 - \exp[-\beta_j \Omega_j])$, where $\beta_j \in \mathbb{C}$. The classical and quantum degrees of freedom are designed to reproduce, respectively, the classical part and the quantum part of the original correlation function, i.e.,

$$
C_{\text{class}}^{\mathbb{E}}(t) = \mathbb{E}[\xi(t_2)\xi(t_1)] \simeq C_{\text{class}}(t),
$$

\n
$$
C_{Q}(t) \simeq \sum_{j=0}^{N_{\text{PM}}} \lambda_j^2 \langle X_j(t_2)X_j(t_1) \rangle
$$

\n
$$
= \sum_{j=0}^{N_{\text{PM}}} \lambda_j^2 e^{-\Gamma_j |t|} [(1 + n_j)e^{-i\Omega_j t} + n_j e^{i\Omega_j t}], \quad (18)
$$

where $t = t_2 - t_1$ and $n_j = 1/(\exp[\beta \Omega_j] - 1)$. Here the first equation is a version of Eq. (15) for finite N_{ξ} , while the second equation corresponds to the pseudomode representation of the correlation function as given in Eq. [\(8\).](#page-3-1) We note that, within the pseudomode model defined by Eq. [\(4\),](#page-2-0) it is not possible to reproduce this quantum part without introducing either some complex conjugation (which, in turn, would lead to different higher-order statistics), Liouville space generalizations [\[98–](#page-41-8)[102\]](#page-41-9) or noncommuting variables (i.e., quantum degrees of freedom, as done in here). Under the approximations in Eq. [\(18\),](#page-4-6) it is possible to write the following stochastic version of the main pseudomode equation:

$$
\rho_S(t) \simeq \mathbb{E}\left[\rho_S^{\xi}(t)\right],\tag{19}
$$

where we defined $\rho_S^{\xi}(t) = Tr_{P M} \rho^{\xi}(t)$. An exact evaluation of this expectation value requires knowledge of $\rho_S^{\xi}(t)$ for all $\xi(t)$, which is, in general, not available. However, for any system observable *O*, we can define the empirical average

$$
\mathcal{O}^{\xi}(t; N_{\text{stoch}}) = \frac{1}{N_{\text{stoch}}} \sum_{j=1}^{N_{\text{stoch}}} \mathcal{O}^{\xi_j}(t) \tag{20}
$$

in terms of the quantity

$$
\mathcal{O}^{\xi_j}(t) = \mathrm{Tr}_S \left[O \rho_S^{\xi_j}(t) \right],\tag{21}
$$

where the label $j = 1, \ldots, N_{\text{stoch}}$ in the field ξ_j characterizes one of the different N_{stoch} realizations of the noise. With use of Eq. (19) , it is clear that this random variable has the correct expectation value, i.e.,

$$
\mathcal{O}(t) \equiv \mathbb{E}\left[\mathcal{O}^{\xi}(t; N_{\text{stoch}})\right] \simeq \text{Tr}_{S}\left[\mathcal{O}\rho_{S}(t)\right] \equiv \mathcal{O}_{\text{true}}.\tag{22}
$$

The model described by Eqs. (16) and (19) constitutes the main result of this work. It defines the dynamics of the reduced density matrix of an open quantum system in terms of a set of N_{PM} quantum pseudomodes and a stochastic field $\xi(t)$ [explicitly defined in Eq. [\(14\)\]](#page-4-1) that reproduce the physical effects of the original bath related to, respectively, the quantum and classical contributions of the full bath correlation [see Eq. (18)]. As the statistics of the classical field can encode any time-symmetric functional dependence [see Eq. (15)], this method can model correlations that are not limited by the decaying-exponential ansatz in Eq. [\(8\).](#page-3-1) In parallel, this model also allows one to increase the accuracy of a deterministic model whenever this is prevented by the impossibility to further increase the Hilbert space dimension. Ultimately, the introduction of randomness in the model requires a characterization of the variance of the result, which we analyze in the next section.

A. Bias and stochastic errors

We start this section by analyzing Eq. (18) in some more detail. There is a conceptual difference between the approximations made in the two lines in Eq. [\(18\).](#page-4-6) On the quantum side [second line in Eq. (18)], the approximation consists in writing the correlation as a finite sum of decaying exponentials, and its accuracy can be increased only by considering more pseudomodes or, in other words, by increasing the dimension of the Hilbert space. On the classical side [first line in Eq. (18)], the approximation error is gauged by the cut-off parameter N_{ξ} (which can, in principle, be tuned to increase the accuracy). At the same time, the presence of stochastic noise in the Schrödinger equation in Eq. [\(16\)](#page-4-0) means that all observables are now random variables whose statistics should be further analyzed.

To quantify these sources of inaccuracy in more detail, we can define the following measure for the total error on the observable *O*:

$$
\Delta \mathcal{O}(t) = \mathbb{E}[|\mathcal{O}^{\xi}(t; N_{\text{stoch}}) - \mathcal{O}_{\text{true}}(t)|]. \tag{23}
$$

Using the triangle inequality, we can obtain an upper bound on this error as

$$
\Delta \mathcal{O}(t) \leq \Delta_{\text{stoch}} \mathcal{O}(t) + \Delta_{\text{bias}} \mathcal{O}(t), \tag{24}
$$

where

$$
\Delta_{\text{stoch}} \mathcal{O}(t) = \mathbb{E}[|\mathcal{O}^{\xi}(t; N_{\text{stoch}}) - \mathcal{O}(t)|],
$$

$$
\Delta_{\text{bias}} \mathcal{O}(t) = |\mathcal{O}(t) - \mathcal{O}_{\text{true}}(t)| \qquad (25)
$$

are the stochastic and bias errors, respectively. As shown in Ref. [\[77\]](#page-40-6) and in Appendix C $1a$, the bias error can be upper bounded by a quantity that scales asymptotically as an exponential in

$$
\Delta C = \int_0^T dt_2 \int_0^{t_2} dt_1 |C_{\text{err}}(t_2, t_1)|, \tag{26}
$$

where

$$
C_{\text{err}}(t_2, t_1) = C_{\text{class}}(t_2 - t_1) + C_Q(t_2 - t_1) - C(t_2 - t_1)
$$
\n(27)

is the approximation error of the original correlation function. As mentioned above, in general, the quality of this approximation can be improved by increasing the cut-off N_{ξ} (for the classical contribution) and the number N_{PM} of pseudomodes (for the quantum contribution). For the models in which the quantum part can be modeled exactly with a finite number of pseudomodes (see Sec. [IV\)](#page-7-0), the bias error in the correlation is due to only the finiteness of the spectral expansion of the classical field and can always be reduced. Specifically, the bias is simply given by the difference between Eq. (12) and Eq. (15) and corresponds to $2\sum_{n=N_{\xi}+1}^{\infty} c_n \cos[n\pi t/T]$, so $\Delta_{bias} \rightarrow 0$ in the $N_{\xi} \rightarrow \infty$ limit.

By analyzing the properties of the random variables involved (see Appendix $C1b$ for specific details), we can also bound the stochastic error by a quantity that scales also bound the stochastic error by a quantity that scales
as $O(1/\sqrt{N_{\text{stoch}}})$. However, as with the bias, the explicit form of this bound asymptotically scales exponentially in time (see Appendix $C1b$), effectively limiting its practicality. However, it is possible to further provide an alternative empirical bound in the form

$$
\Delta_{\text{stoch}}^2 \mathcal{O}(t) \le \sigma_{\mathcal{O}^{\xi}(t; N_{\text{stoch}})}^2 \tag{28}
$$

in terms of the variance of the empirical average $\mathcal{O}^{f}(t; N_{\text{stoch}})$. This variance can be further estimated as

$$
\sigma_{\mathcal{O}^{\xi}(t;N_{\text{stoch}})}^2 = \frac{\sum_j [\mathcal{O}^{\xi_j}(t)]^2}{N_{\text{stoch}}} - \left[\frac{\sum_j \mathcal{O}^{\xi_j}(t)}{N_{\text{stoch}}}\right]^2}{N_{\text{stoch}}}
$$
(29)

up to terms of order $O(1/N_{\text{noise}}^{3/2})$, thereby allowing a numerical estimate. Similarly, it is possible to define an empirical average to estimate the expected correlation in Eq. (15) as

$$
C_{\text{class}}^{\text{emp}}(t_2, t_1) = \frac{1}{N_{\text{stoch}}} \sum_{j=1}^{N_{\text{stoch}}} \xi_j(t_2) \xi_j(t_1), \quad (30)
$$

whose expectation value $\mathbb{E}[C_{\text{class}}^{\text{emp}}(t_2, t_1)] = C_{\text{class}}^{\mathbb{E}}(t_2, t_1),$ and whose variance satisfies the bound $\sigma_{\text{emp}}^2 \leq [|\hat{C}(0)|^2 +$ $|C(t_2 - t_1)|^2]/N_{\text{stoch}}.$

In summary, for all models in which the bias error in reproducing the correlation function is negligible, we can estimate the value of an observable $O(t)$ by using a single realization of the empirical average in Eq. [\(20\),](#page-5-2) which requires us to solve the dynamics of the system $N_{\rm stoch}$ times and whose variance can be estimated with Eq. [\(29\).](#page-6-1) We note that, by use of the stochastic formalism presented here, reaching a regime with negligible bias error is possible. For all models (with rational spectral densities) presented in Sec. [IV](#page-7-0) in which the quantum part of the correlation can be exactly reproduced with use of a finite number of pseudomodes, the bias error can be made arbitrary small by simply increasing the number N_{ξ} of classical spectral components of the field in Eq. [\(15\).](#page-4-5)

B. A zero-temperature stochastic pseudomode

The stochastic pseudomode model presented in the previous section is valid for any decomposition of the correlation function into a classical part and a quantum part as described in Eq. (11) . In this section, we show that it is possible to take advantage of the nonuniqueness of this decomposition so as to define all the quantum degrees of freedom initially at zero temperature. This is consistent with the general intuition that "quantumness" is required to generate zero-temperature effects (or, more precisely, to generate the asymmetric tuning of absorption and emission rates required to model detailed balance at finite temperatures), while stochastic noise can be used to reproduce classical statistical uncertainty.

To achieve this, we follow the straightforward strategy of adapting the pseudomode ansatz to the antisymmetric part of the correlation. We then use this ansatz to characterize a symmetric function $f_s(t)$, leading to a quantum correlation compatible with a zero-temperature model. Explicitly, our starting point is the (unique) decomposition in Eq. [\(9\)](#page-3-3) of the correlation function into a symmetric part and an antisymmetric part. Given its symmetries, and compatibly with the pseudomode ansatz, we assume the following expansion for the antisymmetric contribution in terms of the parameters $a_i, b_i, c_i \in \mathbb{C}, j = 1, \ldots, N_{PM}$:

$$
C_{\rm as}(t) = \sum_{j=1}^{N_{\rm PM}} a_j \sin(b_j t) e^{-c_j |t|}.
$$
 (31)

We note that this is assumption does not imply more restrictions than those required by the pseudomode model as it writes the antisymmetric contribution as a sum of decaying sines. The ansatz is also compatible with a wide range of spectral densities; see Sec. [IV.](#page-7-0) We can now define

$$
f_s(t) = -i \sum_{j=1}^{N_{\text{PM}}} a_j \cos(b_j t) e^{-c|t|},
$$
 (32)

which, inserted in Eq. (11) , leads to the following classical and quantum contributions:

$$
C_{\text{class}}(t) = C_s(t) + f_s(t),
$$

\n
$$
C_Q(t) = C_{\text{as}}(t) - f_s(t) = \sum_{j=1}^{N_{\text{PM}}} ia_j e^{-ib_j t} e^{-c_j |t|},
$$
\n(33)

where we used Eqs. (31) and (32) . Comparing this expression with Eq. [\(18\),](#page-4-6) we can appreciate the presence of only zero-temperature pseudomodes, i.e., $n_i = 0$ for all *j*. More specifically, the parameters of the pseudomode model are $\lambda_j^2 = i a_j$, $\Omega_j = b_j$, and $\Gamma_j = c_j$. It is interesting to explicitly note that the pseudomodes *j* are physical for $b_i, c_i \in$ $\mathbb R$ and for imaginary a_i (compatibly with the imaginary nature of the antisymmetric correlation). We also explicitly note that Eq. [\(32\)](#page-6-3) is not uniquely defined as, for example, an overall sign in Eq. [\(31\)](#page-6-2) can be encoded in either *aj* or b_i .

We conclude by mentioning that the procedure presented in this section is not the only possible one as any of the quantum-classical decompositions described in Sec. [II](#page-3-0) can be more appropriate to model a specific environment. We show this in Appendix D_3 , where, in the case of a pure dephasing environment, the decomposition is chosen by our imposing $f_s(t) = 0$ [instead of Eq. [\(32\)\]](#page-6-3) in Eq. [\(9\).](#page-3-3)

IV. STOCHASTIC PSEUDOMODE MODEL FOR RATIONAL SPECTRAL DENSITIES

In this section, we analyze the stochastic pseudomode method to model Gaussian environments characterized by rational spectral densities. More specifically, we consider spectral densities that can be written as

$$
J_r(\omega) = \frac{p(\omega)}{q(\omega)},\tag{34}
$$

where *p* and *q* are polynomials such that the order of the denominator is strictly higher than the order of the numerator and such that the zeros of the denominator are different from the zeros of the numerator. We further assume that $J_r(\omega) \in \mathbb{R}$ for $\omega \in \mathbb{R}$, that $J_r(-\omega) =$ $-J_r(\omega)$, and that all poles of $J_r(\omega)$ are simple and not located on the real axis. Since these spectral densities are real on the real axis, their poles come in conjugate pairs. Furthermore, antisymmetry implies that the poles come either in imaginary conjugate pairs (labeled by $k_i = 1, ..., N_i$) such as $(\omega_{k_i}, \omega_{-k_i}^{\mathcal{R}})$ for $\text{Re}[\omega_{k_i}] = 0$ and $\text{Im}[\omega_{k_i}] > 0$ or in quadruples (labeled with $k_q = 1, \ldots, N_q$) as $(\omega_{k_q}, \omega_{-k_q}, -\omega_{k_q}, -\omega_{-k_q})$ for Re[ω_{k_q}] > 0. Here we used the notation $\omega_k = \overline{\omega}_{-k}$. We can explicitly note that the total number of poles $N_{\text{poles}} = 2N_i + 4N_q$.

With use of this notation, the antisymmetric part of the correlation in Eq. [\(10\)](#page-3-4) reads

$$
C_{\rm as}(t) = -2i s g(t) \sum_{k_q=1}^{N_q} R_{k_q}^{\mathcal{R}} \cos(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|}
$$

+
$$
2i \sum_{k_q=1}^{N_q} R_{k_q}^{\mathcal{I}} \sin(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|}
$$

-
$$
i s g(t) \sum_{k_i=1}^{N_i} R_{k_i}^{\mathcal{R}} \cos(\omega_{k_i}^{\mathcal{R}} t) e^{-\omega_{k_i}^{\mathcal{I}} |t|}, \qquad (35)
$$

where $R_k = \text{Res}[J_r(\omega); \omega_k]$ denotes the residue of the spectral density at the simple pole $\omega_k \in \mathbb{C}$. Furthermore, we defined $sg(t) = t/|t|$ for $t \neq 0$, and we used the labels \mathcal{R} and *I* to denote the real and imaginary parts of a parameter, respectively. We note that the sign function appearing in this expression makes a direct comparison with the ansatz in Eq. [\(31\)](#page-6-2) not immediately obvious. However, it is possible to make progress by weakening the meaning of the correlation function to a distribution. Since we are ultimately interested in computing the reduced density matrix of the system, the correlation in Eq. (3) always appear inside definite integrals in time, thereby effectively defining it as a functional over the system's observables, i.e., a distribution. This conceptual observation is not just abstract as it allows us to concretely modify the expression on the right-hand side of Eq. [\(35\)](#page-7-1) on any zero-measure subspace of the real axis (by simply reinterpreting the equal sign in the distribution space). These considerations allow us to write Eq. [\(35\)](#page-7-1) (omitting the time dependence on the right-hand side) in terms of an arbitrary energy parameter *W* that is supposed to be much bigger than any frequency that can be associated with the system:

$$
C_{\text{as}} = 2 \sum_{k_q=1}^{N_q} \left\{ i R_{k_q}^{\mathcal{I}} \sin(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|} + R_{k_q}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_q}^{\mathcal{I}}) + 2\omega_{k_c}^{\mathcal{R}}}{2} t\right] e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} + R_{k_q}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_q}^{\mathcal{I}}) - 2\omega_{k_c}^{\mathcal{R}}}{2} t\right] e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} \right\} + 2 \sum_{k_i=1}^{N_i} R_{k_i}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_i}^{\mathcal{I}})}{2} t\right] e^{-(W + \omega_{k_i}^{\mathcal{I}})|t|/2}.
$$
\n(36)

This expression allows a direct comparison with the ansatz in Eq. [\(31\)](#page-6-2) and ultimately implies that $N_{PM} = 3N_q +$ *Ni* zero-temperature pseudomodes are needed to *exactly* reproduce the antisymmetric part of the correlation for this class of spectral densities. We note that, in practice, a smaller number of pseudomodes can be considered at the price of downgrading Eq. [\(31\)](#page-6-2) to a best-fit approximation. While the analytical expression for the antisymmetric contribution to the correlation function above allows us to give an upper bound on the number of pseudomodes, a similar analytical expression for the symmetric part is not as useful as the expansion in Eq. (12) can always be computed numerically. Nonetheless, such an expression can be obtained, and it explicitly reads (for $\beta \in \mathbb{R}$)

$$
C_{s} = -2 \sum_{k_{q}} [R_{k_{q}}^{\beta,R} \sin (\omega_{k_{q}}^{R}|t) + R_{k_{q}}^{\beta,I} \cos (\omega_{k_{q}}^{R}t)] e^{-\omega_{k_{q}}^{I}|t|}
$$

$$
- \sum_{k_{i}=1}^{N_{i}} R_{k_{i}}^{\beta,I} e^{-\omega_{k_{i}}^{I}|t|} + \frac{2i}{\beta} \sum_{k>0} J(\omega_{k}^{M}) e^{-|\omega_{k}^{M}|t|}, \qquad (37)
$$

where $k_q = 1, ..., N_q$ and $R_k^{\beta} = R_k \coth(\beta \omega_k/2)$, and in terms of the Matsubara poles $\omega_k^M = 2\pi i k/\beta$ (*k* > 0)

FIG. 2. Correlations for the Brownian spectral density at zero temperature. In (a),(b) we plot the symmetric [Eq. [\(44\)\]](#page-9-1) and antisymmetric [Eq. (43)] contributions to the correlation. In (c) , (d) we plot the classical [Eq. (46)] and quantum [Eq. (45)] contributions, which are obtained by subtracting or adding the symmetric function given in Eq. [\(32\)\]](#page-6-3). At zero temperature, the classical part of the correlation $C_{\text{class}}(t)$ shown in (c) consists of the Matsubara contribution; see Eq. [\(47\).](#page-10-1) In (c), we further show the empirical average $C_{\text{class}}^{\text{emp}}(t)$ [dashed green line; see Eq. [\(30\)\]](#page-6-4) of the correlation function, its expected value $C_{\text{class}}^{\text{E}}(t)$ [dashed red line; see Eq. [\(15\)\]](#page-4-5), and its variance [in light green; see Eq. [\(C72\)\]](#page-29-0). As the number N_{stoch} of samples increases, the stochastic reconstruction (green) averages to its expected value (red), which, in turn, tends to the exact numerical expression as the number N_{ξ} of spectral components in the fields in Eq. [\(14\)](#page-4-1) approaches infinity. In (d), the quantum contribution $C_Q(t)$ is modeled by a single exponential function and it does not have any definite symmetry under time reversal. Here the parameters are the same as those used in Fig. [3\(a\);](#page-9-5) specifically, $N_{\xi} = 1000$ and $N_{\rm stoch} = 100$.

of coth($\beta \omega/2$). By using the prescriptions described in Sec. [III B,](#page-6-0) we can use Eq. (33) to compute the quantum and classical contributions to the correlations $C_Q(t)$ = $C_{\text{as}}(t) - f_s(t)$ as

$$
C_{Q}(t) = -2 \sum_{k_{q}=1}^{N_{q}} \left\{ R_{k_{q}}^{T} e^{-i\omega_{k_{q}}^{T}t} e^{-\omega_{k_{q}}^{T}} |t| + iR_{k_{q}}^{R} e^{-i[\omega_{k_{q}}^{R} - i(W - \omega_{k_{q}}^{T})/2]t} e^{-(W + \omega_{k_{q}}^{T})|t|/2} + iR_{k_{q}}^{R} e^{-i[-\omega_{k_{q}}^{R} - i(W - \omega_{k_{q}}^{T})/2]t} e^{-(W + \omega_{k_{q}}^{T})|t|/2} \right\}
$$

+
$$
2i \sum_{k_{i}=1}^{N_{i}} R_{k_{i}}^{R} e^{-i[-i(W - \omega_{k_{i}}^{T})/2]t} e^{-(W + \omega_{k_{i}}^{T})|t|/2}
$$
(38)

and

$$
C_{\text{class}} = i \sum_{k_q=1}^{N_q} [\Delta R_{k_q} e^{i\omega_{k_q}|t|} - \Delta' R_{k_q} e^{-i\tilde{\omega}_{k_q}|t|}] + i \sum_{k_l=1}^{N_l} \Delta R_{k_l} e^{i\omega_{k_l}|t|} + \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|} \tag{39}
$$

in terms of the quantities $\Delta R_{k_x} = R_{k_x}^{\beta} - R_{k_x}$ and $\Delta' R_{k_x} =$ $\bar{R}^{\beta}_{k_x} + R_{k_x}$ (*x* = *q*, *i*). The quantum correlation corresponds to a decomposition like the one presented in Eq. (18) , which can be modeled by pseudomodes initially at zero temperature. On the other hand, the explicit expression for the classical correlation can further be used to explicitly compute the coefficients for the spectral decomposition of the field ξ in Eq. [\(14\)](#page-4-1) as

$$
c_n = i \sum_{k_q=1}^{N_q} [\Delta R_{k_q} L(i\omega_{k_q}) - \Delta' R_{k_q} L_n(-i\bar{\omega}_{k_q})] + i \sum_{k_i=1}^{N_i} \Delta R_{k_i} L_n(i\omega_{k_i}) + \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) L_n(-|\omega_k^M|),
$$
\n(40)

where

$$
L_n(\omega) = (e^{\omega T} e^{in\pi} - 1) \frac{\omega T}{(\omega T)^2 + (n\pi)^2}.
$$
 (41)

V. EXAMPLES

In this section, we exemplify the model by considering two specific choices of spectral densities. First, we test the stochastic method against the fully quantized, deterministic pseudomode model using an underdamped Brownian

FIG. 3. Dynamics of a two-level system with Hamiltonian $H_S = (\omega_s/2)\sigma_z$ and coupling operator $s = \sigma_x$ strongly coupled to a bath with a narrow and broad Brownian spectral density (insets) at zero temperature. As the blue line, the evolution follows a standard pseudomode model in which all degrees of freedom are quantized (one mode for the quantum contribution and two modes for the classical one). The dashed black line represents evolution without the contribution from the Matsubara correlation. As the dashed red line, the evolution of the empirical average in Eq. [\(20\)](#page-5-2) for $N_{\text{stoch}} = 100$ is evaluated with the stochastic pseudomode model involving a single harmonic oscillator to model the quantum contribution. The horizontal dashed gray line represents the value of the observable for the ground state of a Rabi model with Hamiltonian H_B and zero fields. In (b), the failure to reach this value can be interpreted as due to hybridization with residual modes in the environment (as a consequence of the broad resonance), which are correctly taken into account by both the standard pseudomode model and the stochastic pseudomode model; see Ref. [\[80\]](#page-41-1) for more details about the effects of the Matsubara terms in the deterministic pseudomode model. In (a), the parameters are $ω_0 = ω_s$, $γ = 0.05ω_s$, $λ = (0.2/√2π)ω_s^{3/2}$, *N*_ξ = 1000, and *N*_{stoch} = 100. In (*b*), the parameters are $\omega_0 = \omega_s$, $\gamma = \omega_s$, $\lambda = (1/\sqrt{2\pi})\omega_s^{3/2}$, $N_\xi = 100$, and $N_{\text{stoch}} = 1000$. To further highlight the different hybridization properties of the two cases, we used different initial conditions for the two-level system [excited state in (a) and ground state in (b)].

spectral density. We then focus on an Ohmic spectral density with exponential cut-off which lies outside the domain of rational spectral densities analyzed analytically in the previous sections.

A. Underdamped Brownian spectral density

The spectral density

$$
J^B(\omega) = \frac{\gamma \lambda^2 \omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2},\tag{42}
$$

defined in terms of the frequency parameters ω_0 and γ < $2\omega_0$ and an overall strength λ (having dimension of frequency to the power 3/2), describes a structured environment characterized by an underdamped resonance having frequency $\Omega = \sqrt{\omega_0^2 - \Gamma^2}$ and a broadening $\Gamma = \gamma/2$. It has the form described in Sec. [IV](#page-7-0) of a rational function with a Ohmic numerator (linear in ω) and a polynomial cut-off with poles located at $\pm \Omega \pm i\Gamma$. For this spectral density, the antisymmetric and symmetric parts of the correlation are

$$
C_{\text{as}}^{B}(t) = -i\frac{\lambda^{2}}{2\Omega}\sin(\Omega t)e^{-\Gamma|t|}
$$
 (43)

and

$$
C_s^B(t) = \frac{\lambda^2}{4\Omega} \coth (\beta(\Omega + i\Gamma)/2) e^{i\Omega|t|} e^{-\Gamma|t|}
$$

$$
- \frac{\lambda^2}{4\Omega} \coth (\beta(-\Omega + i\Gamma)/2) e^{-i\Omega|t|} e^{-\Gamma|t|}
$$

$$
+ \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|}, \qquad (44)
$$

where $\omega_k^M = 2\pi i k/\beta$. Following Eq. [\(32\),](#page-6-3) we can define $f_s^B(t) = -(\lambda^2/2\Omega)\cos(\Omega t)e^{-\Gamma|t|}$ so that the quantum and classical parts of the correlation read

$$
C_Q^B(t) = C_{\text{as}}^B(t) - f_s^B(t) = \frac{\lambda^2}{2\Omega} e^{-i\Omega t} e^{-\Gamma|t|}
$$
 (45)

and

$$
C_{\text{class}}^{B}(t) = \frac{\lambda^{2}}{4\Omega} \coth (\beta(\Omega + i\Gamma)/2) e^{i\Omega|t|} e^{-\Gamma|t|}
$$

$$
- \frac{\lambda^{2}}{4\Omega} \coth (\beta(-\Omega + i\Gamma)/2) e^{-i\Omega|t|} e^{-\Gamma|t|}
$$

$$
- \frac{\lambda^{2}}{2\Omega} \cos(\Omega t) e^{-\Gamma|t|} + \frac{2i}{\beta} \sum_{k>0} J^{B}(\omega_{k}^{M}) e^{-|\omega_{k}^{M}|t|},
$$
(46)

respectively. It is interesting to note that, in the $\beta \to \infty$ limit, simplifications in the classical correlation occur,

FIG. 4. Dynamics of a two-level system with Hamiltonian $H_S = (\omega_s/2)\sigma_z$ and coupling operator $s = \sigma_x$ strongly coupled to an underdamped Brownian bath at finite temperature. As the blue line, the evolution follows the standard pseudomode model described in Eq. [\(48\)](#page-10-2) in which all degrees of freedom are quantized [for a total of five modes, i.e., the ones described in Eq. [\(D42\)](#page-35-0) and two fitting the Matsubara contribution to the correlation]. As the dashed red line, the evolution of the empirical average in Eq. (20) for $N_{\text{stoch}} = 500$ is evaluated with the stochastic pseudomode model involving a single harmonic oscillator to model the quantum contribution. The standard deviation from Eq. [\(29\)](#page-6-1) is, for these parameters, not visible. The horizontal dashed gray line represents the value of the observable at thermal equilibrium. The parameters are $\omega_0 = \omega_s$, $\gamma = 0.1\omega_s$, $λ = (0.2/\sqrt{2\pi})\omega_s^{3/2}, β = 2/\omega_s,$ and $N_\xi = 500$.

resulting in the usual expression

$$
C_{\text{class}}^B(t) \stackrel{\beta \to \infty}{=} \frac{i}{\pi} \int_0^\infty dx J^B(ix) e^{-x|t|}, \tag{47}
$$

which involves only the so-called Matsubara contribution. In Fig. [2,](#page-8-1) we show an example of these correlations at zero temperature.

The dynamics of a system coupled to a bath with the spectral density in Eq. [\(42\)](#page-9-6) can be computed through a traditional pseudomode model in which quantum modes are used to both exactly describe the quantum contributions *and* to approximate the Matsubara series in Eq. [\(46\).](#page-9-3) A minimal number of $1 + N_{\text{Mats}}$ pseudomodes are needed in the zero-temperature limit (where N_{Mats} is the number of Matsubara modes). In contrast, the stochastic pseudomode model requires only a *single quantum degree of freedom initially at zero temperature* to model an underdamped Brownian environment *at any temperature*. More specifically, the model reads

$$
\dot{\rho} = -i[H_B, \rho] + D_B[\rho],\tag{48}
$$

where

$$
H_B = H_S + \xi^B(t) s + \lambda_{\text{res}} \sigma_x (a + a^{\dagger}) + \Omega_{\text{res}} a^{\dagger} a \qquad (49)
$$

FIG. 5. Dynamics of a two-level system with Hamiltonian $H_S = (\omega_s/2)\sigma_z$ and coupling operator $s = \sigma_x$ coupled to an Ohmic spectral density (inset) at zero temperature. For the dashed green line and the dashed red line we used the stochastic model (averaged $N_{\text{stoch}} = 10^3$ and $N_{\text{stoch}} = 10^4$ times, respectively), where two quantum pseudomodes account for the antisymmetric part of the correlation, see also Fig. 10 for further details. This result is compared with the solution of the HEOM [\[32\]](#page-39-14), where the full correlation function is approximated as a linear combination of 20 decaying exponentials. This value is chosen to check the results of the presented method with respect to a nearly exact case. The bound on the estimated standard deviation obtained from Eq. [\(29\)](#page-6-1) is shown in light red. The parameters are $N_{\text{PM}}^{\Omega} = 2$, $\alpha = 2/100$, $\omega_c = 3\omega_s$, and $N_{\xi} = 1000$.

in terms of the parameters $\lambda_{res} = \sqrt{\lambda^2/2\Omega}$ and $\Omega_{res} = \Omega$, and where

$$
D_B[\rho] = \Gamma_{\rm res}[2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a],\tag{50}
$$

is a zero-temperature dissipator written as a function of the decay rate $\Gamma_{\text{res}} = \Gamma$. The fields $\xi^{B}(t)$ can be explicitly defined by use of Eq. [\(14\)](#page-4-1) together with the analytical expression in Eq. $(D49)$ for the coefficients c_n . To test the method, in Figs. [3](#page-9-5) and [4](#page-10-3) we show the dynamics of a single two-level system with Hamiltonian $H_S = (\omega_s/2)\sigma_z$ and coupling operator $s = \sigma_x$. The stochastic model results are compared with those obtained by solving the fully quantized pseudomode model both at zero temperature and at finite temperature and for different regimes involving strongly and weakly coupled resonances with different broadening.

B. Ohmic spectral density with exponential cut-off

In this section, we consider the spectral density

$$
J^{\Omega}(\omega) = \pi \alpha \omega e^{-\omega/\omega_c},\tag{51}
$$

which shows an Ohmic behavior at low frequencies characterized by the strength parameter $\alpha \in \mathbb{R}$ and by an exponential decay characterized by the frequency cut-off ω*^c* [\[120\]](#page-42-2). While the transcendental form of this spectral density does not allow us to use the results presented in Sec. [IV](#page-7-0) for rational functions, it is still possible to follow the

FIG. 6. Dynamics of a two-level system coupled to three baths characterized by different spectral densities at different temperatures (see the inset). As the cyan line, the dynamics was computed with use of the HEOM. Dashed curves were computed with use of the stochastic pseudomode model averaging over $N_{\text{stoch}} = 10$ (yellow) and $N_{\text{stoch}} = 10^4$ (red) realizations for the classical noise. The horizontal dashed red, green, and blue lines correspond to the thermal occupation which the qubit would have at the temperature of each individual bath. The horizontal dashed gray line corresponds the occupation it would have in the steady state when hybridization effects with the environment are ignored, obtained with the expression given in Ref. [\[126\]](#page-42-3).

procedure in Sec. [III B](#page-6-0) to define the stochastic pseudomode model using numerical optimization. Specifically, it is possible to find the parameters $\{a_j^{\Omega}, b_j^{\Omega}, c_j^{\Omega}\}\$ that better approximate the antisymmetric part of the correlation

$$
C_{\text{as}}^{\Omega}(t) = -2i\alpha\omega_c^2 \frac{\omega_c t}{(1+\omega_c^2 t^2)^2} \simeq \sum_{j=1}^{N_{\text{PM}}^{\Omega}} a_j^{\Omega} \sin(b_j^{\Omega} t) e^{-c_j^{\Omega} |t|}.
$$
\n(52)

We note that, it with respect to the fully quantized pseudomode model, the procedure presented here has the advantage of not having to fit the symmetric part of the correlation, which also contains all information about the temperature of the original environment. In Fig. [5](#page-10-4) we show an example in which the dynamics of a two-level system is computed by use of two pseudomodes together with classical stochastic fields. We compared this result against the hierarchical equations of motion solved with use of the BoFiN package [\[32](#page-39-14)[,121–](#page-42-4)[124\]](#page-42-5).

VI. MULTIPLE BATHS AT DIFFERENT TEMPERATURES

It is interesting to note that, in the case of an underdamped Brownian spectral density, the Hilbert space of the stochastic pseudomode model augments the system with only a single extra pseudomode initialized in the vacuum for any temperature of the original environment. This should be compared with the deterministic pseudomode method, which, as shown in Eq. ($D40$), requires $3 + N_{Mats}$ pseudomodes $[125]$, where N_{Mats} is the number of modes

FIG. 7. Using the example and parameters from Fig. [3\(b\),](#page-9-5) we calculate the von Neumann entropy of the reduced system state as a function of time. The solid black curve shows the result from a deterministic pseudomode (PM) model with a single quantum pseudmode and where the Matsubara, or classical, contribution to the bath correlation function is omitted entirely. The solid blue curve represents the result for the same situation but with the Matsubara contribution included as quantum pseudomodes. Ad the dashed purple curve we show the result for the hybrid stochastic pseudomode model, where the quantum part of the correlation function is the same as that for the solid black curve, but the Matsubara part is captured by classical stochastic fields, with $N_{\text{stoch}} = 1000$. In both the deterministic approach and the hybrid stochastic approach the addition of the imaginary-valued Matsubara contribution reduces the system entropy.

corresponding to a fit with *N*_{Mats} exponentials for the Matsubara contribution to the correlation; see Eq. [\(D40\).](#page-35-1) This might result in a considerable reduction of the Hilbert space when the system is coupled to multiple baths at different temperatures. We analyze this case in Fig. [6,](#page-11-2) where a single two-level system is coupled to three independent Brownian baths at different temperatures.

In Fig. [6,](#page-11-2) we compare the steady-state value of $\langle \sigma_z \rangle$ with the values the spin would have when in equilibrium with each bath. Using the elegant formalism in Ref. [\[126\]](#page-42-3), we further show that the steady state is different from the one expected for a system weakly coupled to all three baths. The averaging over the statistics of the field completes the full characterization of the effects due to hybridization with the quantum degrees of the original bath. To further test the method, in Appendix $\overline{D}3$, we present the results for an environment causing pure decoherence, i.e., when the system interaction operator commutes with the system Hamiltonian.

VII. VON NEUMANN ENTROPY

The hybrid pseudomode model described in this article is an effective method, i.e., its only goal is to reproduce the *effects* of the environment on the system, rather than the system-bath full dynamics. It does so by introducing ancillary degrees of freedom that are not directly related to the original environment. This allows us to extend the regime of the associated parameters to unphysical values as long as the reduced density matrix of the system remains physical. As a consequence, despite the effective nature of these degrees of freedom, it is still meaningful to estimate relevant quantities that are a function of such a reduced dynamics. One important example is the von Neumann entropy

$$
S(t) = -\mathrm{Tr}_S \rho_S(t) \log \rho_S(t), \tag{53}
$$

which can be used as a measure of the information contained in the system and the correlation between bipartite systems. For example, in our context, it can be considered as a measure of system-bath entanglement when the initial state of the bath is at zero temperature, and the initial state of the system is a pure state.

In normal circumstances, one might expect that the presence of stochastic noise might drive a system to a higher-entropy state, i.e., it would increase its information disorder. It is then interesting to test whether this intuition remains true for the kind of noise needed to model the classical contribution to the correlation function of a quantum bath considered here. In the case of a zero-temperature bath characterized by an underdamped Brownian spectral density, the driving field is purely imaginary. In Fig. [7,](#page-11-3) we show that this unphysical field cause a decrease in the von Neumann entropy of the reduced state of the system.

While the effective nature of the fields prevents a direct physical interpretation, the meaning of this result can still be found in the description of the properties associated with different contributions to the correlation function of a physical environment. For example, any approximation that ignores the Matsubara contribution of a Brownian environment at zero temperature will correspond to an overestimation of the disorder in the reduced state of the system, due to a breaking of the detailed balance condition of that environment. In turn, by using unphysical, imaginary fields, one can correctly reduce such a disorder to the correct physical balance.

VIII. CONCLUSIONS

In this article, we analyzed a decomposition of the effects of a Gaussian bosonic bath on a system into quantum and classical contributions. We used this decomposition to define a stochastic version of the bosonic pseudomode method in which classical noise complements a discrete set of harmonic degrees of freedom to model non-Markovian open quantum systems. This ultimately results in a reduction of the number of ancillary quantum resources needed for the classical simulation of the original environment, which can become critical to model highly structured open quantum systems in the presence of multiple baths at different temperatures.

Ohmic, pure dephasing, multiple baths at different **7** (Sec. VI)

FIG. 8. Summary. Given a linear interaction between a system and a Gaussian environment, the system dynamics is a function of the correlation of the environmental coupling operator. Different models rely on different approximations for the correlation. For example, the deterministic pseudomode model assumes an ansatz given by a sum of decaying exponentials, which introduces a bias error. By using a classical or quantum decomposition, it is possible to consider an additional stochastic driving to model, on average, more general correlations. In this case, the observables are stochastic variables whose variance scales as the inverse of the number of noise realizations. Numerical examples for different specific models are provided.

Furthermore, all temperature effects of the original environment can be encoded into properties of the classical noise, allowing the remaining quantum degrees of freedom to be, initially, at zero temperature. For a class of rational spectral densities, all parameters of the stochastic pseudomode model are explicitly provided without the need for any best-fit optimization for all temperatures of the original bath, thereby simplifying the modeling stage.

We tested the method for Ohmic spectral densities with polynomial and exponential decay against the deterministic pseudomode method and the hierarchical equations of motion, respectively. The possibility to encode all temperature effects in the statistics of the driving field even for multiple baths leads to improved handling of the computational resources with respect to the fully deterministic pseudomode model. We further observed interesting features related to the unphysicality of this field, which, despite its noisy nature, decreases the von Neumann entropy of the system-environment partition. This shows that the simplicity in the interpretation of this method can lead to new interesting ways to explore non-Markovian effects, such as the entanglement structure in open quantum systems.

In summary, see Fig. [8,](#page-12-0) our hybrid method allows one to model the nonperturbative effects of a bosonic bath on a system's dynamics with an approach that balances conceptual simplicity (it requires only averaging over the solutions of a Lindblad-like equation) and numerical accuracy, while using a limited amount of quantum resources with respect to deterministic algorithms, such as the regular pseudomode model and the regular HEOM.

Beyond numerical simulations, despite the purely effective nature of the degrees of freedom involved, the quantum-classical decomposition presented here could also be useful in analyzing the interplay between quantum and classical effects induced by environments in the context of quantum thermodynamics [\[127](#page-42-7)[,128\]](#page-42-8), quantum control [\[32](#page-39-14)[,129](#page-42-9)[,130\]](#page-42-10), and quantum transport [\[131](#page-42-11)[–134\]](#page-42-12). In this direction, we provide evidence that the imaginary nature of the stochastic field characterizes effects that tend to decrease the von Neumann entropy of the reduced system state.

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APPENDIX A: INFLUENCE SUPEROPERATOR

In this section, we derive an expression for the influence superoperator (see also Refs. [\[135–](#page-42-13)[137\]](#page-42-14)) appearing in Eq. [\(2\)](#page-2-2) that encodes all the effects of a bosonic Gaussian environment linearly interacting with a quantum system. The proof does not use any path-integral technique.

1. A canonical derivation

Here we present a canonical (i.e., purely operator-based) derivation of the bosonic influence superoperator. We consider system *S* coupled to bosonic environment *B* as

$$
H = HS + HI + HB, \t(A1)
$$

where H_S is the system Hamiltonian and $H_B = \sum_k \omega_k b_k^{\dagger} b_k$ characterizes the energy ω_k of each environmental mode b_k . We suppose the system-environment coupling to be in the form $H_I = sX$, where *s* is a system operator and *X* is an interaction operator linearly expanded by $\{b_k^{\dagger}, b_k\}$. Meanwhile, we assume the initial state can be denoted as $\rho(0) = \rho_S(0) \otimes \rho_B(0)$, where $\rho_S(0)$ is the initial state of the system and $\rho_B(0)$ is a Gaussian state of the bosonic environment (for example, a thermal equilibrium state at inverse temperature β). We further suppose that the initial state of the environment is invariant under the free dynamics, i.e., $\rho_B(0) = U_0(t)\rho_B(0)U_0^{\dagger}(t)$ in terms of the free propagator $U_0(t) = \exp[-i(H_S + H_B)t]$

In the interaction picture, the Schrödinger equation

$$
\dot{\rho} = -i[H_I(t), \rho] \tag{A2}
$$

can be formally solved as

$$
\rho(t) = \mathcal{T}\left[e^{-i\int_0^t d\tau H_I^{\times}(\tau)}\right]\rho(0),\tag{A3}
$$

where $H_I(t) = U_0^{\dagger}(t)H_I U_0(t)$, and where we further defined $O^{\times}[\cdot] = [O, \cdot]$ as the superoperator associated with the commutation with the operator *O*. The time-ordering operator *T* acts on superoperators as

$$
\mathcal{T}\left[O^{\times}(t_1)O^{\times}(t_2)\right] = O^{\times}(t_1)O^{\times}(t_2)\theta(t_1 - t_2)
$$

$$
+ O^{\times}(t_2)O^{\times}(t_1)\theta(t_2 - t_1), \quad (A4)
$$

where θ is the step function defined as 1 for $x > 0$, 1/2 for $x = 0$, and 0 otherwise.

We are now interested in analyzing the reduced density matrix for the system, i.e., $\rho_S(t) = Tr_B[\rho(t)]$, which, with use of Eq. $(A3)$, takes the form

$$
\rho_S(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \text{Tr}_B \left[\mathcal{T} \int_0^t dt_1 \cdots \int_0^t dt_n H_I^\times(t_1) - \cdots H_I^\times(t_n) \rho(0) \right]. \tag{A5}
$$

We can now consider the explicit form of the interaction Hamiltonian in the interaction frame, i.e., $H_I(t) = s(t) \otimes$ *X*(*t*), where $s(t) = e^{iH_St}se^{-iH_St}$ and $X(t) = e^{iH_Bt}Xe^{-iH_Bt}$, and use it in Eq. $(A5)$. In this way, the first nontrivial term can be written as

$$
H_I^{\times}(t) [\rho_S(0) \otimes \rho_B(0)] = \sum_{i=1}^2 \mathcal{S}_i^i [\rho_S(0)] \otimes \mathcal{X}_i^i [\rho_B(0)],
$$
\n(A6)

where $S_t^1[\cdot] = s(t) \cdot$, $S_t^2[\cdot] = - \cdot s(t)$, $X_t^1[\cdot] = X(t) \cdot$, and X_t^2 [·] = *X* (*t*). With use of this notation in Eq. [\(A5\),](#page-13-2) the reduced density matrix takes the form

$$
\rho_S(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \rho_n(t),
$$
\n(A7)

where $\rho_0(t) = Tr_B[\rho(0)]$ and

$$
\rho_n(t) = \int_0^t dt_1 \cdots \int_0^t dt_n \sum_{i_1,\dots,i_n} \text{Tr}_B
$$

$$
\times \left[T \mathcal{X}_{t_1}^{i_1} \cdots \mathcal{X}_{t_n}^{i_n} \rho_B(0) \right] T \mathcal{S}_{t_1}^{i_1} \cdots \mathcal{S}_{t_n}^{i_n} \rho_S(0) \quad \text{(A8)}
$$

for $n > 0$. To make progress, we now take advantage of the Gaussianity of the state $\rho_B(0)$, which translates into the following version of Wick's theorem for superoperators (see Appendix [A 4\)](#page-17-1):

$$
\operatorname{Tr}\left[\mathcal{I}\mathcal{X}_{t_1}^{i_1}\cdots\mathcal{X}_{t_{2N}}^{i_{2N}}\rho_B\right]=\sum_{C\in P_{2N}}\prod_{(l,m)\in C}\operatorname{Tr}\left[\mathcal{I}\mathcal{X}_{t_l}^{i_l}\mathcal{X}_{t_m}^{i_m}\rho_B\right],\tag{A9}
$$

where the traces are intended on the bath *B*, where we omitted the time label in the state $\rho_B(0)$, and where P_{2N} is the collection of all possible sets (full contractions *C*) whose elements are *N* disjoint pairs (i.e., contractions) taken from $\{1, \ldots, 2N\}$. The cardinality of P_{2N} is $(2N - 1)!! = (2N)!/(2^N N!)$, i.e., the number of different ways to fully contract the set $\{1,\ldots,2N\}$. We further have that $\text{Tr}_B\left[\mathcal{TX}_{t_1}^{i_1}\cdots\mathcal{X}_{t_{2N+1}}^{i_{2N+1}}\rho_B\right]=0$. We refer to Appendix [A 4](#page-17-1) for a detailed proof of this version of Wick's theorem written in terms of time-ordered superoperators.

Using Wick's theorem in Eq. [\(A8\),](#page-13-3) we obtain

$$
\rho_{2N}(t) = \sum_{C \in P_{2N}} \int_{0}^{t} dt_{1} \cdots \int_{0}^{t} dt_{2N} \prod_{(l,m) \in C} \sum_{i_{l},i_{m}} Tr_{B} \left[T \mathcal{X}_{t_{l}}^{i_{l}} \mathcal{X}_{t_{m}}^{i_{m}} \rho_{B}(0) \right] T \left[S_{t_{1}}^{i_{1}} \cdots S_{t_{2N}}^{i_{2N}} \right] \rho_{S}(0)
$$
\n
$$
= \sum_{C \in P_{2N}} T \left[\int_{0}^{t} dt_{1} \cdots \int_{0}^{t} dt_{2N} \prod_{(l,m) \in C} \sum_{i_{l},i_{m}} Tr_{B} \left[T \mathcal{X}_{t_{l}}^{i_{l}} \mathcal{X}_{t_{m}}^{i_{m}} \rho_{B}(0) \right] S_{t_{1}}^{i_{1}} \cdots S_{t_{2N}}^{i_{2N}} \right] \rho_{S}(0)
$$
\n
$$
= \sum_{C \in P_{2N}} T \left[\int_{0}^{t} dt_{1} \cdots \int_{0}^{t} dt_{2N} \prod_{(l,m) \in C} \left(\sum_{i_{l},i_{m}} Tr_{B} \left[T \mathcal{X}_{t_{l}}^{i_{l}} \mathcal{X}_{t_{m}}^{i_{m}} \rho_{B}(0) \right] S_{t_{l}}^{i_{l}} S_{t_{m}}^{i_{m}} \right) \right] \rho_{S}(0)
$$
\n
$$
= T \left\{ \sum_{C \in P_{2N}} \left(\int_{0}^{t} dt_{2} \int_{0}^{t} dt_{1} \sum_{i_{2},i_{1}} Tr_{B} \left[T \mathcal{X}_{t_{2}}^{i_{2}} \mathcal{X}_{t_{1}}^{i_{1}} \rho_{B}(0) \right] S_{t_{2}}^{i_{2}} S_{t_{1}}^{i_{1}} \right)^{N} \rho_{S}(0) \right\}
$$
\n
$$
= T \left\{ \frac{(2N)!}{N!} \left(\frac{1}{2} \int_{0}^{t} dt_{2} \int_{0}^{t} dt_{1} \sum_{i_{2},i_{1}} Tr_{B} \left[T \mathcal{X}_{t_{2}}^{i_{2}} \mathcal{X}_{t_{1}}^{i_{1}} \rho_{B}(0) \right] S_{t_{2}}^{i_{2}}
$$

Using this result in Eq. $(A7)$, we obtain

$$
\rho_S(t) = \mathcal{T} \left\{ \sum_{N=0}^{\infty} \frac{(-1)^N}{N!} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 \sum_{i_2, i_1} \text{Tr}_B \left[\mathcal{X}_{t_2}^{i_2} \mathcal{X}_{t_1}^{i_1} \rho_B(0) \right] \mathcal{S}_{t_2}^{i_2} \mathcal{S}_{t_1}^{i_1} \right)^N \right\} \rho_S(0)
$$

= $\mathcal{T} \operatorname{Exp} \left\{ - \int_0^t dt_2 \int_0^{t_2} dt_1 \sum_{i_2, i_1} \text{Tr}_B \left[\mathcal{X}_{t_2}^{i_2} \mathcal{X}_{t_1}^{i_1} \rho_B(0) \right] \mathcal{S}_{t_2}^{i_2} \mathcal{S}_{t_1}^{i_1} \right\} \rho_S(0)$
= $\mathcal{T} e^{\mathcal{F}(t, s, C(t))} \rho_S(0)$ (A11)

in terms of the superoperator

$$
\mathcal{F}(t,s,C(t))[\cdot] = -\int_0^t dt_2 \int_0^{t_2} dt_1 \sum_{i_2,i_1} \text{Tr}_B \left[\mathcal{X}_{t_2}^{i_2} \mathcal{X}_{t_1}^{i_1} \rho_B(0) \right] S_{t_2}^{i_2} S_{t_1}^{i_1}[\cdot]
$$

\n
$$
= -\int_0^t dt_2 \int_0^{t_2} dt_1 C(t_2,t_1) \left[s(t_2)s(t_1)[\cdot] - s(t_1)[\cdot]s(t_2) \right] + C(t_1,t_2) \left[[\cdot]s(t_1)s(t_2) - s(t_2)[\cdot]s(t_1) \right]
$$

\n
$$
= \int_0^t dt_2 \int_0^{t_2} dt_1 C(t_2-t_1) \left[s(t_1) \cdot s(t_2) \right] - C(t_1-t_2) \left[\cdot s(t_1), s(t_2) \right], \tag{A12}
$$

which proves Eq. [\(2\)](#page-2-2) and which depends on the correlation function

$$
C(t_2, t_1) = Tr_B [X(t_2)X(t_1)\rho_B(0)]
$$

=
$$
\sum_k g_k^2 Tr_B [(a^{\dagger}e^{i\omega t_2} + ae^{-i\omega t_2})(a^{\dagger}e^{i\omega t_1} + ae^{-i\omega t_1})\rho_B(0)] = \int d\omega \frac{J(\omega)}{\pi} [(2n(\omega) + 1)\cos(\omega t) - i\sin(\omega t)]
$$
 (A13)

of the environmental interaction operator $X(t)$. Here $J(\omega) = \pi \sum_{k} g_k^2 \delta(\omega - \omega_k)$ and $t = t_2 - t_1$, so, using $2n(\omega) + 1 = \coth \beta \omega/2$, we get Eq. [\(3\).](#page-2-5) The invariance of the initial environmental state under free dynamics implies the stationarity of the correlation, i.e.,

$$
C(t_2, t_1) = \text{Tr}_B \left[X(t_2) U_0^{\dagger}(t_1) X(0) U_0(t_1) \rho_B(0) \right]
$$

\n
$$
= \text{Tr}_B \left[X(t_2) U_0^{\dagger}(t_1) X(0) \rho_B(0) U_0(t_1) \right]
$$

\n
$$
= \text{Tr}_B \left[U_0(t_1) X(t_2) U_0^{\dagger}(t_1) X(0) \rho_B(0) \right]
$$

\n
$$
= \text{Tr}_B \left[X(t_2 - t_1) X(0) \rho_B(0) \right]
$$

\n
$$
\equiv C(t). \tag{A14}
$$

In summary, the effects on the reduced dynamics of a Gaussian bosonic environment linearly coupled to a quantum system can be fully described by an influence superoperator that depends on the system coupling operator *s* and the correlation function $C(t)$ of the environmental coupling operator. This directly implies the equivalence between the reduced dynamics of any open quantum system sharing the same *s* and *C*(*t*); see Ref. [\[79\]](#page-41-18).

In the following, we further improve on this derivation to allow for a general linear system-bath interaction.

2. Generalized interaction

It is worth noting that the result proven in Eq. $(A10)$ can be generalized to the case where the system and the environment interact through a more general form of the interaction term, i.e., performing the substitution

$$
H_I \mapsto H_I' = \sum_{\alpha} s^{\alpha} X^{\alpha}, \tag{A15}
$$

in Eq. [\(A1\),](#page-13-5) where s^{α} and X^{α} define a collection of system and environmental interaction operators. Under the replacement above, Eq. [\(A6\)](#page-13-6) takes the more general form

$$
H_I^{'\times}(t)\left[\rho_S(0)\otimes\rho_B(0)\right] = \sum_{\tilde{\alpha}} \mathcal{S}_t^{\tilde{\alpha}}\left[\rho_S(0)\right] \otimes \mathcal{X}_t^{\tilde{\alpha}}\left[\rho_B(0)\right],\tag{A16}
$$

where $\bar{\alpha} \equiv (i, \alpha)$ is a multi-index and where $S_t^{(1, \alpha)}[\cdot] =$ $s^{\alpha}(t) \cdot$, $S_t^{(2,\alpha)}[\cdot] = - \cdot s^{\alpha}(t), \; \mathcal{X}_t^{(1,\alpha)}[\cdot] = X^{\alpha}(t) \cdot$, and $\mathcal{X}_t^{(2,\alpha)}$ $[\cdot] = X^{\alpha}(t)$. As a consequence, we can follow all the calculations done in the previous section by simply replacing the upper indexes *i* with multi-indexes, i.e., $i \mapsto \alpha' =$ (i, α) , to get

$$
\rho'_{S}(t) = T e^{\mathcal{F}'(t,\{s\},\{C(t)\})} \rho_{S}(0), \tag{A17}
$$

where $\rho'_{S}(t)$ is the reduced density matrix for the system when the interaction Hamiltonian with the environment takes the generalized form $H_I'(t)$ above, and where

$$
\mathcal{F}' = -\int_0^t dt_2 \int_0^{t_2} dt_1 \sum_{\alpha'_1, \alpha'_2} \text{Tr}_B \left[\mathcal{X}_{t_2}^{\alpha'_2} \mathcal{X}_{t_1}^{\alpha'_1} \rho_B(0) \right] \mathcal{S}_{t_2}^{\alpha'_2} \mathcal{S}_{t_1}^{\alpha'_1},\tag{A18}
$$

in which we omitted the functional dependencies $(t, \{s\}, \{C(t)\})$ from \mathcal{F}' . We note that these dependencies highlight that in this case the influence superoperator depends on the whole set $\{s\}$ of s^{α} operators and the whole set $\{C(t)\}\$ of correlation functions $C_{\alpha\beta}$, which can be defined by further noting that

$$
\mathcal{F}' = -\int_{0}^{t} dt_{2} \int_{0}^{t_{2}} dt_{1} \mathcal{G}'(t_{2}, t_{1}),
$$

\n
$$
\mathcal{G}' = \sum_{i_{1}, i_{2}, \alpha_{1}, \alpha_{2}} \text{Tr}_{\beta} \left[\mathcal{X}_{t_{2}}^{i_{2}, \alpha_{2}} \mathcal{X}_{t_{1}}^{i_{1}, \alpha_{1}} \rho_{\beta} \right] \mathcal{S}_{t_{2}}^{i_{2}, \alpha_{2}} \mathcal{S}_{t_{1}}^{i_{1}, \alpha_{1}} \n= \sum_{\alpha, \beta} \text{Tr}_{\beta} \left[\mathcal{X}_{t_{2}}^{\alpha} \mathcal{X}_{t_{1}}^{\beta} \rho_{\beta} \right] s_{t_{2}}^{\alpha} s_{t_{1}}^{\beta} [\cdot] + \text{Tr}_{\beta} \left[\rho_{\beta} \mathcal{X}_{t_{1}}^{\beta} \mathcal{X}_{t_{2}}^{\alpha} \right] [\cdot] s_{t_{1}}^{\beta} s_{t_{2}}^{\alpha} - \text{Tr}_{\beta} \left[\mathcal{X}_{t_{1}}^{\beta} \rho_{\beta} \mathcal{X}_{t_{2}}^{\alpha} \right] s_{t_{1}}^{\beta} [\cdot] s_{t_{2}}^{\alpha} - \text{Tr}_{\beta} \left[\mathcal{X}_{t_{2}}^{\alpha} \rho_{\beta} \mathcal{X}_{t_{1}}^{\beta} \right] s_{t_{2}}^{\alpha} [\cdot] s_{t_{1}}^{\beta} \n= \sum_{\alpha, \beta} \text{Tr}_{\beta} \left[\mathcal{X}_{t_{2}}^{\alpha} \mathcal{X}_{t_{1}}^{\beta} \rho_{\beta} \right] [s_{t_{2}}^{\alpha}, s_{t_{1}}^{\beta} [\cdot]] - \text{Tr}_{\beta} \left[\rho_{\beta} \mathcal{X}_{t_{1}}^{\beta} \mathcal{X}_{t_{2}}^{\alpha} \right] [s_{t_{2}}^{\alpha}, [\cdot] s_{t_{1}}^{\beta}] = \sum_{\alpha, \beta} C^{\alpha\beta} (t_{2}, t_{1}) [s_{t_{2}}^{\alpha}, s_{t_{1}}^{\beta} [\cdot]] - C^{\beta\alpha} (t_{1}, t_{2}) [s_{t_{2}}^{\alpha}, [\cdot] s_{t_{1}}^{\beta}].
$$
\n(A19)

030316-16

Explicitly, we defined the correlation functions as

$$
C^{\alpha\beta}(t_2, t_1) = \mathrm{Tr}_B \left[X_{t_2}^{\alpha} X_{t_1}^{\beta} \rho_{\beta} \right]. \tag{A20}
$$

In conclusion, the influence superoperator for the generalized interaction Hamiltonian H_I' can be written as

$$
\mathcal{F}'[\cdot] = \int_0^t dt_2 \int_0^{t_2} dt_1 \sum_{\alpha,\beta} \left\{ C^{\beta\alpha}(t_1, t_2) [s_{t_2}^{\alpha}, \cdot s_{t_1}^{\beta}] -C^{\alpha\beta}(t_2, t_1) [s_{t_2}^{\alpha}, s_{t_1}^{\beta}] \right\}.
$$
 (A21)

a. Quantum white noise limit

Here we exemplify the results above in the case where the environment can be modeled as quantum white noise (i.e., frequency-independent spectral density nonzero for both positive and negative energies, and frequencyindependent Bose-Einstein occupation number) and interacts with the system in a "rotating-wave" fashion, i.e., $H_I^{\text{RW}} = s^+ A(0) + s^- A^{\dagger}(0)$, where $s^+ = (s^-)^{\dagger}$ and $A(t) =$ $\sum_k g_k b_k(t)$. In this case, only two of the four correlations in Eq. [\(A20\)](#page-16-0) are nonzero, i.e.,

$$
C^{+-}(t_2, t_1) = \text{Tr}_B \left[A_{t_2}^{\dagger} A_{t_1} \rho_{\beta} \right] = \sum_k g_k^2 n_k e^{i\omega_k t}
$$

$$
= 2\Gamma n \delta(t),
$$

$$
C^{-+}(t_2, t_1) = \text{Tr}_B \left[A_{t_2} A_{t_1}^{\dagger} \rho_{\beta} \right] = \sum_k g_k^2 (n_k + 1) e^{-i\omega_k t}
$$

$$
= 2\Gamma(n + 1) \delta(t), \qquad (A22)
$$

and, similarly, $C^{++}(t_2, t_1) = C^{--}(t_2, t_1) = 0$, where $t =$ $t_2 - t_1$ and where we used $\int_{-\infty}^{\infty} d\omega e^{i\omega t} = 2\pi \delta(t)$ together with the quantum white noise conditions

$$
J(\omega) = \pi \sum_{k} g_k^2 \delta(\omega - \omega_k) = \Gamma,
$$

$$
n_k = n.
$$
 (A23)

By using these expressions in Eq. [\(A21\),](#page-16-1) we obtain

$$
\mathcal{G}'[\cdot] = C^{+-}(t)[s_{t_2}^-, s_{t_1}^+] - C^{-+}(t)[s_{t_2}^-, s_{t_1}^+] \n+ C^{-+}(t)[s_{t_2}^+, s_{t_1}^-] - C^{+-}(t)[s_{t_2}^+, s_{t_1}^-] \n= \Gamma \delta(t) \left\{ n[s_{t_1}^-, s_{t_1}^+] - (n+1)[s_{t_1}^-, s_{t_1}^+] \right\} \n+ (n+1)[s_{t_1}^+, s_{t_1}^-] - n[s_{t_1}^+, s_{t_1}^-] \right\} \n= \Gamma \delta(t) \left\{ n \left[2s_{t_1}^-, s_{t_1}^+ - s_{t_1}^+ s_{t_1}^- - s_{t_1}^+ s_{t_1}^- \right] \right\} \n+ (n+1) \left[2s_{t_1}^+, s_{t_1}^- - s_{t_1}^- s_{t_1}^+ - s_{t_1}^- s_{t_1}^+ \right] \right\}, \quad \text{(A24)}
$$

which, when inserted in Eq. [\(A17\),](#page-15-0) gives a Lindblad equation in the Schrödinger picture, i.e.,

$$
\dot{\rho}'_S(t) = -i[H_s, \rho'_S(t)] + \Gamma D[\rho'_S(t); s^-]
$$
 (A25)

in terms of the dissipator

$$
D[\cdot; O] = n \left[2O \cdot O^{\dagger} - \cdot O^{\dagger}O - O^{\dagger}O \cdot \right] + (n+1) \left[2O^{\dagger} \cdot O - \cdot OO^{\dagger} - OO^{\dagger} \cdot \right], \quad (A26)
$$

where *O* is a generic system operator.

3. Classical environment

The results presented in the previous section include the possibility that part of the environment is made by a classical stochastic process. To explicitly see this, we can consider, in Eq. $(A1)$, the replacement

$$
H_I \mapsto H_I + H_I^{\text{class}},\tag{A27}
$$

where $H_I^{\text{class}} = s\xi(t)$ in terms of a classical stochastic field ξ(*t*) that complements the original quantum environment *B* with additional classical noise. In the following, we denote the average with respect to the underlying probability distribution of the field $\xi(t)$ by $E[\cdot]$. We further suppose the stochastic process $\xi(t)$ to be Gaussian (i.e., all statistical moments depend on the second-order moment by Wick's theorem), to be stationary (i.e., the second-order moment is invariant under translation in time of both its augments), and to have zero mean (i.e., $\mathbb{E}[\xi(t)] = 0$). With the replacement in Eq. $(A27)$, all the reasoning in Appendix [A](#page-13-0) continues to hold as long as we perform the substitution $Tr_B \mapsto \mathbb{E} Tr_B$. As a result, the correlation appearing in Eq. [\(A13\)](#page-15-1) takes a further contribution

$$
C(t_2, t_1) \mapsto C(t_2, t_1) + C_{\text{class}}(t_2, t_1), \tag{A28}
$$

where

$$
C_{\text{class}}(t_2, t_1) = \mathbb{E}[\xi(t_2)\xi(t_1)]. \tag{A29}
$$

The hypothesis of stationarity for the process $\xi(t)$ implies that $C_{\text{class}}(t_2, t_1) = C_{\text{class}}(t)$ for $t = t_2 - t_1$. Furthermore, since the field $\xi(t)$ is classical, it has trivial commutation relations ([$\xi(t_2)$, $\xi(t_1)$] = 0), and the correlation satisfies the additional constraint

$$
C_{\text{class}}(t) = \mathbb{E}[\xi(t_2)\xi(t_1)] = \mathbb{E}[\xi(t_1)\xi(t_2)]
$$

= $C_{\text{class}}(-t)$, (A30)

i.e., it is symmetric under time reversal.

Even more explicitly, using the same reasoning as above, we can generalize the interaction term considered in Appendix $A₂$ with the addition of a classical stochastic field, i.e., further generalizing Eq. $(A15)$ using

$$
H'_I \mapsto H'_I + H_I^{\text{class}}.\tag{A31}
$$

This ultimately results in an additional term in the influence superoperator of the form

$$
\mathcal{F}' \mapsto \mathcal{F}' + \mathcal{F}(t, s, C_{\text{class}}(t)). \tag{A32}
$$

4. Wick's theorem for time-ordered superoperators

To optimize space, whenever not explicitly stated, all traces in this section are assumed to be over the bath *B*. Common derivations of Wick's theorem (see Ref. [\[138\]](#page-42-15), page 243) show how to reduce *n*-point correlation functions involving fields linear in bosonic creation and annhilation operators in terms of two-point correlation functions. Using the notation presented in this article, we can, for example, write

$$
\langle X(t_1)\cdots X(t_{2N})\rangle = \sum_{C\in P_{2N}} \prod_{(l,m)\in C} \text{Tr}_B\left[X(t_l)X(t_m)\rho_B\right],\tag{A33}
$$

where $\langle \cdot \rangle \equiv \text{Tr}_{B}[\cdot \rho_{B}(0)]$ and where $\rho_{B}(0)$ is a Gaussian state such that $Tr_B[X(t)\rho_B] = 0$, and where P_{2N} is the collection of all possible sets (full contractions *C*) whose elements are *N* disjoint pairs (i.e., contractions) taken from {1, ... , 2*N*}. We further have that $Tr_B[\mathcal{X}(t_1)\cdots\mathcal{X}(t_{2N+1})\rho_B]=0$. In this section, we show that Wick's theorem can also be written in terms of timeordered superoperators linear in the fields *X* (*t*). More specifically, we are interested in correlations taking the form

$$
C_{2N} = \mathrm{Tr}_{B}\left[\mathcal{I}\mathcal{X}_{t_1}^{i_1}\cdots\mathcal{X}_{t_{2N}}^{i_{2N}}\rho_B\right],\tag{A34}
$$

where $\mathcal{X}_t^1[\cdot] = X(t)$ and $\mathcal{X}_t^2[\cdot] = X(t)$. To begin, we can write

$$
C_{2N} = \text{Tr}_B \left[\mathcal{X}_{t_{P_T(1)}}^{i_{P_T(1)}} \cdots \mathcal{X}_{t_{P_T(2N)}}^{i_{P_T(2N)}} \rho_B \right], \tag{A35}
$$

where P_T is a permutation of $\{1, \ldots, 2N\}$ such that $t_{P_T(1)} \ge$ $\cdots \geq t_{P_T(2N)}$. Now, depending on the value of their upper indexes, the superoperators act on the left or the right of the density matrix, so

$$
C_{2N} = \text{Tr} \left[\prod_{j:ip_{T}(j)=1} \mathcal{X}_{tp_{T}(j)}^{ip_{T}(j)} \prod_{k:ip_{T}(k)=2} \mathcal{X}_{tp_{T}(k)}^{ip_{T}(k)} \rho_{B} \right]
$$

=
$$
\text{Tr} \left[\prod_{k:ip_{T}(k)=2} X(t_{p_{T}(k)}) \prod_{j:ip_{T}(j)=1} X(t_{p_{T}(j)}) \rho_{B} \right],
$$
(A36)

where we used the cyclic property of the trace to bring the operators on the right of the density matrix back to the left. We further note that this procedure has caused the fields labeled by *k* indexes to be antiordered in time and indicate this by the overbar in $\bar{P}_T(k)$. It is now possible to invoke the usual version of Wick's theorem given in Eq. [\(A33\).](#page-17-2) In doing so, we obtain three different types of contraction:

(1) Contractions between indexes *j* (which we denote as j_1 and j_2), whose contribution to Wick's theorem can be written as

$$
Tr[X(t_{P_T(j_1)})X(t_{P_T(j_2)})\rho_B] = Tr[X_{t_{P_T(j_1)}}^1 X_{t_{P_T(j_2)}}^1 \rho_B]
$$

=
$$
Tr[T X_{t_{j_1}}^1 X_{t_{j_2}}^1 \rho_B].
$$
 (A37)

(2) Contractions between indexes *k* (which we denote as k_1 and k_2) whose contribution to Wick's theorem can be written as

$$
Tr[X(t_{\bar{P}_T(k_1)})X(t_{\bar{P}_T(k_2)})\rho_B] = Tr[X_{t_{P_T(k_1)}}^2 X_{t_{P_T(k_2)}}^2 \rho_B]
$$

= Tr[$\mathcal{I} X_{t_{k_1}}^2 X_{t_{k_2}}^2 \rho_B$]. (A38)

(3) Contractions between indexes *j* and *k*, whose contribution to Wick's theorem can be written as

$$
Tr_B[X(t_{\bar{P}_T(k)})X(t_{P_T(j)})\rho_B] = Tr_B[\mathcal{X}_{t_{\bar{P}_T(k)}}^2 \mathcal{X}_{t_{P_T(j)}}^1 \rho_B]
$$

=
$$
Tr_B[\mathcal{I} \mathcal{X}_{t_k}^2 \mathcal{X}_{t_j}^1 \rho_B],
$$
(A39)

where we note that the time-ordering is irrelevant as the superoperators commute.

As a consequence, using Wick's theorem for operators in Eq. $(A33)$ together with Eqs. $(A37)$ – $(A39)$, we can write

$$
\operatorname{Tr}\left[\mathcal{TX}_{t_1}^{i_1}\cdots\mathcal{X}_{t_{2N}}^{i_{2N}}\rho_B\right]=\sum_{C\in P_{2N}}\prod_{(l,m)\in C}\operatorname{Tr}\left[\mathcal{TX}_{t_l}^{i_l}\mathcal{X}_{t_m}^{i_m}\rho_B\right],\tag{A40}
$$

which proves Eq. $(A9)$. Since the number of superoperators present in the correlation is equal to the number of corresponding operators, the hypothesis $Tr_B[X(t)\rho_B] = 0$ together with Wick's theorem for operators allow us to also conclude that $\text{Tr}_B \left[T \mathcal{X}_{t_1}^{i_1} \cdots \mathcal{X}_{t_{2N}}^{i_{2N+1}} \rho_B \right] = 0.$

APPENDIX B: PSEUDOMODE MODEL

In this section, we provide details for the pseudomode model. In particular, we derive the pseudo-Schrödinger equation in Eq. (5) , which supports the main correspondence presented in Eq. [\(4\).](#page-2-0)

Following Refs. [\[79,](#page-41-18)[80\]](#page-41-1), to characterize a pseudomode model, we proceed in two logical steps. First, we define an open quantum system for which there exists a specific interaction operator whose correlation function can be expressed as a sum of decaying exponentials. As a consequence, this open quantum system can be used to define a structured environment that simulates physical baths whose correlation function can be expressed in such a functional form. Second, we show that the reduced density matrix for a system interacting with this environment can be equivalently computed by solving the pseudomode Lindblad master equation in Eq. [\(5\).](#page-2-4)

1. Open quantum system

We consider a model in which the system directly couples with *N*_{PM} pseudomodes, each of which interacts with its own residual environment made out of bosonic modes as

$$
H_T = H_{\text{PM}} + H_{\text{PM-RE}}^I + H_{\text{RE}},\tag{B1}
$$

where

$$
H_{\rm PM} = H_S + Xs + \sum_{j=1}^{N_{\rm PM}} \Omega_j a_j^{\dagger} a_j,
$$

$$
X = \sum_j \lambda_j X_j,
$$
 (B2)

where H_S is the system Hamiltonian and we considered N_{PM} pseudomodes a_i having frequency $\Omega_i \in \mathbb{C}$. The system-pseudomode interaction is characterized by a generic system operator *s* and an interaction operator *X*, where $\lambda_j \in \mathbb{C}$ and $X_j = a_j + a_j^{\dagger}$. We further suppose that each pseudomode a_i is associated with an independent residual environment made out by a collection of bosonic modes b_{jk} having frequency ω_{jk} so that $H_{\text{RE}} =$ $\sum_{j} \sum_{k} \omega_{jk} b_{jk}^{\dagger} b_{jk}$. To highlight their importance, we now describe the interaction of each pseudomode with its residual environment and the initial condition in the "pseudomode–residual environment" (PM-RE) space in more detail.

(1) We assume the interaction with the *j* th pseudomode to be written in following rotating-wave form:

$$
H_{\text{PM-RE}}^{I,j} = \sum_{k} g_{jk}(a_j b_{jk}^{\dagger} + a_j^{\dagger} b_{jk}), \quad (B3)
$$

so $H_{\text{PM-RE}}^{I} = \sum_{j=1}^{N_{\text{PM}}} H_{\text{PM-RE}}^{I,j}$.

(2) We assume the spectral density characterizing the *j* th residue environment to be a constant and to be defined for both negative and positive frequencies, i.e.,

$$
J_j(\omega) = \pi \sum_k g_{jk}^2 \delta(\omega - \omega_{jk}) \equiv \Gamma_j.
$$
 (B4)

(3) We assume the initial state in the PM-RE space to be

$$
\rho_{\text{PM-RE}}(0) \propto \prod_{j=1}^{N_{\text{PM}}} \exp \times \left[-\beta_j \Omega_j a_j^{\dagger} a_j - \beta_{jk} \sum_k \omega_{jk} b_{jk}^{\dagger} b_{jk} \right], \quad (B5)
$$

where we omitted the factor needed to ensure $Tr_{PM-RE}\rho_{PM-RE}(0) = 1$. To allow the invariance of the initial state under the free dynamics in the PM-RE space, i.e., under the Hamiltonian

$$
H_{\text{PM}}^{\text{free}} = H_{\text{PM-RE}}^I + H_{\text{RE}} + \sum_{j=1}^{N_{\text{PM}}} \Omega_j a_j^{\dagger} a_j
$$

=
$$
\sum_{j=1}^{N_{\text{PM}}} \left[\Omega_j a_j^{\dagger} a_j + \sum_k \omega_{jk} b_{jk}^{\dagger} b_{jk} + g_{jk} (a_j b_{jk}^{\dagger} + a_j^{\dagger} b_{jk}) \right],
$$
 (B6)

we consider a quantum white noise setting in which the expectation value of the occupation of each pseudomode is frequency independent, i.e.,

$$
\langle b_{jk}^{\dagger} b_{jk} \rangle = \langle a_j^{\dagger} a_j \rangle = n_j. \tag{B7}
$$

Here the expectation values are taken with respect to Eq. [\(B5\),](#page-18-0) which further implies the constraints

$$
\beta_j \Omega_j = \beta_{jk} \omega_{jk} = \ln \frac{1 + n_j}{n_j}.
$$
 (B8)

Using these relations, we can write Eq. $(B5)$ as $\rho_{\text{PM-RE}}(0) \propto \prod_{j=1}^{N_{\text{PM}}} \exp \left[-\ln(1 + 1/n_j) N_{\text{PM-RE}}^j \right],$ where $N_{\text{PM-RE}}^j = a_j^{\dagger} a_j + \sum_k b_{jk}^{\dagger} b_{jk}$ is the total number of excitations of the *j* th pseudomode and its residual environment. Since the Hamiltonian $H_{\text{PM-RE}}^{I}$ describes a rotating-wave interaction, and there is no interaction between the pseudomodes a_j , we have $[H_{\text{PM-RE}}^{\text{free}}, \sum_j N_{\text{PM-RE}}^j] = 0$, which, in turn, implies

$$
[H_{\text{PM-RE}}^{\text{free}}, \rho_{\text{PM-RE}}(0)] = 0, \tag{B9}
$$

i.e., the initial state is invariant under the free PM-RE dynamics.

We now consider the correlation function

$$
C(t+s,s) = \text{Tr}_{\text{PM-RE}}[X(t+s)X(s)\rho_{\text{PM-RE}}(0)], \quad (B10)
$$

where $X(t) = U^{\dagger}(t)XU(t)$, where $U(t) = e^{-iH_{PM}^{\text{free}}t}$. Using Eq. [\(B9\),](#page-18-1) we can prove that this correlation is stationary, i.e,

$$
C(t + s, s) = Tr[U^{\dagger}(t + s)XU(t)XU(s)\rho_{\text{PM-RE}}(0)]
$$

= Tr[U^{\dagger}(t)XU(t)XU(s)\rho_{\text{PM-RE}}(0)U^{\dagger}(s)]
= Tr[X(t)X(0)\rho_{\text{PM-RE}}(0)] := C(t), (B11)

where, for notational convenience, we omitted the labels PM ⊗ RE under the trace operator. We now compute $C(t)$ explicitly by considering the Heisenberg equations of motion

$$
\dot{a}_j(t) = i[H_{\text{PM}}^{\text{free}}, a_j] = -i\left(\Omega_j a_j + \sum_k g_{jk} b_{jk}\right),
$$

$$
\dot{b}_{jk}(t) = i[H_{\text{PM}}^{\text{free}}, b_{jk}] = -i\left(g_{jk} a_j + \omega_{jk} b_{jk}\right) \qquad (B12)
$$

with initial conditions $a_j(0)$ and $b_{jk}(0)$ at $t = 0$. By introducing the Laplace transformation $a_i[s]$ and $b_{ik}[s]$ of the operators, we can write

$$
a_j[s] = F_j[s]a_j(0) - iF_j[s] \sum_k G_{jk}[s]b_{jk}(0), \quad (B13)
$$

where

$$
F_j[s] = \frac{1}{s + i\Omega_j + \sum_k \frac{g_{jk}^2}{s + i\omega_{jk}}}
$$

=
$$
\frac{1}{s + i\Omega_j + \frac{1}{i\pi} \int d\omega \frac{J_j(\omega)}{\omega - is}}
$$

=
$$
\frac{1}{s + i\Omega_j + \Gamma_j sg(t)},
$$

$$
G_{jk}[s] = \frac{g_{jk}}{s + i\omega_{jk}},
$$
 (B14)

where we used Eq. [\(B4\)](#page-18-2) and where $sg(t) = t/|t|$ for $t \neq 0$. We can now use the inverse Laplace transform to find

$$
a_j(t) = a_j(0)e^{-i\Omega_j t - \Gamma_j|t|}
$$

- $i \sum_k g_{jk}b_{jk}(0) \int_0^t d\tau e^{-i\Omega_j \tau - \Gamma_j|\tau|} e^{-i\omega_{jk}(t-\tau)},$
(B15)

where we used the convolution theorem. Because of the stationarity condition in Eq. $(B11)$, we can use the formula above to directly compute the correlation as

$$
C(t) = \text{Tr}[X(t)X(0)] = \sum_{j} \lambda_j^2 \left(\text{Tr}[a_j^{\dagger}(t)a_j(0)] + \text{Tr}[a_j(t)a_j^{\dagger}(0)] \right)
$$

=
$$
\sum_{j} \lambda_j^2 \left[n_j e^{i\Omega_j t} + (n_j + 1)e^{-i\Omega_j t} \right] e^{-\Gamma_j |t|}.
$$
 (B16)

Despite our having already reached the main goal of this section with the expression above, it is interesting to also compute the correlation directly, i.e., without assuming (or, in our case, previously proving) translational invariance in time. This will highlight the role of the quantum fluctuations in the residual environment so as to effectively obtain stationarity. To do this, we write, with the help of Eq. [\(B15\),](#page-19-1)

$$
C(t_2, t_1) = \text{Tr}[X(t_2)X(t_1)]
$$

\n
$$
= \sum_j \lambda_j^2 \left\{ e^{i\Omega_j (t_2 - t_1) - \Gamma_j (|t_2| + |t_1|)} \text{Tr}[a_j^{\dagger}(0) a_j(0)] + e^{-i\Omega_j (t_2 - t_1) - \Gamma_j (|t_2| + |t_1|)} \text{Tr}[a(t_2) a^{\dagger}(t_1)] \right\}
$$

\n
$$
+ \sum_j \lambda_j^2 \sum_k g_{jk}^2 \text{Tr}[b_{jk}^{\dagger}(0) b_{jk}(0)] \int_0^{t_2} d\bar{\tau} \int_0^{t_1} d\tau e^{i\omega_{jk}(t_2 - \bar{\tau} - t_1 + \tau)} e^{i\Omega_j \bar{\tau} - \Gamma_j |\bar{\tau}|} e^{-i\Omega_j \tau - \Gamma_j |\tau|}
$$

\n
$$
+ \sum_j \lambda_j^2 \sum_k g_{jk}^2 \text{Tr}[b_{jk}(0) b_{jk}^{\dagger}(0)] \int_0^{t_2} d\bar{\tau} \int_0^{t_1} d\tau e^{i\omega_{jk}(t_2 - \bar{\tau} - t_1 + \tau)} e^{i\Omega_j \bar{\tau} - \Gamma_j |\bar{\tau}|} e^{-i\Omega_j \tau - \Gamma_j |\tau|}.
$$
 (B17)

Using Eqs. [\(B7\)](#page-18-3) and [\(B5\),](#page-18-0) we can write the last two two lines in Eq. [\(B17\)](#page-19-2) as π times an integral over frequencies, which can be evaluated, giving rise to $2\pi \delta(\bar{\tau} - [t_2 - t_1 + \tau])$. This allows us to further compute one of the integrals in time to obtain, assuming $t_2 > t_1$,

$$
C(t_2, t_1) = \text{Tr}[X(t_2)X(t_1)]
$$

\n
$$
= \sum_j \lambda_j^2 \left\{ n_j e^{i\Omega_j (t_2 - t_1)} + (n_j + 1)e^{-i\Omega_j (t_2 - t_1)} \right\} e^{-\Gamma_j (|t_2| + |t_1|)}
$$

\n
$$
+ 2 \sum_j \lambda_j^2 \Gamma_j \left\{ n_j \int_0^{t_1} d\tau e^{i\Omega_j (t_2 - t_1) - \Gamma_j |t_2 - t_1 + \tau|} e^{-\Gamma_j |\tau|} + (1 + n_j) \int_0^{t_1} d\tau e^{-i\Omega_j (t_2 - t_1) - \Gamma_j |t_2 - t_1 + \tau|} e^{-\Gamma_j |\tau|} \right\}
$$

\n
$$
= \sum_j \lambda_j^2 \left\{ n_j e^{i\Omega_j (t_2 - t_1)} + (n_j + 1)e^{-i\Omega_j (t_2 - t_1)} \right\} e^{-\Gamma_j (t_2 - t_1)},
$$
\n(B18)

which, indeed, shows how the fluctuations in the residual bath variables are essential to generate the $t_2 - t_1$ dependence for stationarity.

2. Lindblad master equation

Here we show that the reduced system dynamics can be computed by solving a Lindblad master equation in the S-PM space. We do this by considering the Hamiltonian in Eq. [\(B1\)](#page-18-4) and by tracing the residual environment. This can be done with use of the results in Appendix A_2 , which rely on the following correlations for the residual environment operator $B = \sum_{j,k} g_{j,k} b_{j,k}$:

$$
C_{1}^{RE}(t_{2}, t_{1}) = Tr_{B} [B^{\dagger}(t_{2})B(t_{1})\rho_{B}]
$$

\n
$$
= \sum_{j,k} g_{j,k}^{2} e^{i\omega_{kj} (t_{2} - t_{1})} Tr_{B} [b_{j,k}^{\dagger} b_{j,k} \rho_{B}]
$$

\n
$$
= \frac{1}{\pi} \sum_{j} \int d\omega J_{j}(\omega) n_{j} e^{i\omega t}
$$

\n
$$
= 2 \sum_{j} \Gamma_{j} n_{j} \delta(t),
$$

\n
$$
C_{2}^{RE}(t_{2}, t_{1}) = Tr_{B} [B(t_{2})B^{\dagger}(t_{1}) \rho_{B}]
$$

\n
$$
= 2 \sum_{j} \Gamma_{j} (1 + n_{j}) \delta(t),
$$
 (B19)

where $B(t) = e^{iH_{\text{RE}}t}Be^{-iH_{\text{RE}}t}$ and $t = t_2 - t_1$. The reduced dynamics in the S-PM space can be obtained with use of Eq. [\(A19\),](#page-15-4) i.e., $\rho_S(t) = T e^{\mathcal{F}^{RE}(t)} \rho_S(0)$. The corresponding *G*RE is given by

$$
\mathcal{G}^{\text{RE}}(t_2, t_1) = \sum_{j=1}^{N_{\text{PM}}} 2\Gamma_j n_j \delta(t) D(a_j(t_2), a_j(t_1)) + 2\Gamma_j (1 + n_j) \delta(t) D(a_j^{\dagger}(t_2), a_j^{\dagger}(t_1))
$$
 (B20)

and the corresponding \mathcal{F}^{RE} is given by

$$
\mathcal{F}^{\text{RE}}(t') = -\int_0^{t'} dt_2 \int_0^{t_2} dt_1 \mathcal{G}(t_2, t_1)
$$

=
$$
\sum_{j=1}^{N_{\text{PM}}} \int_0^{t'} dt_2 - \Gamma_j (1 + n_j) D(a_j^{\dagger}(t_2), a_j^{\dagger}(t_2))
$$

-
$$
\Gamma_j n_j D(a_j(t_2), a_j(t_2)),
$$
 (B21)

where we defined

$$
D(a, b)[\cdot] = [a, b^{\dagger} \cdot] - [a^{\dagger}, \cdot b], \tag{B22}
$$

and the Heisenberg operator $a_j(t) = e^{iH_{\text{PM}}t} a_j e^{-iH_{\text{PM}}t}$. Going back to the Schrödinger picture, we find the dynamics in the S-PM space takes the following Lindblad form:

$$
\dot{\rho}_{SPM} = -i[H_{PM}, \rho_{SPM}] + L[\rho_{SPM}], \quad (B23)
$$

where

$$
L[\cdot] = \sum_{j} \Gamma_{j} (1 + n_{j}) \left(2a_{j} [\cdot] a_{j}^{\dagger} - \{ a_{j}^{\dagger} a_{j}, \cdot \} \right)
$$

$$
+ \sum_{j} \Gamma_{j} n_{j} \left(2a_{j}^{\dagger} [\cdot] a_{j} - \{ a_{j} a_{j}^{\dagger}, \cdot \} \right). \tag{B24}
$$

To finish this section, we show that the correlation in Eq. [\(B16\)](#page-19-3) can be computed with use of the influence superoperator formalism. To do this, we consider the free dynamics in the PM-RE space as described by the Hamiltonian $H_{\text{PM}}^{\text{free}}$. The translational invariance of $C(t)$ in Eq. [\(B11\)](#page-19-0) allows us to write it as

$$
C(t) = \text{Tr}_{\text{PM}\otimes\text{RE}}[XU(t)X\rho_{\text{PM-RE}}(0)U^{\dagger}(t)]
$$

=
$$
\text{Tr}_{\text{PM}}[X\text{Tr}_{\text{RE}}[U(t)X\rho_{\text{PM-RE}}(0)U^{\dagger}(t)]], \quad (B25)
$$

which, in turn, allows us to use the results in Appendix $A₂$ with the unphysical initial condition $X \rho_{PM-RE}(0)$. We can then use Eq. $(A19)$, where the influence superoperator can

be calculated with use of steps similar to those used to get Eq. [\(B21\).](#page-20-0) We can then write

$$
C(t) = \text{Tr}_{PM}[Xe^{\mathcal{L}_{PM}t}[X \rho_{PM}(0)]]
$$

=
$$
\text{Tr}_{PM}[e^{\mathcal{L}_{PM}^{\dagger}}[X]X \rho_{PM}(0)],
$$
 (B26)

where $\rho_{PM}(t) = Tr_{RE}[U(t)\rho_{PM}(0) \otimes \rho_{RE}(0)U^{\dagger}(t)]$ and $\mathcal{L}_{PM}[\cdot] = -i \sum_{j=1}^{N_{PM}} [\Omega_j a_j^{\dagger} a_j, \cdot] + L[\cdot],$ where $\mathcal{L}_{PM}^{\dagger}$ is the adjoint operator of \mathcal{L}_{PM} .

$$
\mathcal{L}_{\text{PM}}^{\dagger}[\cdot] = \sum_{j=1}^{N_{\text{PM}}} i[\Omega_j a_j^{\dagger} a_j, \cdot] + \Gamma_j n_j \left(2a_j[\cdot]a_j^{\dagger} - \{a_j a_j^{\dagger}, \cdot\}\right) + \Gamma_j (1 + n_j) \left(2a_j^{\dagger}[\cdot]a_j - \{a_j^{\dagger} a_j, \cdot\}\right). \tag{B27}
$$

By using the identities

$$
\mathcal{L}_{PM}^{\dagger}[a_j] = -(i\Omega_j + \Gamma_j)a_j,
$$

\n
$$
\mathcal{L}_{PM}^{\dagger}[a_j^{\dagger}] = (i\Omega_j - \Gamma_j)a_j^{\dagger},
$$
\n(B28)

we can write the correlation as

$$
C(t) = \sum_{j=1}^{N_{\text{PM}}} \text{Tr}_{\text{PM}}[e^{\mathcal{L}_{\text{PM}}^{\dagger}}[X_j] \sum_{j=1}^{N_{\text{PM}}} X_j \rho_{\text{PM}}(0)]
$$

$$
= \sum_{j=1}^{N_{\text{PM}}} \lambda_j^2 \{e^{(-i\Omega_j - \Gamma_j)t} \langle a_j a_j^{\dagger} \rangle + e^{(i\Omega_j - \Gamma_j)t} \langle a_j^{\dagger} a_j \rangle \}
$$

$$
= \sum_{j=1}^{N_{\text{PM}}} \lambda_j^2 e^{-\Gamma_j t} \left(e^{-i\Omega_j t} (n_j + 1) + e^{i\Omega_j t} n_j \right). \quad (B29)
$$

We note that we could have obtained the same result by using the more general expression given by Eq. (6) in Ref. $[79]$, i.e.,

$$
C(t+s,s) = \text{Tr}_{\text{PM}}\{Xe^{\mathcal{L}t}\big[Xe^{\mathcal{L}s}[\rho_{\text{PM}}(0)]\big]\},\tag{B30}
$$

where $X = \sum_{j=1}^{N_{\text{PM}}} \lambda_j x_j$. Since the initial state is invariant under *L*, i.e., $e^{Lt} \rho_{PM}(0) = \rho_{PM}(0)$, this is equivalent to Eq. [\(B26\).](#page-21-0)

APPENDIX C: COMPLEMENTING PSEUDOMODES WITH CLASSICAL STOCHASTIC FIELDS

In this section, we analyze how to replace some of the quantum degrees of freedom in the pseudomode model with classical stochastic fields.

We consider a modification of the pseudomode model presented in Eq. [\(B1\)](#page-18-4) defined by adding classical stochastic noise to the system, i.e.,

$$
H_T^{\xi} = H_{\text{PM}}^{\xi} + H_{\text{PM-RE}}^I + H_{\text{RE}},\tag{C1}
$$

where $H_{\text{PM}}^{\xi} = H_{\text{PM}} + s\xi(t)$. Here the field $\xi(t)$ is supposed to have all the properties outlined in Appendix [A 3,](#page-16-3) i.e., Gaussianity, stationarity, and zero mean. We then proceed by characterizing this model following the two logical steps already used in Appendix [B,](#page-17-0) i.e., we first find the correlation of the interacting operator of the model and then describe the master equation that can be used to simulate the reduced density matrix.

The correlation of the model in Eq. $(C1)$ can be found by simply considering the results provided in Appendixes [B 1](#page-18-5) and $\overline{A}3$. Equation $(A28)$ tells us that the stochastic open quantum system in Eq. $(C1)$ has correlations given by

$$
C_{\text{PM+class}} = C_{\text{PM}} + C_{\text{class}},\tag{C2}
$$

where

$$
C_{PM}(t_2, t_1) = \text{Tr}_{PM\text{-RE}}[X_{PM}(t_2)X_{PM}(t_1)\rho_{PM\text{-RE}}(0)]
$$

=
$$
\sum_{j=1}^{N_{PM}} \lambda_j^2 [(1 + n_j)e^{-i\Omega_j t} + n_j e^{i\Omega_j t}]e^{-\Gamma_j |t|},
$$

$$
C_{\text{class}}(t_2, t_1) = \mathbb{E}[\xi(t_2)\xi(t_1)],
$$
 (C3)

with $X_{\text{PM}}(t) = \sum_{j=1}^{N_{\text{PM}}} \lambda_j X_j(t)$ and where C_{PM} is the correlation of the pure pseudomode model; see Eq. [\(B16\).](#page-19-3)

In our second step, we present a master equation to compute the reduced system dynamics. To do this, we can simply adapt the results presented in Appendix $B2$ by incorporating the action of the stochastic field into the system, i.e., by considering $H_{PM} \rightarrow H_{PM} + s\xi(t)$. This leads to the Lindblad equation for the S-PM system:

$$
\dot{\rho}^{\xi}(t) = -i[H_{\rm PM} + s\xi(t), \rho^{\xi}(t)] + \sum_{j=0}^{N_{\rm PM}} D_j[\rho^{\xi}(t)], \quad \text{(C4)}
$$

where

$$
D_j[\cdot] = \Gamma_j[(1 + n_j)(2a_j \cdot a_j^{\dagger} - a_j^{\dagger} a_j \cdot \cdot \cdot a_j^{\dagger} a_j) + n_j(2a_j^{\dagger} \cdot a_j - a_j a_j^{\dagger} \cdot \cdot \cdot a_j a_j^{\dagger})].
$$
 (C5)

Each Lindblad operator D_i acts only on the *j* th pseudomode's space. The reduced system dynamics can be computed by tracing the pseudomodes and averaging over the stochastic noise, i.e.,

$$
\rho_S(t) = \mathbb{E}\left[\text{Tr}_{PM}[\rho^{\xi}(t)]\right].\tag{C6}
$$

In practice, it might not be possible to compute this exact average over the stochastic field. In these cases, the equation above must be replaced with an empirical average as

$$
\rho_S^{\xi}(t; N_{\text{stoch}}) = \frac{1}{N_{\text{stoch}}} \sum_{j=1}^{N_{\text{stoch}}} \text{Tr}_{\text{PM}}[\rho^{\xi_j}(t)], \qquad (C7)
$$

where $\xi_j(t)$ indicates one of the N_{stoch} realizations of the stochastic process. This highlights the fact that to take advantage of this formalism, the resulting density matrix is now a random variable. In turn, this means that, on top of the deterministic sources of error due to potential imprecision in modeling the correlation of the original environment, here we also need to take into account further uncertainties due to the statistical properties of the stochastic variable $\rho_S^{\xi}(t; N_{\text{stoch}})$. The analysis of these deterministic and stochastic errors is the focus of the next section.

1. Error analysis

It is important to note that by replacing the exact average in Eq. $(C6)$ with the "empirical" one in Eq. $(C7)$, we are effectively introducing a potential error in the model. Intuitively, we can divide the sources of imprecision in the pseudomode model into two classes. One is a "bias" due to errors in approximating the correlation of the original environment $C(t)$ with C_{PM} in Eq. [\(C2\).](#page-21-3) The second source of error is due to the stochastic nature of Eq. $(C7)$. In the following we estimate more precisely the combined effects of these two error contributions.

To be more specific, we consider physical quantities in the form of the empirical average $O^{\xi}(t; N_{\text{stoch}})$ = $Tr_S \left[O \rho_S^{\xi}(t; N_{\text{stoch}}) \right]$ for a generic system operator *O* and we can further define $O^{\xi}(t) \equiv O^{\xi}(t; 1)$. Using Eq. [\(C7\),](#page-22-1) we can further write

$$
O^{\xi}(t; N_{\text{stoch}}) = \frac{1}{N_{\text{stoch}}} \sum_{j=1}^{N_{\text{stoch}}} \text{Tr}_{S} \left[O \rho_{S}^{\xi_{j}}(t) \right], \qquad (C8)
$$

which better highlights its nature of stochastic variable, where we defined $\rho_S^{\xi_j}(t) = \text{Tr}_{PM}[\rho^{\xi_j}(t)]$. Its expectation value is given by

$$
O(t) = \mathbb{E}[O^{\xi}(t; N_{\text{stoch}})] \equiv \mathbb{E}[O^{\xi}(t)],
$$
 (C9)

which is the stochastic-error-free estimate of the true expectation value $O_{true}(t)$ and is affected only by the bias error in reproducing the original correlation function. This can be quantified more explicitly by defining the following measure for the total error:

$$
\Delta O(t) = \mathbb{E}[|O^{\xi}(t; N_{\text{stoch}}) - O_{\text{true}}(t)|], \tag{C10}
$$

which with use of the triangle inequality takes the form

$$
\Delta O(t) \leq \Delta_{\text{stoch}} O(t) + \Delta_{\text{bias}} O(t), \tag{C11}
$$

where

$$
\Delta_{\text{stoch}} O(t) = \mathbb{E}[|O^{\xi}(t; N_{\text{stoch}}) - O(t)|],
$$

\n
$$
\Delta_{\text{bias}} O(t) = |O(t) - O_{\text{true}}(t)|.
$$
 (C12)

In the following, we analyze these two sources of error separately.

a. Bias

The bias error is due to the inaccuracy in reconstructing the original correlation function, i.e., it depends on the difference $\Delta C(t) = C(t) - C_{PM+\text{class}}$, where $C(t)$ is the correlation of the original environment and *C*_{PM+class} is the pseudomode model correlation in Eq. $(C2)$. While this bias can, in principle, originate from both classical and quantum pseudomode contributions, the classical part can usually be defined to achieve any accuracy by increasing the number of modes in the spectral expansion of the stochastic fields. As a consequence, the bias error is usually dominated by the functional form of the pseudomode correlation as a finite sum of decaying exponentials; see Eq. $(C3)$.

To estimate the bias, we closely follow Ref. [\[77\]](#page-40-6) and represent the derivation of one of its results. We do this for self-consistency and to explicitly avoid using any reference to path-integral techniques. We start by interpreting *O*(*t*) in Eq. [\(C9\)](#page-22-2) as obtained by tracing over an environment made out of the tensor product of the original bath *B* and an auxiliary "error bath" B_{err} . This auxiliary bath is supposed to be Gaussian and to have correlations given by $C_{\text{err}}(t) =$ $C_{PM+\text{class}}(t) - C(t)$. This allows us to consider $S' = S + B$ (system plus original bath) as a new system and use the results in Appendix [A.](#page-13-0) We have

$$
\Delta_{bias} O(t) = |{\rm Tr}_{S'} O(t) \mathcal{T} e^{\Delta \mathcal{F}} \rho(0) - {\rm Tr}_{S'} \mathcal{T} O(t) \rho(0)|,
$$
\n(C13)

where $O(t) = e^{iHt} Oe^{-iHt}$ with the Hamiltonian defined in Eq. [\(1\)](#page-2-3) in the *S* + *B* space, and where $\Delta \mathcal{F} = \mathcal{F}[t, s, C_{\text{err}}(t)]$ is the result of tracing out B_{err} using the definition in Eq. [\(A12\).](#page-14-1) Here $\rho(0) = \rho_S(0)\rho_B$; see the definitions in Sec. [I.](#page-2-1) By expanding the exponential and by the triangle inequality, we get

$$
\Delta_{\text{bias}} O(t) = \left| \sum_{n=1}^{\infty} \frac{1}{n!} \text{Tr}_{S'} O(t) \mathcal{T} (\Delta \mathcal{F})^n \rho(0) \right|
$$

$$
\leq \sum_{n=1}^{\infty} \frac{1}{n!} |\text{Tr}_{S'} O(t) \mathcal{T} (\Delta \mathcal{F})^n \rho(0)|. \qquad (C14)
$$

Using Eq. [\(A12\),](#page-14-1) we can write $\Delta \mathcal{F}$ as

$$
\Delta \mathcal{F} = \int_0^t dt_2 \int_0^{t_2} dt_1 \sum_{j=1}^4 (\Delta C)_j \hat{\hat{s}}_j, \qquad (C15)
$$

where, explicitly, $(\Delta C)_j = C_{\text{err}}(t_2 - t_1)(\delta_{j1} + \delta_{j2}) - C_{\text{err}}(t_1 - t_2)(\delta_{j3} + \delta_{j4})$ and where $\hat{\hat{s}}_1[\cdot] = s(t_1)[\cdot]s(t_2), \hat{\hat{s}}_2[\cdot] =$ $-[·]s(t_2)s(t_1), \hat{s}_3[·] = s(t_1)s(t_2)[·]$, and $\hat{s}_4[·] = -s(t_2)[·]s(t_1)$. This leads to

$$
\Delta_{bias} O(t) \leq \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{j_1,..,j_n} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 \right)^n |Tr_{S'} O(t) \mathcal{T}(\Delta C)_{j_1} \cdots (\Delta C)_{j_n} \hat{S}_{j_1} \cdots \hat{S}_{j_n} \rho(0)|
$$

\n
$$
\leq \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{j_1,..,j_n} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 \right)^n |(\Delta C)_{j_1}| \cdots |(\Delta C)_{j_n}| |Tr_{S'} O(t) \mathcal{T} \hat{S}_{j_1} \cdots \hat{S}_{j_n} \rho(0)|
$$

\n
$$
\leq \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{j_1,..,j_n} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 \right)^n |(\Delta C)_{j_1}| \cdots |(\Delta C)_{j_n}| |O(t) \mathcal{T} \hat{S}_{j_1} \cdots \hat{S}_{j_n} \rho(0)||_1,
$$
 (C16)

in which we used an abuse of notation in labeling time dependencies to achieve a leaner notation and where we used the fact that the trace norm $|| \cdot ||_1$ does not increase under a partial trace; see Eq. (17) in Ref. [\[139\]](#page-42-16) and Appendix [C1c.](#page-25-0) We now act with the time ordering so that all the superoperators \hat{s} are correctly ordered. We then note that each term $\hat{\hat{s}}_{j_1}\cdots\hat{\hat{s}}_{j_n}\rho(0)$ involves 2*n* operators *s*(*t*), some of which will be placed before and some of which will be placed after $\rho(0)$. We can then use Eq. [\(C37\)](#page-26-0) multiple times to write

$$
\Delta_{bias}O(t) \leq \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{j_1, \dots, j_n} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 \right)^n |(\Delta C)_{j_1}| \dots |(\Delta C)_{j_n}| |O||_{\infty} ||s||_{\infty}^{2n} ||\rho(0)||_1
$$

\n
$$
= ||O||_{\infty} \sum_{n=1}^{\infty} \frac{||s||_{\infty}^{2n}}{n!} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 |\sum_j (\Delta C)_j| \right)^n = ||O||_{\infty} \sum_{n=1}^{\infty} \frac{4^n ||s||_{\infty}^{2n}}{n!} \left(\int_0^t dt_2 \int_0^{t_2} dt_1 |C_{\text{err}}(t_2, t_1)| \right)^n
$$

\n
$$
= ||O||_{\infty} \left\{ \exp \left[4||s||_{\infty} \int_0^t dt_2 \int_0^{t_2} dt_1 |C_{\text{err}}(t_2, t_1)| \right] - 1 \right\};
$$
\n(C17)

see Eq. (6) in Ref. [\[77\]](#page-40-6). Here we used the fact that Schatten norms are unitarily invariant, $||\rho(0)||_1 = 1$, and the fact that each ΔC_i takes the form given in Eq. [\(3\)](#page-2-5) so that $|\Delta C_i| = |C_{\text{err}}(t_2, t_1)|$.

b. Stochastic error

In this subsection, we consider the stochastic error

$$
\Delta_{\text{stoch}} O(t) = \mathbb{E}[|O^{\xi}(t; N_{\text{stoch}}) - \mathbb{E}[O^{\xi}(t)]|]. \tag{C18}
$$

Unfortunately, it is not possible to analyze this uncertainty using the same techniques as used in the previous section. We cannot directly consider the influence superoperator in the context of the "empirical" average equation [\(C7\)](#page-22-1) of the stochastic noise since, in this case, Wick's theorem holds only on average. For this reason, we need to take one step further back to Eq. $(A7)$ to write

$$
\Delta_{\text{stoch}}O = \mathbb{E}\left[\left|\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_0^t dt_1 \cdots \int_0^t dt_n \left(\frac{1}{N_{\text{stoch}}}\sum_{j=1}^{N_{\text{stoch}}} \xi_{t_1}^j \cdots \xi_{t_n}^j - \mathbb{E}[\xi_{t_1} \cdots \xi_{t_n}]\right) \text{Tr}_{S''}\left[O(t)\mathcal{T}s_{t_1}^{\times} \cdots s_{t_n}^{\times}\rho_S(0)\right]\right]\right]
$$
\n
$$
\leq \mathbb{E}\left[\sum_{n=0}^{\infty}\frac{1}{n!}\int_0^t dt_1 \cdots \int_0^t dt_n \left|\frac{1}{N_{\text{stoch}}}\sum_{j=1}^{N_{\text{stoch}}}\xi_{t_1}^j \cdots \xi_{t_n}^j - \mathbb{E}[\xi_{t_1} \cdots \xi_{t_n}]\right| \left|\text{Tr}_{S''}\left[O(t)\mathcal{T}s_{t_1}^{\times} \cdots s_{t_n}^{\times}\rho_S(0)\right]\right|\right]
$$
\n
$$
\leq \sum_{n=0}^{\infty}\frac{1}{n!}\int_0^t dt_1 \cdots \int_0^t dt_n \left|\mathbb{E}\left|\frac{1}{N_{\text{stoch}}}\sum_{j=1}^{N_{\text{stoch}}}\xi_{t_1}^j \cdots \xi_{t_n}^j - \mathbb{E}[\xi_{t_1} \cdots \xi_{t_n}]\right|^2 \left|\text{Tr}_{S''}\left[O(t)\mathcal{T}s_{t_1}^{\times} \cdots s_{t_n}^{\times}\rho_S(0)\right]\right|,\tag{C19}
$$

where we omitted the time dependence on the left-hand side and where S'' is the composition of the system S and the deterministic pseudomode open quantum system. We also used the inequality $\mathbb{E}[|X|] \leq \sqrt{E[|X|^2]}$. This result shows us that the stochastic error depends on the average of the difference between the empirical moments and the true moments. To obtain a more direct bound, we now proceed using rather aggressive inequalities, which will limit the result to short times. To start, we write

$$
\mathbb{E}\left|\frac{1}{N_{\text{stoch}}}\sum_{j=1}^{N_{\text{stoch}}}\xi_{t_1}^j\cdots\xi_{t_n}^j - \mathbb{E}[\xi_{t_1}\cdots\xi_{t_n}]\right|^2
$$
\n
$$
= \frac{1}{N_{\text{noise}}^2}\mathbb{E}\left[\sum_{j,k}\overline{\xi_{t_1}^j\cdots\xi_{t_n}^j}\xi_{t_1}^k\cdots\xi_{t_n}^k\right] - \left|\mathbb{E}[\xi_{t_1}\cdots\xi_{t_n}]\right|^2,
$$
\n(C20)

and we note that contributions of Wick's theorem to the first term in which *k* and *j* fields are never contracted will end up simplifying with the term $|\mathbb{E}[\xi_{t_1} \cdots \xi_{t_n}]|^2$ (also considering that for odd *n* the expectation value $\mathbb{E}[\xi_{t_1} \cdots \xi_{t_n}]$ is just zero). We are then left with contributions in which at least one contraction happens between *k* and *j* fields, which generates a δ_{ik} and is consequently proportional to 1/*N*stoch, which already allows us to conclude that

$$
\Delta_{\text{stoch}} O(t) = O\left(\frac{1}{\sqrt{N_{\text{stoch}}}}\right). \tag{C21}
$$

Furthermore, each of the resulting correlation terms arising from the contractions considered above can be upper bounded by $C_{\text{class}}^{\text{max}} = \max_{t' \in [0,t]} \tilde{C}_{\text{class}}(t')$, where we used the definition in Eq. [\(C71\).](#page-29-1) We note that for real correlations $C_{\text{class}}(t') \in \mathbb{R}$, we have $C_{\text{class}}^{\text{max}} = \max_{t' \in [0,t]} C_{\text{class}}(t')$. With these definitions, we can write

$$
\Delta_{\text{stoch}}O \le \frac{||O||_{\infty}}{\sqrt{N_{\text{stoch}}}} \sum_{n=1}^{\infty} \frac{\sqrt{(2n-1)!!} (2||s||_{\infty} t \sqrt{C_{\text{class}}^{\text{max}}})^n}{n!}
$$

$$
\le \frac{||O||_{\infty}}{\sqrt{N_{\text{stoch}}}} F(||s||_{\infty} t \sqrt{2C_{\text{class}}^{\text{max}}}), \qquad (C22)
$$

where we omitted the time dependence on the left-hand side and in terms of the function

$$
F(x) = \sum_{n=1}^{\infty} \sqrt{\frac{(2n)!}{(n!)^3}} x^n,
$$
 (C23)

which is subexponential in the asymptotic limit, and where we used the same techniques as in Sec. $C1a$ to analyze the term $\left[\text{Tr}_{S''}\left[O(t)\mathcal{T}s_{h}^{\times} \cdots s_{h}^{\times}\rho_{S}(0)\right]\right]$ and also considered that $(2n - 1)!! = (2n)!/(2ⁿn!)$ overestimates the number of contractions when *n* is even. The practical applicability of this expression is limited within a timescale given by $1/(||s||_{\infty}\sqrt{2C_{\text{class}}^{\text{max}}})$. Whenever this expression does not give a useful bound, it is always possible to compute an empirical variance following the bound

$$
\Delta_{\text{stoch}}^2 O(t) \le \mathbb{E}[\left|O^{\xi}(t; N_{\text{stoch}}) - \mathbb{E}[O^{\xi}(t)]\right|^2]
$$

= $\mathbb{E}\{[O^{\xi}(t; N_{\text{stoch}})]^2\} - \mathbb{E}^2[O^{\xi}(t; N_{\text{stoch}})],$ (C24)

where we used the inequality $\mathbb{E}^2[|X|] \le E[|X|^2]$ and the fact that $\mathbb{E}[O^{\xi}(t)]^2$ is the expectation value of the random variable $O^{\xi}(t; N_{\text{stoch}})$, which can be directly checked using the definition in Eq. [\(C8\).](#page-22-3)

In abstract terms, given a random variable *X* having finite expectation value $\mu_X = \mathcal{E}[X]$ and finite variance $\sigma_X^2 = \mathbb{E}[X^2] - \mathbb{E}^2[X]$, it is possible to estimate μ_X by making a single extraction of the empirical average random variable

$$
Y = \frac{1}{N} \sum_{k=1}^{N} X_k.
$$
 (C25)

 $\mathbb{E}[Y] = \mu_X$ and

$$
\sigma_Y^2 = \mathbb{E}[Y^2] - \mathbb{E}^2[Y]
$$

= $\frac{1}{N^2} \sum_{k,\bar{k}} \mathbb{E}[X_k X_{\bar{k}}] - \mu_X^2$
= $\frac{N \mathbb{E}[X^2] + (N^2 - N) \mathbb{E}^2[X]}{N^2} - \mu_X^2$
= $\frac{E[X^2] - E^2[X]}{N} = \frac{\sigma_X^2}{N}.$ (C26)

For large *N*, a single extraction of *Y* gives a good approximation to μ_X . The variance σ_X^2 can instead be estimated by a single extraction of the random variable

$$
Z = \frac{1}{N} \sum_{k} X_k^2 - \left(\frac{1}{N} \sum_{k} X_k\right)^2.
$$
 (C27)

$$
\mathbb{E}[Z] = \frac{1}{N} \sum_{k} \mathbb{E}[X_{k}^{2}] - \frac{1}{N^{2}} \sum_{k,\bar{k}} \mathbb{E}[X_{k}X_{\bar{k}}]
$$

\n
$$
= \frac{1}{N} \sum_{k} \mathbb{E}[X_{k}^{2}] - \frac{1}{N} \mathbb{E}[X^{2}] - \frac{N^{2} - N}{N^{2}} \mathbb{E}^{2}[X]
$$

\n
$$
= \left(1 - \frac{1}{N}\right) (\mathbb{E}[X^{2}] - \mathbb{E}^{2}[X])
$$

\n
$$
= \left(1 - \frac{1}{N}\right) \sigma_{X}^{2}.
$$
 (C28)

The variance σ_Z^2 of *Z* depends on the higher momentum of the variable *X* and goes to zero as $N \to \infty$. This can be proven without computing all terms explicitly. We have

$$
\mathbb{E}[Z^2] = \frac{1}{N^2} \sum_{k\bar{k}} \mathbb{E}[X_k^2 X_{\bar{k}}^2] + \frac{1}{N^4} \sum_{k\bar{k}l\bar{l}} \mathbb{E}[X_k X_{\bar{k}} X_l X_{\bar{l}}] - \frac{2}{N^3} \sum_{k\bar{l}\bar{l}} \mathbb{E}[X_k^2 X_l X_{\bar{l}}].
$$
 (C29)

The leading order in this expression (constant in *N*) is obtained when all the labels of the stochastic variables are different from each other. Such a term can be directly computed and it is equal to $\mathbb{E}^2[X^2] + \mathbb{E}^4[X]$ – $2\mathbb{E}[X^2]\mathbb{E}^2[X] = \sigma_X^4 = \mathbb{E}^2[Z]$, where the last equality does not take into account terms *O*(1/*N*). The remaining terms are of higher order in 1/*N* and depend on higher momentum of the random variable *X* . Supposing these momenta are finite, we then obtain the result that

$$
\sigma_Z^2 = \mathbb{E}[Z^2] - \mathbb{E}^2[Z] = O\left(\frac{1}{N}\right). \tag{C30}
$$

To resume, these results show that a single extraction of the variables *Y* and *Z* can be used to estimate the expectation value and variance of the variable *X* .

In our case, we can identify $X \mapsto O^{\xi}(t) \equiv O^{\xi}(t; 1)$ and $Y \mapsto O^{\xi}(t; N_{\text{stoch}})$, which leads to

$$
\Delta_{\text{stoch}}^2 O(t) \le \frac{\sigma_{O^{\xi}(t)}^2}{N_{\text{stoch}}} = \frac{\mathbb{E}[Z]}{N_{\text{stoch}}} + O\left(\frac{1}{N_{\text{noise}}^2}\right). \tag{C31}
$$

where we used Eq. [\(C28\)](#page-24-0) to relate the right-hand side to the expectation value of $Z \mapsto \frac{1}{N} \sum_{k} [O^{\xi}(t)_{k}]^{2}$ – $(\frac{1}{N}\sum_{k} O^{\xi}(t)_{k})^{2}$, which can be estimated numerically. By Chebyshev's inequality, the probability that *Z* is $k\sigma_Z$ distant from the expectation value $\mathbb{E}[Z]$ is less than $1/k^2$. Because of Eq. [\(C30\),](#page-25-1) this implies that

$$
\Delta_{\text{stoch}}^2 O_s(t) \le \frac{\tilde{Z}}{N_{\text{stoch}}} + O\left(\frac{1}{N_{\text{noise}}^{3/2}}\right),\tag{C32}
$$

with probability almost 1. Here \tilde{Z} is a single realization of the random variable *Z*.

To finish, it is instructive to explicitly compute the first terms in Eq. [\(C19\)](#page-23-1) under the same considerations as below that expression. At second order, we have

$$
\Delta_{\text{stoch}}^2 O(t) \le ||O||_{\infty} [\mu_1(t) + \mu_2(t)],\tag{C33}
$$

where

$$
\mu_1(t) = 2||s||_{\infty} \int_0^t dt_1 \sqrt{\frac{1}{N_{\text{noise}}^2} \sum_{j,k} \mathbb{E}[\bar{\xi}_{t_1}^j \xi_{t_1}^k] - |E[\xi_{t_1}]|^2}
$$

\n
$$
= \frac{2||s||_{\infty}\sqrt{\tilde{C}_{\text{class}}(0)t}}{\sqrt{N_{\text{stoch}}}},
$$

\n
$$
\mu_2(t) = \frac{4||s||_{\infty}^2}{2!} \int_0^t dt_1 \int_0^t dt_2 \sqrt{\frac{1}{N_{\text{noise}}^2} \sum_{j,k} \mathbb{E}[\bar{\xi}_{t_2}^j \xi_{t_1}^j \xi_{t_2}^k \xi_{t_1}^k] - |E[\xi_{t_1} \xi_{t_2}]|^2}
$$

\n
$$
= \frac{2||s||_{\infty}^2}{\sqrt{N_{\text{stoch}}}} \int_0^t dt_1 \int_0^t dt_2 \sqrt{\tilde{C}_{\text{class}}^2(0) + \tilde{C}_{\text{class}}^2(t_2 - t_1)}.
$$

\n(C34)

c. Some properties of the trace norm

In this section, we report two important properties of the trace norm. To begin, we start by defining the Schatten *p*norm as

$$
||A||_p = \left(\sum_{j=1}^{N_A} |\sigma_j^p(A)|\right)^{1/p}, \qquad (C35)
$$

where $A: \mathbb{R}^{N_A} \to \mathbb{R}^{N_A}$, $N_A \in \mathbb{N}$, $N_A > 0$. Here $\sigma_i(A)$ is the *j* th singular value of *A*, i.e., the *j* th eigenvalue of the operator $|A| = (A^{\dagger}A)^{1/2}$. We further denote

$$
||A||_{\infty} = \max_{j} \sigma_j(A). \tag{C36}
$$

In our case, to apply this formalism, we consider a regularization of the total Hilbert space (for example, by truncating the number and dimension of all harmonic Hilbert spaces).

Given these definitions, we first state the Hölder inequality for Schatten norms **[**see Ref. [\[140\]](#page-42-17), Eq. (IV.42), page 95**]**, which reads

$$
||AB||_1 \le ||A||_p ||B||_q,\tag{C37}
$$

where *A* and *B* are generic operators, where $p, q \in \mathbb{N}$ $(p, q \ge 1)$, with $1/p + 1/q = 1$, and where $|| \cdot ||_p$ is the Schatten *p*-norm.

For self-consistency and for better relation to the present content, we now also report the proof given in Ref. [\[139\]](#page-42-16) showing that the trace norm does not increase under the partial trace. Following Ref. [\[139\]](#page-42-16), we define an operator *Q* acting on a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ of dimension $n_A n_B$. We consider the partial trace with respect to *B*, i.e., $Q_A =$ $Tr_B[Q]$. We further consider an orthonormal basis $|e_i\rangle_A$ and $|f_{\alpha}\rangle_B$ with $i = 0, \ldots, n_A - 1$ and $\alpha = 0, \ldots, n_B - 1$. Using these definitions, we can write the operator *Q* as

$$
Q = \sum_{\alpha,\beta=0}^{n_{B}-1} \sum_{i,j=0}^{n_{A}-1} |e_{i}\rangle \langle e_{j} | Q_{ij}^{\alpha\beta} |f_{\alpha}\rangle \langle f_{\beta} | \qquad (C38)
$$

in terms of $Q_{ij}^{\alpha\beta} \in \mathbb{C}$. We now define the following generalization *X* and *Z* of the Pauli operators acting on the space *B*:

$$
Z |f_{\alpha}\rangle = e^{2\pi i \alpha/n_B} |f_{\alpha}\rangle,
$$

\n
$$
X |f_{\alpha}\rangle = |f_{\alpha+1}\rangle,
$$
 (C39)

where the "closed boundary conditions" $|f_{n_A}| = |f_0\rangle$ are intended. Taking the conjugate of the definitions above, we get $\langle f_{\alpha} | (Z^{\dagger}Z) | f_{\beta} \rangle = \langle f_{\alpha} | (X^{\dagger}X) | f_{\beta} \rangle = \delta_{\alpha\beta}$, impliying that both *X* and *Z* are unitary. We also have

$$
Z(Q) := \frac{1}{n_B} \sum_{\eta=0}^{n_B-1} (\mathbb{I}_A \otimes Z^{\eta}) Q (\mathbb{I}_A \otimes Z^{\eta})^{\dagger}
$$

\n
$$
= \sum_{\eta=0}^{n_B-1} \sum_{\alpha,\beta=0}^{n_B-1} \sum_{i,j=0}^{n_A-1} \frac{e^{2\pi i \eta (\alpha-\beta)/n_B}}{n_B}
$$

\n
$$
\times |e_i\rangle \langle e_j| Q_{ij}^{\alpha\beta} |f_\alpha\rangle \langle f_\beta|
$$

\n
$$
= \sum_{\alpha,\beta=0}^{n_B-1} \sum_{i,j=0}^{n_A-1} |e_i\rangle \langle e_j| Q_{ij}^{\alpha\beta} \delta_{\alpha\beta} |f_\alpha\rangle \langle f_\beta|
$$
 (C40)

and

$$
X(Z(Q)) := \sum_{\eta=0}^{n_B-1} (\mathbb{I}_A \otimes X^{\eta}) Z(Q) (\mathbb{I}_A \otimes X^{\eta})^{\dagger}
$$

\n
$$
= \sum_{\eta=0}^{n_B-1} \sum_{\alpha,\beta=0}^{n_B-1} \sum_{i,j=0}^{n_A-1} \langle e_i | Q_{ij}^{\alpha\beta} \delta_{\alpha\beta} | f_{\alpha+\eta} \rangle
$$

\n
$$
\times |e_i \rangle \langle f_{\beta+\eta} |
$$

\n
$$
= \sum_{\alpha=0}^{n_B-1} \sum_{i,j=0}^{n_A-1} |e_i \rangle \langle e_j | \sum_{\alpha} Q_{ij}^{\alpha\alpha} \mathbb{I}_B
$$

\n
$$
= \text{Tr}_B(Q) \otimes \mathbb{I}_B. \qquad (C41)
$$

At the same time, we also have

$$
X(Z(Q)) = \frac{1}{n_B} \sum_{\eta, \eta' = 0}^{n_B - 1} (\mathbb{I}_A \otimes X^{\eta'} Z^{\eta}) Q(\mathbb{I}_A \otimes Z^{\eta \dagger} X^{\eta' \dagger})
$$

$$
= \frac{1}{n_B} \sum_{\eta, \eta' = 0}^{n_B - 1} (\mathbb{I}_A \otimes X^{\eta'} Z^{\eta}) Q(\mathbb{I}_A \otimes X^{\eta'} Z^{\eta})^{\dagger}.
$$
(C42)

Taking the norm of Eqs. [\(C41\)](#page-26-1) and [\(C42\),](#page-26-2) and considering that *X* and *Z* are unitary, we get

$$
||\text{Tr}_B(Q) \otimes \mathbb{I}_B||_p \le \frac{n_B^2}{n_B} ||Q||_p = n_B ||Q||_p. \qquad (C43)
$$

At the same time, the singular values of $Tr_B(Q) \otimes \mathbb{I}_B$ are n_B degenerate, which gives

$$
||\text{Tr}_B(Q) \otimes \mathbb{I}_B||_p = \left[n_B \sum_j \sigma_j^p(\text{Tr}_B(Q))\right]^{1/p}
$$

$$
= n_B^{1/p} ||\text{Tr}_B(Q)||_p. \tag{C44}
$$

Together, Eqs. [\(C43\)](#page-26-3) and [\(C44\)](#page-26-4) imply

$$
n_B^{1/p} ||{\rm Tr}_B(Q)||_p \le n_B ||Q||_p, \qquad (C45)
$$

which leads to

$$
||\text{Tr}_B(Q)||_p \le n_B^{(p-1)/p} ||Q||_p, \qquad (C46)
$$

so for $p = 1$,

$$
||\text{Tr}_B(Q)||_1 \le ||Q||_1. \tag{C47}
$$

2. Spectral representation of classical correlations

In this section, we introduce a spectral representation to define a stationary Gaussian stochastic field ξ(*t*) characterized by a vanishing mean and by a symmetric correlation function $C(t')$. To add extra clarity, we use *t* to denote times within the domain $t \in [0, T]$, while we use a prime symbol to denote variables that can be written as the difference between two times, which implies $t' \in [-T, T]$.

Our main goal is to define the field $\xi(t)$ in such a way to satisfy $\mathbb{E}[\xi(t)] = 0$ and $\mathbb{E}[\xi(t_2)\xi(t_1)] = C(t_2 - t_1)$, where $C(-t') = C(t').$

Since we are interested in simulating the dynamics of a system for times within the domain [0, *T*], we take advantage of the structure of $L^2(-T, T)$ functional spaces (characterizing the domain of the difference between two times, i.e., $t' = t_2 - t_1 \in [-T, T]$ by defining the inner product $\langle f, g \rangle_T$ between two functions $f, g : [-T, T] \to \mathbb{C}$ as

$$
\langle f, g \rangle_T = \frac{1}{2T} \int_{-T}^{T} d\tau \bar{f}(\tau) g(\tau), \qquad (C48)
$$

where the overbar denotes complex conjugation. In this space, we can define the orthonormal basis $\phi_n(t') = e^{in\pi t'/T}$ that fulfills

$$
\langle \phi_n, \phi_m \rangle_T = \delta_{n,m}, \qquad (C49)
$$

and it has the property that

$$
\phi_n(t_2 - t_1) = \phi_n(t_2)\phi_{-n}(t_1). \tag{C50}
$$

With this formalism at hand, a stationary correlation can be decomposed as

$$
C(t') = \sum_{n=-\infty}^{\infty} c_n \phi_n(t'), \qquad (C51)
$$

where $c_n = \langle \phi_n, C \rangle_T$. The symmetry $C(t') = C(-t')$, together with $\phi_n(-t') = \phi_{-n}(t')$, implies the constraint $c_{-n} = c_n$, which simply reflects the fact that the function $C(t')$ can be expanded with use of cosine functions and that

$$
c_n = \frac{1}{2T} \int_{-T}^{T} d\tau \cos(n\pi \tau/T) C(t).
$$
 (C52)

Using Eq. [\(C50\),](#page-27-1) we can further write

$$
C(t_2 - t_1) = \sum_{n = -\infty}^{\infty} c_n \phi_n(t_2) \phi_{-n}(t_1)
$$

=
$$
\sum_{n,m = -\infty}^{\infty} \phi_m(t_2) C_{mn} \phi_n(t_1),
$$
 (C53)

where $C_{mn} = c_m \delta_{n,-m}$. This matrix is symmetric because of the constraint $c_{-n} = c_n$ and hence we can diagonalize it as

$$
C_{mn} = \sum_{j=-\infty}^{\infty} O_{mj} d_j O_{jn}, \qquad (C54)
$$

where O_{mj} is the (possibly complex) orthogonal matrix made out of the *m*th element of the *j* th eigenvector with eigenvalue d_i of the matrix C_{mn} . In this case, the eigenvectors are just trigonometric functions that can be expressed as

$$
O_{mj} = \delta_{j0}\delta_{m0} + \theta(j)[\delta_{j,m} + \delta_{j,-m}]/\sqrt{2}
$$

$$
-\theta(-j)[\delta_{j,m} - \delta_{j,-m}]/\sqrt{2}, \qquad (C55)
$$

corresponding to the eigenvalues

$$
d_j = \delta_{j0}c_0 + c_j[\theta(j) - \theta(-j)], \qquad (C56)
$$

where $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ otherwise. We note that the sign in front of the eigenvectors in Eq. $(C55)$ can be chosen arbitrarily. As we will see later, the minus sign in the second line in Eq. $(C55)$ is designed to allow a cleaner expression for the fields. Plugging Eq. [\(C54\)](#page-27-3) into Eq. [\(C53\),](#page-27-4) we can write

$$
C(t_2 - t_1) = \sum_{n,m,j=-\infty}^{\infty} \phi_m(t_2) O_{mj} d_j O_{jn} \phi_n(t_1)
$$

=
$$
\sum_{j=-\infty}^{\infty} \phi_j^C(t_2) d_j \phi_j^C(t_1),
$$
 (C57)

where

$$
\phi_j^C(t) = \sum_{n = -\infty}^{\infty} O_{jn} \phi_n(t)
$$

= $\delta_{j0} + \sqrt{2} [\theta(j) \cos(n\pi t/T) + \theta(-j) i \sin(n\pi t/T)].$ (C58)

We explicitly note that the last line in the above equation holds only when the eigenvectors can be organized in a, possibly complex, orthogonal matrix, which is a consequence of the symmetry under time reversal of the original correlation. *This is a manifestation of the fact that the construction shown here is prevented for "nonclassical" correlations, i.e., correlations that are not symmetric under time reversal*. Using Eqs. [\(C56\)](#page-27-5) and [\(C58\)](#page-27-6) in Eq. [\(C57\),](#page-27-7) we can further be more explicit and write

$$
C(t_2 - t_1) = c_0 + 2 \sum_{n=1}^{\infty} c_n [\cos(n\pi t_2/T) \cos(n\pi t_1/T)
$$

$$
- i^2 \sin(n\pi t_2/T) \sin(n\pi t_1/T)]
$$

$$
= c_0 + 2 \sum_{n=1}^{\infty} c_n [\cos(n\pi t_2/T) \cos(n\pi t_1/T)
$$

$$
+ \sin(n\pi t_2/T) \sin(n\pi t_1/T)],
$$
 (C59)

whose correctness can be directly checked by noting that Eq. [\(C51\)](#page-27-8) can be written as

$$
C(t') = c_0 + 2 \sum_{n=1}^{\infty} c_n \cos[n\pi(t_2 - t_1)/T],
$$
 (C60)

which, indeed, corresponds to Eq. [\(C59\)](#page-28-0) by use of the trigonometric identity $\cos(\alpha - \beta) = \cos(\alpha) \cos(\beta) +$ $sin(\alpha) sin(\beta)$. As already noted above, the whole construction of this section would be prevented if the correlation has a term proportional to a sine function as the analogue of the trigonometric identity above contains nonfactorizable products of cosines and sines.

We are now in a position to finally define the stochastic variable $\xi(t)$ as the following spectral representation:

$$
\xi(t) = \sum_{j=-\infty}^{\infty} \xi_j \sqrt{d_j} \phi_j^C(t), \qquad (C61)
$$

where $\xi_i \in \mathcal{N}(0, 1)$ are independent Gaussian variables with unit variance and zero mean. This immediately implies that $\mathbb{E}[\xi(t)] = 0$. Furthermore, we can use Eq. [\(C57\)](#page-27-7) to show that

$$
\mathbb{E}[\xi(t_2)\xi(t_1)] = \sum_{j,j'} \mathbb{E}[\xi_j \xi_{j'}]\sqrt{d_j d_{j'}} \Phi_j^C(t_2) \Phi_{j'}^C(t_1)
$$

=
$$
\sum_j d_j \Phi_j^C(t_2) \Phi_j^C(t_1)
$$

=
$$
C(t_2 - t_1).
$$
 (C62)

Using Eqs. $(C56)$ and $(C58)$ in Eq. $(C61)$, we can write the fields in the following more explicit form:

$$
\xi(t) = \sqrt{c_0} \xi_0 + \sum_{n=1}^{\infty} \sqrt{2c_n} [\xi_n \cos(n\pi t/T)
$$

$$
+ \xi_{-n} \sin(n\pi t/T)]. \tag{C63}
$$

Here we note that the plus sign in front of the sine is due to our previous sign choice in Eq. [\(C55\).](#page-27-2) We can further check explicitly that these fields indeed have the correct statistics by writing

$$
\mathbb{E}[\xi(t_2)\xi(t_1)] = c_0 + 2\sum_{n=1}^{\infty} c_n[\cos(n\pi t_2/T)\cos(n\pi t_1/T) + \sin(n\pi t_2/T)\sin(n\pi t_1/T)]
$$

= $c_0 + 2\sum_{n=1}^{\infty} c_n \cos[n\pi(t_2 - t_1)/T]$, (C64)

where we again used the identity $cos(\alpha - \beta) = cos(\alpha)$ $\cos(\beta) + \sin(\alpha)\sin(\beta)$. It is interesting to note that the presence of *antisymmetric* functions (the sines) in the definition of the field $\xi(t)$ is essential in reproducing the stationarity of the *symmetric* correlation $C(t')$.

As an example, we compute the spectral representation above for terms in the correlations taking the form of a symmetric exponential, i.e.,

$$
C^{\text{decay}}(t_2 - t_1) = \alpha^2 e^{\omega |t_2 - t_1|}, \tag{C65}
$$

in terms of the frequencylike parameter $\omega \in \mathbb{C}$. Here the superscript "decay" indicates that, usually, correlations of this kind are used to model purely decaying contributions such as the Matsubara ones (for $\omega \in \mathbb{R}$ and $\omega < 0$). However, they can also be used to model resonant effects through $cos(\omega t) = (e^{i\omega|t|} + e^{-i\omega|t|})/2$). By using Eq. [\(C52\),](#page-27-9) we find

$$
c_n^{\text{decay}} = \frac{1}{2T} \int_{-T}^{T} d\tau \ e^{\omega \tau} \cos\left(\frac{n\pi \tau}{T}\right) = L_n(\omega) \qquad (C66)
$$

in terms of the function

$$
L_n(\omega) = (e^{\omega T} e^{in\pi} - 1) \frac{\omega T}{(\omega T)^2 + (n\pi)^2}.
$$
 (C67)

It is interesting to finish this section with an analysis of the first two moments of the empirical expectation value for the correlation, i.e., the random variable

$$
C_{\text{class}}^{\text{emp}}(t_2, t_1) = 1/N_{\text{stoch}} \sum_{j} \xi_j(t_2) \xi_j(t_1), \tag{C68}
$$

which constitutes an estimate of the true average in Eq. [\(C62\)](#page-28-2) by averaging over *N*_{stoch} independent realizations of the noise $\xi_j(t)$, $j = 1, ..., N_{\text{stoch}}$. The expectation value is simply the expected value of the correlation

$$
\mathbb{E}[C_{\text{class}}^{\text{emp}}(t_2, t_1)] = \frac{1}{N_{\text{stoch}}} \sum_{j} \mathbb{E}[\xi_j(t_2)\xi_j(t_1)]
$$

$$
= C_{\text{class}}(t_2 - t_1), \tag{C69}
$$

while the variance is given by

$$
\sigma_{emp}^{2} = \mathbb{E}\left[|C_{\text{class}}^{emp}(t_{2}, t_{1}) - \mathbb{E}[C_{\text{class}}^{emp}(t_{2}, t_{1})]^{2}\right]
$$
\n
$$
= \mathbb{E}[|C_{\text{class}}^{emp}(t_{2}, t_{1})|^{2}] - |C_{\text{class}}(t_{2}, t_{1})|^{2}
$$
\n
$$
= \frac{1}{N_{\xi}^{2}} \sum_{j,k} \mathbb{E}[\bar{\xi}_{j}(t_{2})\bar{\xi}_{j}(t_{1})\xi_{k}(t_{2})\xi_{k}(t_{1})]
$$
\n
$$
- |C_{\text{class}}(t_{2}, t_{1})|^{2}
$$
\n
$$
= \frac{1}{N_{\xi}^{2}} \sum_{j,k} \{\mathbb{E}[\bar{\xi}_{j}(t_{2})\bar{\xi}_{j}(t_{1})]\mathbb{E}[\xi_{k}(t_{2})\xi_{k}(t_{1})]
$$
\n
$$
+ \mathbb{E}[\bar{\xi}_{j}(t_{2})\xi_{k}(t_{2})]\mathbb{E}[\bar{\xi}_{j}(t_{1})\xi_{k}(t_{2})]
$$
\n
$$
+ \mathbb{E}[\bar{\xi}_{j}(t_{2})\xi_{k}(t_{1})]\mathbb{E}[\bar{\xi}_{j}(t_{1})\xi_{k}(t_{2})]
$$
\n
$$
- |C_{\text{class}}(t_{2}, t_{1})|^{2}
$$
\n
$$
= [|\tilde{C}(0)|^{2} + |\tilde{C}(t_{2} - t_{1})|^{2}] / N_{\text{stoch}}, \qquad (C70)
$$

where we used Wick's theorem and the real version of the correlation *C*(*t*) can be defined as

$$
\tilde{C}(t) = \mathbb{E}[\bar{\xi}(t_2)\xi(t_1)]
$$

= $|c_0| + 2\sum_{n=1}^{\infty} |c_n| \cos(n\pi t/T),$ (C71)

where we used Eq. $(C63)$. Using Eq. $(C60)$, we finally find

$$
\sigma_{\rm emp}^2 \leq [|C_{\rm class}(0)|^2 + |C_{\rm class}(t_2 - t_1)|^2]/N_{\rm stoch}.
$$
 (C72)

APPENDIX D: A CLASS OF RATIONAL SPECTRAL DENSITIES

To be more specific, we now study this decomposition for a subclass *M* of spectral densities that are real and asymmetric on the real axis and meromorphic in the overall complex plane. We further suppose all $2N_p > 1$ poles (we later show this number needs to be even and suppose there is at least one such couple) to be simple (and not located on the real axis) apart from a pole of order $N_{\infty} < 2N_p$ at infinity. We now consider three basic facts about functions in *M*:

(1) The poles of $J(\omega) \in M$ come in complex-conjugate pairs having complex-conjugate residues. To show this, we consider a region *D* that contains all the poles. The Schwarz reflection principle tells us that $J(\bar{\omega}) = J(\omega)$ for $\omega \in D$. For any pole ω_k in the upper (or lower) complex plane \mathbb{C} , we can write the Laurent series $J(\omega) = \sum_{j=-\infty}^{\infty} a_j (\omega - \omega_k)^j$, where a_{-1} represents the residue at ω_k . With use of the Schwarz reflection principle, this implies that $J(\omega) = \sum_{j=-\infty}^{\infty} \bar{a}_j (\omega - \bar{\omega}_k)^j$, i.e., the point $\bar{\omega}_k$ is

also a pole whose residue is the complex conjugate of the one evaluated at ω_k . This immediately implies that the number of poles is even, i.e., it can be written as $2N_p$. In the following we use the notation (ω_k, ω_{-k}) to denote the complexconjugate pairs of poles, i.e., $\omega_{-k} = \bar{\omega}_k$. We will further use $k > 0$ ($k < 0$) to denote poles in the upper (lower) complex plane so that the full set of poles can be written as $\{\omega_k\}$ for $k \in \mathbb{Z}_{N_p}^0$, where $\mathbb{Z}_{N_p}^0 = \{-N_p, \ldots, -1, 1, \ldots, N_p\}$ and where all ω_k are distinct.

(2) Since $J(\omega)$ is meromorphic with single poles located in the finite complex plane, $\prod_{k \in \mathbb{Z}_{N_p}^0} (\omega \omega_k$)*J*(ω) is analytical in $\mathbb C$ and it has a pole of order N_{∞} at infinity. This implies that such a function is an N_{∞} -order polynomial $p(\omega)$, so

$$
J(\omega) = \frac{p(\omega)}{\prod_{k \in \mathbb{Z}_{N_p}^0} (\omega - \omega_k)}.
$$
 (D1)

Imposing $J(\omega) \in \mathbb{R}$ for $\omega \in \mathbb{R}$ implies that all coefficients in the polynomial *p* are real, i.e., $\bar{p}(\omega)$ = $p(\bar{\omega})$ (since the roots ω_k appearing in the denominator come in complex-conjugate pairs). It is now possible to write this expression in terms of a sum of rational functions with polynomials of degree 1 in the denominator. To see this, we note that $1/\prod_k(\omega - \omega_k) = \sum_j \kappa v_j / \prod_{k \neq j} (\omega - \omega_k)$, where $\sum_{k} v_k = 0$ and $\kappa = -1/\sum_{k} (v_k \omega_k)$. By proceeding iteratively in this way, we find a decomposition of the kind $1/\prod_k(\omega - \omega_k) = \sum_k c_k/(\omega - \omega_k)$ in terms of some coefficients $c_k \in \overline{\mathbb{C} \cdot \mathbb{C}}$ Ultimately this leads to

$$
J(\omega) = p(\omega) \sum_{k \in \mathbb{Z}_{N_p}^0} \frac{c_k}{(\omega - \omega_k)}.
$$
 (D2)

This expression also allows us to find a more explicit expression for the coefficients c_k . The residue at any of the points ω_k can be computed both from Eq. [\(D2\)](#page-29-2) as $p(\omega_k)c_k$ and from Eq. [\(D1\)](#page-29-3) as $p(\omega_k)/\prod_{j\neq k}(\omega_k \omega_j$). Equating these two results, we find that $c_k =$ $1/\prod_{j\neq k}(\omega_k - \omega_j)$. Furthermore, the residue at ω_k explicitly reads

$$
R_k \equiv \text{Res}[J(\omega); \omega_k]
$$

= $p(\omega_k)/\prod_{j \neq k} (\omega_k - \omega_j),$ (D3)

so

$$
R_{-k} = \text{Res}[J(\omega); \omega_{-k}]
$$

=
$$
\frac{p(\bar{\omega}_k)}{\prod\limits_{j \neq -k} (\bar{\omega}_k - \omega_j)}
$$

=
$$
\frac{p(\bar{\omega}_k)}{(\bar{\omega}_k - \omega_k) \prod\limits_{j \neq -k,k} (\bar{\omega}_k - \bar{\omega}_j)}
$$

=
$$
\bar{R}_k,
$$
 (D4)

checking explicitly what was proved in (1) and where we used the fact that all poles come in complex-conjugate pairs.

(3) The antisymmetry hypothesis on $J(\omega)$ imposes further constraints on the set of poles $\{\omega_k\}$ and on the polynomial $p(\omega)$. Because of antisymmetry, we need to require

$$
J(\omega) = \frac{J(\omega) - J(-\omega)}{2}
$$

=
$$
\frac{p(\omega)}{2\prod_{k}(\omega - \omega_{k})} - \frac{p(-\omega)}{2\prod_{k}(-\omega - \omega_{k})}
$$
 (D5)

To continue, we can distinguish between two kinds of pole. For imaginary ω_k , both denominators contain the same $\omega^2 + |\omega_k|^2$ factor. For general complex poles ω_k , we can apply a greatest common divisor to show that in Eq. [\(D1\)](#page-29-3) for an antisymmetric spectral density the poles come either in complex-conjugate pairs (if ω_k is purely imaginary) or in quadruples (ω_k and $-\omega_k$ and their conjugate pairs, see Fig. [9\)](#page-30-0). Furthermore, the polynomial $p(x)$ must be antisymmetric.

This has immediate implications in the expression for the residues when the poles come in quadruples. To show this, we denote by k the label such that $\omega_{\tilde{k}} = -\omega_{-k} = -\bar{\omega}_k$ so that \tilde{k} has the same sign as *k* and so that the quadruples of poles are $(\omega_k, \omega_{-k}, \omega_{\tilde{k}}, \omega_{\widetilde{(-k)}})$. We have

$$
R_{\tilde{k}} = \text{Res}[J(\omega); \omega_{\tilde{k}}]
$$

=
$$
\frac{p(-\bar{\omega}_k)}{\prod_{j \neq \tilde{k}} (-\bar{\omega}_k - \omega_j)}
$$

=
$$
\frac{p(-\bar{\omega}_k) \left[\prod_{j \neq \tilde{k}, k, -k, \tilde{k} \neq \tilde{k}} (-\bar{\omega}_k - \bar{\omega}_j) \right]^{-1}}{(-\bar{\omega}_k - \omega_k)(-\bar{\omega}_k + \omega_k)(-\bar{\omega}_k - \bar{\omega}_k)}
$$

FIG. 9. The poles of the spectral densities considered in this section come either in quadruples $(\omega_k, \bar{\omega}_k, -\omega_k, -\bar{\omega}_k)$, represented in blue, or in couples $(\omega_k, \bar{\omega}_k)$, represented in red.

$$
p(\bar{\omega}_k) \left[\prod_{j \neq \bar{k}, k, -k, \overline{(-k)}} (\bar{\omega}_k + \bar{\omega}_j) \right]^{-1}
$$

\n
$$
= \frac{\overline{(\bar{\omega}_k + \omega_k)(\bar{\omega}_k - \omega_k)(\bar{\omega}_k + \bar{\omega}_k)}}{(\bar{\omega}_k + \bar{\omega}_k) \left[\prod_{j \neq \bar{k}, k, -k, \overline{(-k)}} (\bar{\omega}_k - \bar{\omega}_j) \right]^{-1}}
$$

\n
$$
= \frac{\overline{(\bar{\omega}_k + \omega_k)(\bar{\omega}_k - \omega_k)(\bar{\omega}_k + \bar{\omega}_k)}}{(\bar{\omega}_k + \omega_k)(\bar{\omega}_k - \omega_k)(\bar{\omega}_k + \bar{\omega}_k)}
$$

\n
$$
= R_{-k}
$$

\n
$$
= \bar{R}_k, \qquad (D6)
$$

where we used the fact that an even number of labels *j* is present and that, given the symmetries of the poles, a change in sign in all ω_i is just formal.

A similar proof holds to show that the residues of poles coming in conjugate pairs $(\omega_{k_i}, \omega_{-k_i})$ are real. We have

$$
R_{k_i} = \text{Res}[J(\omega); \omega_{k_i}]
$$

=
$$
\frac{p(\omega_{k_i})}{(\omega_{k_i} - \bar{\omega}_{k_i}) \prod_{k \neq \pm k_i} (\omega_{k_i} - \omega_k)},
$$
 (D7)

where $p(\omega_{k_i})/(\omega_{k_i} - \bar{\omega}_{k_i})$ is real by the antisymmetry of *p* and the fact that ω_{k_i} is imaginary. The remaining roots $k \neq k_i$ come either in couples or in quadruples. In both cases $(\omega_{k_i} - \omega_k)(\omega_{k_i} - \bar{\omega}_k)$ and $(\omega_{k_i} - \omega_k)(\omega_{k_i} - \omega_k)$ $\bar{\omega}_k(\omega_{k_i} + \omega_k)(\omega_{k_i} + \bar{\omega}_k)$ are real by construction.

We can now compute

$$
C_{\rm as}(t) = -\frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega J(\omega) \sin(\omega t)
$$

=
$$
\frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega J(\omega) (e^{-i\omega t} - e^{i\omega t}),
$$
 (D8)

where we used Eq. (10) together with the antisymmetry of $J(\omega)$. Since the degree N_{∞} of the polynomial $p(\omega)$ is smaller than the degree N_{poles} of the polynomial in the denominator (i.e., $N_{\infty} < N_{\text{poles}}$), Eq. [\(D1\)](#page-29-3) implies that $\lim_{\omega\to\infty} J(\omega) \to 0$, which allows us to use the Jordan lemma to write

$$
C_{\text{as}}(t) = -\frac{i\theta(t)}{2} \sum_{k < 0} \text{Res} \left[J(\omega) e^{-i\omega t}; \omega_k \right] \\
+ \frac{i\theta(-t)}{2} \sum_{k > 0} \text{Res} \left[J(\omega) e^{-i\omega t}; \omega_k \right] \\
- \frac{i\theta(t)}{2} \sum_{k > 0} \text{Res} \left[J(\omega) e^{i\omega t}; \omega_k \right] \\
+ \frac{i\theta(-t)}{2} \sum_{k < 0} \text{Res} \left[J(\omega) e^{i\omega t}; \omega_k \right], \qquad (D9)
$$

where $\text{Res}[g(\omega); \omega^*]$ denotes the residue of the function $g(\omega)$ at the point ω^* . Now that the Jordan lemma has been used, we can use Eqs. $(D3)$ and $(D4)$ to write

$$
C_{\rm as}(t) = -\frac{i}{2} \sum_{k>0} \theta(t) [R_k e^{i\omega_k t} + \bar{R}_k e^{-i\bar{\omega}_k t}]
$$

$$
+ \frac{i}{2} \sum_{k>0} \theta(-t) [R_k e^{-i\omega_k t} + \bar{R}_k e^{i\bar{\omega}_k t}].
$$
 (D10)

We now describe an environment made out of pseudomodes able to exactly reproduce the correlation $C_{as}(t)$. To achieve this, we first write Eq. $(D10)$ in the following slightly more explicit form:

$$
C_{\rm as}(t) = -\frac{i}{2} \sum_{k>0} \theta(t) [R_k e^{i\omega_k^{R}t} + \bar{R}_k e^{-i\omega_k^{R}t}] e^{-\omega_k^{T}t} + \frac{i}{2} \sum_{k>0} \theta(-t) [R_k e^{-i\omega_k^{R}t} + \bar{R}_k e^{i\omega_k^{R}t}] e^{\omega_k^{T}t} = -i\text{sg}(t) \sum_{k>0} R_k^{R} \cos(\omega_k^{R}t) e^{-\omega_k^{T}|t|} + i \sum_{k>0} R_k^{T} \sin(\omega_k^{R}t) e^{-\omega_k^{T}|t|}, \qquad (D11)
$$

where the indexes R and I denote the real and imaginary parts of a variable. It is important to note that the sum over poles that belong to the same quadruple

 $(\omega_k, \omega_{-k}, -\omega_k, -\omega_{-k})$ or pure-imaginary pairs $(\omega_k, \omega_{-k}),$ if present, can be further reduced or simplified. To do this, we partition the $2N_p$ poles into N_q quadruples and N_i imaginary couples so that $2N_p = 4N_q + 2N_i$. We can now write

$$
C_{\rm as}(t) = -2i s g(t) \sum_{k_q=1}^{N_q} R_{k_q}^{\mathcal{R}} \cos(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|}
$$

+ $2i \sum_{k_q=1}^{N_q} R_{k_q}^{\mathcal{I}} \sin(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|}$
- $i s g(t) \sum_{k_i=1}^{N_i} R_{k_i}^{\mathcal{R}} \cos(\omega_{k_i}^{\mathcal{R}} t) e^{-\omega_{k_i}^{\mathcal{I}} |t|},$ (D12)

where we used Eq. ($D6$), and where $k_q > 0$ labels poles coming in quadruples $(\omega_{k_q}, \omega_{-k_q}, -\omega_{k_q}, -\omega_{-k_q})$ and such that $\text{Re}[\omega_{k_q}] \ge 0$ and $\text{Im}[\omega_{k_q}] > 0$. Similarly, $k_i > 0$ labels poles coming in pairs $(\omega_{k_i}, \omega_{-k_i})$ and such that $\text{Im}[\omega_{k_i}] > 0$ and $\text{Re}[\omega_{k_i}] = 0$.

To characterize a pseudomode model able to reproduce the correlation above, we need to find the explicit parameters that allows to write $C_{PM}(t) = C_{as}(t)$, where $C_{PM}(t)$ is given in Eq. [\(B16\).](#page-19-3) However, the presence of the sign function in Eq. [\(D11\)](#page-31-1) requires a few further preliminary steps. First, we write Eq. [\(D11\)](#page-31-1) as

$$
C_{\text{as}}(t) = -i\text{sg}(t) \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) (e^{-\omega_k^{\mathcal{I}}|t|} - e^{-W|t|})
$$

$$
-i\text{sg}(t) \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) e^{-W|t|}
$$

$$
+ i \sum_{k>0} R_k^{\mathcal{I}} \sin(\omega_k^{\mathcal{R}} t) e^{-\omega_k^{\mathcal{I}}|t|}, \qquad (D13)
$$

where we introduced an arbitrary frequency scale *W*. We can now use the identity

$$
sg(t) = \frac{\exp[-a(|t| - t)] - \exp[-a(t + |t|)]}{1 - \exp[-2a|t|]}, \quad (D14)
$$

where *a* is an arbitrary nonzero frequency. By imposing $a \rightarrow (W - \omega_k^{\mathcal{I}})/2$ for each different *k*, we get

$$
C_{\text{as}} = -i \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) [e^{(W-\omega_k^{\mathcal{I}})t/2} - e^{-(W-\omega_k^{\mathcal{I}})t/2}]
$$

$$
\times e^{-(W+\omega_k^{\mathcal{I}}) |t|/2} - i \text{sg}(t) \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) e^{-W|t|}
$$

+
$$
i \sum_{k>0} R_k^{\mathcal{I}} \sin(\omega_k^{\mathcal{R}} t) e^{-\omega_k^{\mathcal{I}}|t|}
$$

$$
= 2 \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) \sin\left[\frac{-i(W - \omega_k^{\mathcal{I}})t}{2}\right]
$$

$$
\times e^{-(W + \omega_k^{\mathcal{I}})|t|/2}
$$

-
$$
i \operatorname{sg}(t) \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) e^{-W|t|}
$$

+
$$
i \sum_{k>0} R_k^{\mathcal{I}} \sin(\omega_k^{\mathcal{R}} t) e^{-\omega_k^{\mathcal{I}}|t|},
$$
 (D15)

where we omitted the time dependence on the lefthand side. Using the identity $sin(x) cos(y) = [sin(x +$ y) + sin($x - y$)]/2, we finally obtain

$$
C_{\rm as} = \sum_{k>0} R_k^{\mathcal{R}} \sin \left[\frac{-i(W - \omega_k^{\mathcal{I}}) + 2\omega_k^{\mathcal{R}}}{2} t \right] e^{-(W + \omega_k^{\mathcal{I}})|t|/2} + \sum_{k>0} R_k^{\mathcal{R}} \sin \left[\frac{-i(W - \omega_k^{\mathcal{I}}) - 2\omega_k^{\mathcal{R}}}{2} t \right] e^{-(W + \omega_k^{\mathcal{I}})|t|/2} + i \sum_{k>0} R_k^{\mathcal{I}} \sin(\omega_k^{\mathcal{R}} t) e^{-\omega_k^{\mathcal{I}}|t|} - i s g(t) \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) e^{-W|t|}.
$$
 (D16)

As noted before, the sum over poles that belong to the same quadruple $(\omega_k, \omega_{-k}, -\omega_k, -\omega_{-k})$ or pure-imaginary pairs (ω_k, ω_{-k}) can be further reduced or simplified using Eq. [\(D6\)](#page-30-2) to write

$$
C_{\text{as}} = 2 \sum_{k_q=1}^{N_q} \left\{ i R_{k_q}^{\mathcal{I}} \sin(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|} + R_{k_q}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_q}^{\mathcal{I}}) + 2\omega_{k_q}^{\mathcal{R}}}{2} t\right] e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} + R_{k_q}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_q}^{\mathcal{I}}) - 2\omega_{k_q}^{\mathcal{R}}}{2} t\right] e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} \right\} + \sum_{k_i=1}^{N_i} \left\{ i R_{k_i}^{\mathcal{I}} \sin(\omega_{k_i}^{\mathcal{R}} t) e^{-\omega_{k_i}^{\mathcal{I}} |t|} + 2R_{k_i}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_i}^{\mathcal{I}})}{2} t\right] e^{-(W + \omega_{k_i}^{\mathcal{I}})|t|/2} \right\} - i s g(t) \sum_{k>0} R_k^{\mathcal{R}} \cos(\omega_k^{\mathcal{R}} t) e^{-W|t|}, \qquad (D17)
$$

where we omitted the time dependence on the left-hand side. We further note that for *W* much bigger than any inverse timescale present in the model, the last term is effectively nonzero only at $t = 0$. However, in the context presented here, the correlation can always be interpreted as a *distribution*, i.e., as a functional over functions of time (in the domain [0, *t*]). This can be seen explicitly by expanding Eq. $(A17)$ in series and using it to compute the expectation value of a system observable. In this case, the correlation always appears inside an integral that further involves functions of time related to the system, i.e., it can be interpreted as a linear operator over the space of such functions over the time domain. As a distribution, the correlation can always be redefined over discrete domains, thereby justifying the ignoring of the last term in the previous expression to write

$$
C_{\rm as} = 2 \sum_{k_q=1}^{N_q} \left\{ iR_{k_q}^{\mathcal{I}} \sin(\omega_{k_q}^{\mathcal{R}} t) e^{-\omega_{k_q}^{\mathcal{I}} |t|} + R_{k_q}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_q}^{\mathcal{I}}) + 2\omega_{k_q}^{\mathcal{R}}}{2} t\right] e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} + R_{k_q}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_q}^{\mathcal{I}}) - 2\omega_{k_q}^{\mathcal{R}}}{2} t\right] e^{-(W + \omega_{k_l}^{\mathcal{I}})|t|/2} \right\} + 2 \sum_{k_i=1}^{N_l} R_{k_i}^{\mathcal{R}} \sin\left[\frac{-i(W - \omega_{k_i}^{\mathcal{I}})}{2} t\right] e^{-(W + \omega_{k_i}^{\mathcal{I}})|t|/2},
$$
\n(D18)

where we omitted the time dependence on the left-hand side. The resulting expression for the antisymmetric correlation can then be expressed as

$$
C_{\rm as}(t) = \sum_{j=1}^{N_{\rm as}} g_j^{\rm as} \sin(\Omega_j^{\rm as} t) e^{-\Gamma_j^{\rm as}|t|}
$$
 (D19)

in terms of the parameters $g_j^{\text{as}}, \Omega_j^{\text{as}}, \Gamma_j^{\text{as}} \in \mathbb{C}$, which can be explicitly read by direct comparison with Eq. [\(D18\).](#page-32-0) Here $N_{\text{as}} = 3N_q + N_i$ denotes the maximum number of terms in this decomposition. This immediately implies the possibility to use $N_{\text{PM}}^{\text{rational}} = N_{\text{as}}$ pseudomodes to reproduce the effects of this correlation. However, to reproduce sine functions with the expression for the pseudomode correlation given in Eq. [\(B16\),](#page-19-3) with a minimal (i.e., *N*as) number of modes, one needs to impose what is, arguably, the highest level of unphysicality on the bosonic occupation numbers. If we label generic pseudomode parameters with an asterisk, reproducing a sine function requires $n^* = -1/2$, which does not allow an obvious truncation scheme for the thermal state that describes the initial state of the pseudomode (since its temperature would be required to satisfy $\beta^* \Omega^* = i \pi$). While alternative solutions might be found (as simple as increasing the number of pseudmodes), in this article we chose a strategy based on the fact that we are always free to reshape the antisymmetric part of the correlation by adding a symmetric function as long as we compensate it with classical stochastic fields; see

Appendix [C.](#page-21-5) This allows us to model Eq. $(D19)$ using N_{PM}_{PM} pseudomodes initially at zero temperature. By explicitly defining the following symmetric function as described in Sec. [III B,](#page-6-0)

$$
f_{s} = -i \sum_{j=1}^{N_{\text{PM}}} g_{j}^{\text{as}} \cos(\Omega_{j}^{\text{as}} t) e^{-\Gamma_{j}^{\text{as}} |t|}
$$

\n
$$
= 2 \sum_{k_{q}=1}^{N_{q}} \left\{ R_{k_{q}}^{T} \cos(\omega_{k_{q}}^{T} t) e^{-\omega_{k_{q}}^{T} |t|} -i R_{k_{q}}^{T} \cos\left[\frac{-i(W - \omega_{k_{q}}^{T}) + 2\omega_{k_{q}}^{T}}{2} t \right] e^{-(W + \omega_{k_{q}}^{T})|t|/2} -i R_{k_{q}}^{T} \cos\left[\frac{-i(W - \omega_{k_{q}}^{T}) - 2\omega_{k_{q}}^{T}}{2} t \right] e^{-(W + \omega_{k_{q}}^{T})|t|/2} \right\}
$$

\n
$$
-2i \sum_{k_{i}=1}^{N_{i}} R_{k_{i}}^{T} \cos\left[\frac{-i(W - \omega_{k_{i}}^{T}) - 2\omega_{k_{i}}^{T}}{2} t \right] e^{-(W + \omega_{k_{i}}^{T})|t|/2}, \tag{D20}
$$

where we omitted the time dependence on the left-hand side, we obtain, using Eq. (33) , the following quantum contribution to the correlation:

$$
C_Q(t) = C_{as}(t) - f_s(t)
$$

\n
$$
= -2 \sum_{k_q=1}^{N_q} \left\{ R_{k_q}^{\mathcal{I}} e^{-i\omega_{k_q}^{\mathcal{R}_t} t} e^{-\omega_{k_q}^{\mathcal{I}} |t|} + iR_{k_q}^{\mathcal{R}} e^{-i[\omega_{k_q}^{\mathcal{R}} - i(W - \omega_{k_q}^{\mathcal{I}})/2]t} e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} + i R_{k_q}^{\mathcal{R}} e^{-i[-\omega_{k_q}^{\mathcal{R}} - i(W - \omega_{k_q}^{\mathcal{I}})/2]t} e^{-(W + \omega_{k_q}^{\mathcal{I}})|t|/2} \right\}
$$

\n
$$
+ 2i \sum_{k_i=1}^{N_i} R_{k_i}^{\mathcal{R}} e^{-i[-i(W - \omega_{k_i}^{\mathcal{I}})/2]t} e^{-(W + \omega_{k_i}^{\mathcal{I}})|t|/2}, \quad (D21)
$$

which corresponds to a decomposition like the one presented in Eq. [\(B29\),](#page-21-6) which can be modeled by pseudomodes initially at zero temperature.

1. Symmetric correlation

In this subsection, we explicitly compute the symmetric part of the correlation for the subset of spectral densities *M*. We do this for completeness as the stochastic fields needed to reproduce this part of the correlation can be computed without reference to any analytical form; see Appendix [C 2.](#page-27-0)

We want to compute, see Eq. (10) ,

$$
C_s(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega J(\omega) \coth(\beta \omega/2) \cos(\omega t)
$$

=
$$
\frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega J(\omega) \coth(\beta \omega/2) (e^{-i\omega t} + e^{i\omega t})
$$
(D22)

for $J(\omega) \in \mathcal{M}$. We have

$$
C_s(t) = -\frac{i\theta(t)}{2} \sum_{k>0} \text{Res} [J(\omega) \coth(\beta \omega/2) e^{-i\omega t}; \tilde{\omega}_k]
$$

+
$$
\frac{i\theta(-t)}{2} \sum_{k>0} \text{Res} [J(\omega) \coth(\beta \omega/2) e^{-i\omega t}; \tilde{\omega}_k]
$$

+
$$
\frac{i\theta(t)}{2} \sum_{k>0} \text{Res} [J(\omega) \coth(\beta \omega/2) e^{i\omega t}; \tilde{\omega}_k]
$$

-
$$
\frac{i\theta(-t)}{2} \sum_{k<0} \text{Res} [J(\omega) \coth(\beta \omega/2) e^{i\omega t}; \tilde{\omega}_k].
$$
 (D23)

Here we denoted by $\tilde{\omega}_k$ the collection of both the poles ω_k of $J(\omega)$ as described in the previous section and the Matsubara poles $\omega_k^M = 2\pi i k/\beta$, $k \in \mathbb{Z} - \{0\}$, of coth($\beta \omega/2$). 0 is not a pole for the composite $J(\omega)$ coth $\beta \omega/2$ because it is canceled by asymmetric $p(\omega)$, whose degree is larger than 1.

If simple poles of $J(\omega)$ and Matsubara poles have no intersection, using the fact that $\text{Res}_{\omega_k^M} \coth(\beta \omega/2) = 2/\beta$, we can write

$$
C_s(t) = \frac{i}{2} \sum_{k>0} \theta(t) [R_k^{\beta} e^{i\omega_k t} - R_k^{\prime \beta} e^{-i\bar{\omega}_k t}]
$$

+
$$
\frac{i}{2} \sum_{k>0} \theta(-t) [R_k^{\beta} e^{-i\omega_k t} - R_k^{\prime \beta} e^{i\bar{\omega}_k t}]
$$

+
$$
\frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|},
$$
 (D24)

where $R_k^{\beta} = R_k \coth(\beta \omega_k/2)$ and $R_k^{\prime \beta} = \bar{R}_k \coth(\beta \bar{\omega}_k/2)$, which is the conjugate of R_k^{β} for real β . We also took advantage of the fact that $\omega_{-k}^{\tilde{M}} = -\omega_k^M$. For real temperatures, we can further write

$$
C_s(t) = -\sum_{k>0} [R_k^{\beta,\mathcal{R}} \sin(\omega_k^R |t|) + R_k^{\beta,\mathcal{I}} \cos(\omega_k^R t)]e^{-\omega_k^{\mathcal{I}}|t|}
$$

+
$$
\frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|}.
$$
 (D25)

By partitioning the sum into poles belonging to couples and quadrupoles, we have

$$
C_{s} = -2 \sum_{k_{q}} [R_{k_{q}}^{\beta,\mathcal{R}} \sin (\omega_{k_{q}}^{R}|t|) + R_{k_{q}}^{\beta,\mathcal{I}} \cos (\omega_{k_{q}}^{R}t)] e^{-\omega_{k_{q}}^{\mathcal{I}}|t|}
$$

$$
- \sum_{k_{i}=1}^{N_{i}} R_{k_{i}}^{\beta,\mathcal{I}} e^{-\omega_{k_{i}}^{\mathcal{I}}|t|} + \frac{2i}{\beta} \sum_{k>0} J(\omega_{k}^{M}) e^{-|\omega_{k}^{M}|t|}, \quad (D26)
$$

where $k_q = 1, \ldots, N_q$, and where we used Eq. [\(D6\).](#page-30-2) Noting that Eq. [\(D6\)](#page-30-2) implies that $R_{k_i}^{\beta, \mathcal{I}} = \text{Im}[R_{k_i} \coth(\beta \omega_{k_i}/2)] =$ $-iR_{k_i} \coth(\beta \omega_{k_i}/2) = -iR_{k_i}^{\beta}$, and using the fact that $\omega_{k_i}^{\mathcal{I}} =$ $-i\omega_{k_i}$, together with $\cos(\omega t) = \cos(\omega|t|)$ for all ω , we can further write

Nq

$$
C_{s} = \sum_{k_{q}=1}^{N_{q}} [iR_{k_{q}}^{\beta} e^{i\omega_{k_{q}}|t|} - i\bar{R}_{k_{q}}^{\beta} e^{-i\bar{\omega}_{k_{q}}|t|}] + i \sum_{k_{i}=1}^{N_{i}} R_{k_{i}}^{\beta} e^{i\omega_{k_{i}}|t|} + \frac{2i}{\beta} \sum_{k>0} J(\omega_{k}^{M}) e^{-|\omega_{k}^{M}|t|}. \quad (D27)
$$

Using Eqs. (33) and $(D20)$, we can also find the classical contribution to the correlation function as

$$
C_{\text{class}}(t) = C_s(t) + f_s(t)
$$

\n
$$
= \sum_{k_q=1}^{N_q} [iR_{k_q}^{\beta} e^{i\omega_{k_q}|t|} - i\bar{R}_{k_q}^{\beta} e^{-i\bar{\omega}_{k_q}|t|}]
$$

\n
$$
+ i \sum_{k_i=1}^{N_i} R_{k_i}^{\beta} e^{i\omega_{k_i}|t|} + \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|}
$$

\n
$$
+ \sum_{k_q=1}^{N_q} \left\{ R_{k_q}^{\mathcal{I}} (e^{i\omega_{k_q}|t|} + e^{-i\bar{\omega}_{k_q}|t|})
$$

\n
$$
- iR_{k_q}^{\mathcal{R}} (e^{(-i\omega_{k_q}^{\mathcal{R}} - W)|t|} + e^{(i\omega_{k_q}^{\mathcal{R}} - W)|t|}) \right\}
$$

\n
$$
- i \sum_{k_i=1}^{N_i} R_{k_i}^{\mathcal{R}} (e^{-\omega_{k_i}^{\mathcal{I}}|t|} + e^{-W|t|}), \qquad (D28)
$$

which can be further written as

$$
C_{\text{class}}(t) = \sum_{k_q=1}^{N_q} [i\Delta R_{k_q} e^{i\omega_{k_q}|t|} - i\Delta' R_{k_q} e^{-i\bar{\omega}_{k_q}|t|}] + i \sum_{k_i=1}^{N_i} \Delta R_{k_i} e^{i\omega_{k_i}|t|} + \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|}
$$
\n(D29)

in terms of $\Delta R_{k_x} = R_{k_x}^{\beta} - R_{k_x}$ and $\Delta' R_{k_x} = \bar{R}_{k_x}^{\beta} + R_{k_x}$ ($x =$ q , *i*) and where we used Eq. [\(D7\)](#page-30-3) and ignored terms decaying exponentially in the free parameter *W*.

This explicit expression can also be used to explicitly compute the coefficients for the spectral decomposition of the field ξ ; see Eq. [\(14\).](#page-4-1) We can simply use Eq. [\(D29\)](#page-34-0) in Eq. (13) to obtain

$$
c_n = \sum_{k_q=1}^{N_q} [i\Delta R_{k_q} L(i\omega_{k_q}) - i\Delta' R_{k_q} L_n(-i\bar{\omega}_{k_q})]
$$

+
$$
i\sum_{k_l=1}^{N_l} \Delta R_{k_l} L_n(i\omega_{k_l}) + \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) L_n(-|\omega_k^M|),
$$
(D30)

where, as in Appendix C_2 , we used the identity

$$
\frac{1}{2T} \int_{-T}^{T} d\tau e^{\omega|\tau|} \cos\left(\frac{n\pi \tau}{T}\right) = L_n(\omega), \tag{D31}
$$

for all $\omega \in \mathbb{C}$ in terms of the function

$$
L_n(\omega) = (e^{\omega T} e^{in\pi} - 1) \frac{\omega T}{(\omega T)^2 + (n\pi)^2}.
$$
 (D32)

2. Brownian spectral density

We now specialize the results of the previous section for the Brownian spectral density

$$
J_B(\omega) = \frac{\gamma \lambda^2 \omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2 \omega^2},
$$
 (D33)

characterized by a resonant frequency ω_0 , a width γ (with dimension of frequency), and an overall strength λ (with dimension frequency to the power 3/2, so that, for adimensional system coupling *s*, the correlation has the dimension of energy squared). This spectral density has four poles located at $\pm(\Omega \pm i\Gamma)$, where $\Omega = \sqrt{\omega_0^2 - \Gamma^2}$ and $\Gamma = \gamma/2$. This defines an underdamped limit when ω_0 > γ /2 (poles not located on the imaginary axis) and an overdamped limit when $\omega_0 < \gamma/2$ (poles located on the imaginary axis), which we analyze in the following sections. In both cases, the spectral density in Eq. [\(D33\)](#page-34-1) can be written, in the notation of Eq. $(D1)$, as

$$
J_B(\omega) = \frac{p_B(\omega)}{\prod_{k \in \mathbb{Z}_4^0} (\omega - \omega_k)},\tag{D34}
$$

where $p_B(\omega) = \gamma \lambda^2 \omega$, $\mathbb{Z}_4^0 = \{-2, -1, 1, 2\}$, $\omega_1 = \Omega + i\Gamma$, $\omega_2 = -\Omega + i\Gamma$, and $\omega_{-k} = -\omega_k$.

a. Underdamped limit

The underdamped limit $\Gamma < \omega_0$ implies $\Omega > 0$ and, using Eq. $(D34)$, we can compute the residues at the two poles ω_1 and ω_2 on the upper complex plane as

$$
Res_{\omega_1}J_B(\omega) = \gamma \lambda^2 \frac{\omega_1}{(\omega_1 - \omega_2)(\omega_1 - \omega_{-1})(\omega_1 - \omega_{-2})}
$$

\n
$$
= \gamma \lambda^2 \frac{\omega_1}{(2i\Gamma)(2\omega_1)(2\Omega)}
$$

\n
$$
= -i\frac{\lambda^2}{4\Omega}
$$

\n
$$
Res_{\omega_2}J_B(\omega) = \gamma \lambda^2 \frac{\omega_2}{(\omega_2 - \omega_1)(\omega_2 - \omega_{-1})(\omega_2 - \omega_{-2})}
$$

\n
$$
= \gamma \lambda^2 \frac{\omega_2}{(2i\Gamma)(-2\Omega)(2\omega_2)}
$$

\n
$$
= i\frac{\lambda^2}{4\Omega}.
$$
 (D35)

The imaginary nature of the residues above considerably simplifies the expression in Eq. $(D16)$ for the asymmetric part of the correlation function, which reads

$$
C_{\rm as}(t) = -i\frac{\lambda^2}{2\Omega}\sin(\Omega t)e^{-\Gamma|t|}
$$

=
$$
\frac{\lambda^2}{4\Omega}(e^{-i\Omega t} - e^{i\Omega t})e^{-\Gamma|t|}.
$$
 (D36)

Similarly, the symmetric part of the correlation in Eq. [\(D25\)](#page-33-1) can be written as

$$
C_s(t) = \frac{\lambda^2}{4\Omega} \coth (\beta \omega_1/2) e^{i\omega_1^R |t|} e^{-|\omega_1^I| |t|}
$$

\n
$$
- \frac{\lambda^2}{4\Omega} \coth (\beta \omega_2/2) e^{i\omega_2^R |t|} e^{-|\omega_2^I| |t|}
$$

\n
$$
+ \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M| |t|}
$$

\n
$$
= \frac{\lambda^2}{4\Omega} \coth (\beta(\Omega + i\Gamma)/2) e^{i\Omega |t|} e^{-\Gamma |t|}
$$

\n
$$
- \frac{\lambda^2}{4\Omega} \coth (\beta(-\Omega + i\Gamma)/2) e^{-i\Omega |t|} e^{-\Gamma |t|}
$$

\n
$$
+ \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M| |t|}
$$
 (D37)

in terms of the Matsubara frequencies $\omega_k^M = 2\pi i k/\beta$. In the $\beta \to \infty$ limit, we have

$$
C_{s}(t) \stackrel{\beta \to \infty}{=} \frac{\lambda^{2}}{4\Omega} (e^{i\Omega t} + e^{-i\Omega t})e^{-\Gamma|t|} + \frac{i}{\pi} \int_{0}^{\infty} dx J(ix)e^{-x|t|}.
$$
 (D38)

By defining $R_B = \text{Re}\{\coth[\beta(\Omega + i\Gamma)/2)\}\$ and $I_B =$ Im{coth[β (Ω + *i* Γ)/2)}, we can write the full correlation function as

$$
C(t) = C_s(t) + C_{as}(t)
$$

= $\frac{\lambda^2}{2\Omega} \left(\frac{R_B + 1}{2} e^{-i\Omega t} + \frac{R_B - 1}{2} e^{i\Omega t} \right) e^{-\Gamma|t|}$
+ $\frac{\lambda^2}{4\Omega} \left(I_B e^{-(-i\Omega + \Gamma)|t|} - I_B e^{-(i\Omega + \Gamma)|t|} \right)$
+ $\frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|}.$ (D39)

From this expression, it is possible to define a completely deterministic model on the lines of the one proposed in Ref. [\[80\]](#page-41-1). This can be done by introducing three "resonant" modes a_j , $j = 1, 2, 3$, and N_{Mats} "Matsubara" modes $a_i, j = 4, \ldots 3 + N_{\text{Mats}}$, as

$$
\dot{\rho}^{\text{det}} = -i[H_B^{\text{det}}, \rho^{\text{det}}] + D_B^{\text{det}}[\rho^{\text{det}}],\tag{D40}
$$

where

$$
H_{B}^{\text{det}} = H_{S} + \sum_{j=1}^{3+N_{\text{Mats}}} \lambda_{j} (a_{j} + a_{j}^{\dagger}) s + \Omega_{j} a_{j}^{\dagger} a_{j},
$$

$$
D_{B}^{\text{det}}[\rho] = \sum_{j=1}^{3+N_{\text{Mats}}} \Gamma_{j}[(n_{j} + 1)(2a_{j} \rho a_{j}^{\dagger} - a_{j}^{\dagger} a_{j} \rho - \rho a_{j}^{\dagger} a_{j}) + n_{j} (2a_{j}^{\dagger} \rho a_{j} - a_{j} a_{j}^{\dagger} \rho - \rho a_{j} a_{j}^{\dagger})]
$$
(D41)

as a function of the parameters

$$
\lambda_1 = \sqrt{\frac{\lambda^2}{2\Omega}}, \quad \lambda_2 = \sqrt{\frac{I_B \lambda^2}{4\Omega}}, \quad \lambda_3 = \sqrt{\frac{-I_B \lambda^2}{4\Omega}}, \n\Omega_1 = \Omega, \quad \Omega_2 = 0, \quad \Omega_3 = 0, \n\Gamma_1 = \Gamma, \quad \Gamma_2 = \Gamma - i\Omega, \quad \Gamma_3 = \Gamma + i\Omega, \n n_1 = \frac{R_B - 1}{2}, \quad n_2 = 0, \quad n_3 = 0 \n(D42)
$$

characterizing the resonant modes. We note that other choices that use only two resonant modes initially prepared with complex temperature values are possible [\[141\]](#page-42-18). The parameters characterizing the Matsubara modes can be defined by imposing $n_j = 0$, $\Omega_j = 0$ for $j = 4, \ldots, N_{\text{Mats}}$ and by minimizing the functional difference

$$
\left| \frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) e^{-|\omega_k^M||t|} - \sum_{j=4}^{N_{\text{Mats}}} \lambda_j^2 e^{-\Gamma_j|t|} \right|. \tag{D43}
$$

In contrast, the stochastic method proposed here requires one to solve only the dynamics of the system coupled to a single zero-temperature resonant mode a_0 and driven by a complex stochastic field ξ(*t*) as

$$
\dot{\rho} = -i[H_B, \rho] + D_B[\rho], \qquad (D44)
$$

where

$$
H_B = H_S + \lambda_0 s (a_0 + a_0^{\dagger}) + \Omega_0 a_0^{\dagger} a_0 + \xi(t) s,
$$

$$
D_B[\rho] = \Gamma_0 (2a_0 \rho a_0^{\dagger} - a_0^{\dagger} a_0 \rho - \rho a_0^{\dagger} a_0).
$$
 (D45)

In this case, the parameters for the resonant mode and the statistics of the field can be determined by the following classical-quantum decomposition of the correlation:

$$
C(t) = C_{\text{class}}(t) + C_Q(t), \tag{D46}
$$

where

$$
C_{\text{class}}(t) = C_s(t) - f_s(t),
$$

\n
$$
C_Q(t) = C_{\text{as}}(t) + f_s(t) = \frac{\lambda^2}{2\Omega} e^{-i\Omega t - \Gamma|t|}
$$
 (D47)

in terms of the symmetric function $f_s(t) = C_Q(t) +$ $C_Q(-t)$. Specifically, the parameters in Eq. [\(D45\)](#page-36-1) must then be defined as $\lambda_0 = \sqrt{\lambda^2/2\Omega}$, $\Omega_0 = \Omega$, and $\Gamma_0 = \Gamma$, while the field $\xi(t)$ must be Gaussian and such that

$$
\mathbb{E}[\xi(t_2)\xi(t_1)] = C_{\text{class}}(t_2 - t_1). \tag{D48}
$$

It is actually possible to be even more explicit in the definition of the stochastic field. By using Eq. [\(D35\)](#page-35-2) in Eq. [\(D30\),](#page-34-3) we obtain

$$
c_n = \frac{\lambda^2}{4\Omega} \{ \coth[\beta(\Omega + i\Gamma)/2] - 1 \} L(i\Omega - \Gamma)
$$

+
$$
\frac{\lambda^2}{4\Omega} \{ \coth[\beta(\Omega - i\Gamma)/2] - 1 \} L(-i\Omega - \Gamma)
$$

+
$$
\frac{2i}{\beta} \sum_{k>0} J(\omega_k^M) L_n(-|\omega_k^M|)
$$
 (D49)

in terms of the function $L_n(\omega)$ defined in Eq. [\(D32\).](#page-34-4)

b. Overdamped limit

The overdamped limit $\Gamma > \omega_0$ implies $\Omega^2 < 0$, so the results in the previous section can be adapted with the substitution $\Omega \mapsto i|\Omega|$, with $|\Omega| < \Gamma$. For example, the poles in the upper complex plane are now $\omega_1 = i(\Gamma + \Omega)$ and $\omega_2 = i(\Gamma - \Omega)$ and the residues become

$$
Res_{\omega_1} J_B(\omega) = -\frac{\lambda^2}{4|\Omega|},
$$

$$
Res_{\omega_2} J_B(\omega) = \frac{\lambda^2}{4|\Omega|}.
$$
 (D50)

Using Eq. $(D18)$ and noting that here the poles come in pairs (we have two such pairs, one for each of the poles ω_1

and ω_2 on the upper complex plane) with real residues, we can write

$$
C_{\rm as}(t) = 2 \sum_{k_i} R_{k_i}^{\mathcal{R}} \sin \left[\frac{-i(W - \omega_{k_i}^I)}{2} t \right] e^{-(W + \omega_{k_i}^I) |t|/2}
$$

\n
$$
= 2 \frac{\rm sg(t)}{2i} \sum_{k_i} R_{k_i}^{\mathcal{R}} e^{-\omega_{k_i}^I t}
$$

\n
$$
= 2 \frac{\rm sg(t)}{2i} \frac{\lambda^2}{4|\Omega|} e^{-\Gamma|t|} (e^{|\Omega| |t|} - e^{-|\Omega| |t|})
$$

\n
$$
= i \frac{\lambda^2}{4|\Omega|} e^{-\Gamma|t|} (e^{-|\Omega| t} - e^{|\Omega| t}).
$$
 (D51)

When the poles of the spectral density $J_B(\omega)$ are not located at the poles of coth $(\beta \omega)/2$, the symmetric part of the correlation reads

$$
C_s(t) = -\frac{\lambda^2}{4|\Omega|} \cot\left[\frac{\beta(\Gamma + |\Omega|)}{2}\right] e^{-(\Gamma + |\Omega|)|t|}
$$

+
$$
\frac{\lambda^2}{4|\Omega|} \cot\left[\frac{\beta(\Gamma - |\Omega|)}{2}\right] e^{-(\Gamma - |\Omega|)|t|}
$$

+
$$
\frac{2i}{\beta} \sum_{k>0} J_B(\omega_k^M) e^{-|\omega_k^M||t|}.
$$
 (D52)

When the poles ω_1 and ω_2 are located exactly at one of the Matsubara poles ω_k^M , one can still apply the expression above after regularizing the degeneracy and then taking the limit for such regularization to be zero.

c. Critical-damping limit

When $\Gamma = \omega_0$, we have $\Omega = 0$, implying the presence of a second-order pole in the upper complex plane located at $\omega_1 = \omega_2 = i\Gamma$. The correlation can be computed by either using the residue theorem or simply taking the $\Omega \rightarrow 0$ limit in the corresponding expressions for the underdamped and overdamped limits to obtain

$$
C_{as}(t) = -\frac{i t \lambda^2}{2} e^{-\Gamma|t|}.
$$
 (D53)

Similarly, the symmetric correlation reads

$$
C_{s}(t) = \frac{\lambda^{2}}{4} \frac{\beta + |t| \sin(\beta \Gamma)}{\sin^{2}(\beta \Gamma/2)} e^{-\Gamma|t|}
$$

$$
+ \frac{2i}{\beta} \sum_{k>0} J_{B}(\omega_{k}^{M}) e^{-|\omega_{k}^{M}|t|}. \tag{D54}
$$

3. Ohmic spectral density

In this section, we analyze an Ohmic spectral density

$$
J_{\Omega}(\omega) = \pi \alpha \omega e^{-\omega/\omega_c}, \qquad (D55)
$$

characterized by a strength parameter $\alpha \in \mathbb{R}$ and a cutoff energy scale ω_c . The antisymmetric contribution to the correlation takes the form

$$
C_{\text{as}}^{\Omega}(t) = -\frac{\alpha}{2} \int_0^{\infty} \omega e^{-\omega/\omega_c} (e^{i\omega t} - e^{-i\omega t}) d\omega
$$

=
$$
-2i\alpha \omega_c^2 \frac{\omega_c t}{(1 + \omega_c^2 t^2)^2},
$$
 (D56)

whose behavior interpolates the following limiting regimes:

$$
C_{\text{as}}^{\Omega}(t) \stackrel{t \ll 1/\omega_c}{=} -2i\alpha \omega_c^3 t
$$

$$
\stackrel{t \gg 1/\omega_c}{=} \frac{-2i\alpha \omega_c^2}{(\omega_c t)^3}.
$$
 (D57)

In contrast to the rational case, this contribution does not identically follow the ansatz in Eq. [\(31\).](#page-6-2) However, it is always possible to impose it, i.e., to find the optimal parameters that better approximate the expression

$$
C_{\rm as}^{\Omega}(t) \simeq \sum_{j=1}^{N_{\rm PM}^{\Omega}} a_j^{\Omega} \sin(b_j^{\Omega} t) e^{-c_j^{\Omega} |t|}.
$$
 (D58)

It is interesting to gain some intuition on this procedure by using Eq. $(D57)$ in Eq. $(D58)$ to obtain a rough estimate

of the parameters. By assuming $N_{\text{PM}}^{\Omega} = 1$ and taking the $t \ll 1/\omega_c$ limit on both sides of Eq. [\(D58\),](#page-37-2) we can write the following intuitive expressions:

$$
a_1^{\Omega} \simeq -2i\alpha\omega_c^2, \quad b_1^{\Omega} \simeq \omega_c, \quad c_1^{\Omega} \simeq \omega_c. \tag{D59}
$$

By using these expressions in Eq. [\(33\),](#page-6-5) we can conclude that the quantum contribution to the Ohmic spectral density can be approximated by a single pseudomode with parameters $\lambda^{\Omega} = \sqrt{2\alpha} \omega_c$, $\Omega^{\Omega} = \omega_c$, and $\Gamma^{\Omega} = \omega_c$. In Fig. [11,](#page-38-6) we show the results for the dynamics of the off-diagonal elements of the density matrix of a twolevel system interacting with an environment through a coupling operator that commutes with the system Hamiltonian. Specifically, we chose this pure dephasing model to be characterized by $s = \sigma_z$ and, for simplicity, by $H_s = 0$.

As can be seen from the analysis in Sec. [D3a,](#page-38-7) the dynamics of the coherences of a two-level system in contact with a dephasing environment depends only on the symmetric part of the correlation. It is then interesting to note that if we were to use the protocol defined in Sec. [III B,](#page-6-0) this model would still require a certain number of quantum pseudomodes in order to account for the quantum part of the correlation function. In turn, the classical field would then be defined in terms of the *classical* part of the correlation, which is defined in terms of both the symmetric part and the antisymmetric part. However, the procedure in Sec. [III B](#page-6-0) is not the only possible one. In this case, we can, for example, model the full symmetric part of the correlation using a classical stochastic field [i.e., imposing $f_s(t) = 0$ in the general formalism developed in Sec. [II\]](#page-3-0) and avoid considering any quantum degrees of freedom.

FIG. 10. Correlations for the Ohmic spectral density (see Ref. [\[120\]](#page-42-2) for an analytical expression) at zero temperature. Here the parameters correspond to the ones in Fig. [5.](#page-10-4) The fitting of the antisymmeatric part of the correlation function is done using two sine functions (which corresponds to two pseudomodes).

As expected from the analysis presented in Sec. D 3 a, the resulting dynamics matches the analytical dynamics more since it is the only one that affects the system in this dephasing model [see Eq. [\(D64\)](#page-38-8) and the third line in Eq. [\(D62\)\]](#page-38-9).

a. Pure dephasing

Here we consider the case in which the system-bath interaction Hamiltonian commutes with the system Hamiltonian, i.e., that $[s, H_S]$ in the notation of Appendix [A.](#page-13-0) In this case, the operator *s* is time independent in the interaction picture and the dynamics described by Eq. [\(A11\)](#page-14-2) becomes

$$
\rho_S(t) = e^{\mathcal{F}_{\text{deph}}(t,s,C(t))} \rho_S(0),\tag{D60}
$$

which, importantly, no longer requires a time ordering. The influence superoperator for the pure dephasing case reads

$$
\mathcal{F}_{\text{deph}}[\cdot] = \int_0^t dt_2 \int_0^{t_2} dt_1 \{ C(t_2 - t_1) [s \cdot, s] - C(t_1 - t_2) [s \cdot, s] \}
$$

\n
$$
= \int_0^t dt_2 \int_0^{t_2} dt_1 \{ 2C_s(t_2 - t_1)s \cdot s - C_s(t_2 - t_1) [s^2 + s^2 \cdot] - C_{\text{as}}(t_2 - t_1) [s^2, \cdot] - \Gamma_{\text{deph}}(t) D_{\text{deph}}[\cdot] - i \Omega_{\text{deph}}[s^2, \cdot], \qquad (D61)
$$

FIG. 11. Dynamics of the coherences for a pure dephasing model with Ohmic spectral density at zero temperature for $N_{\text{PM}} = 0$ (dashed red line) against the analytical result (solid blue line). The classical model does not have any pseudomodes and its stochastic field is defined to reproduce the *symmetric* part of the correlation (see Fig. [10\)](#page-37-3) in accordance with the pure dephasing analysis presented in Appendix D_3 a. The initial state of the two-level system is assumed to be an equal superposition of the ground state and the excited state. Specifically, here we plot the off-diagonal elements of the density matrix, which decay exponentially in the parameter $-4\Gamma_{\text{dep}}(t) = -2\alpha \log(1 + \omega_c^2 t^2)$; see Eq. [\(D65\)](#page-38-10) and Ref. [\[1\]](#page-38-0), Eq. (4.51). Other parameters are the same as those in Fig. [5.](#page-10-4) The averaging is done over 10^4 samples.

where we defined

$$
\Omega_{\text{deph}} = -i \int_0^t dt_2 \int_0^{t_2} dt_1 C_{\text{as}}(t_2 - t_1)
$$

= $-\frac{1}{\pi} \int_0^{\infty} d\omega J(\omega) \frac{t\omega - \sin(\omega t)}{\omega^2}$

$$
\Gamma_{\text{deph}} = \int_0^t dt_2 \int_0^{t_2} dt_1 C_s(t_2 - t_1)
$$

= $\frac{1}{\pi} \int_0^{\infty} d\omega J(\omega) \coth (\beta \omega/2) \frac{1 - \cos(\omega t)}{\omega^2}$

$$
D_{\text{deph}}[\cdot] = 2s \cdot s - s^2 \cdot - \cdot s^2, \qquad (D62)
$$

where we used

$$
\int_0^t dt_2 \int_0^{t_2} dt_1 \cos [\omega (t_2 - t_1)] = \int_0^t dt_2 \int_0^{t_2} du \cos (\omega u)
$$

=
$$
\frac{1 - \cos(\omega t)}{\omega^2}
$$

$$
\int_0^t dt_2 \int_0^{t_2} dt_1 \sin [\omega (t_2 - t_1)] = \frac{t\omega - \sin(\omega t)}{\omega^2}.
$$
 (D63)

In the special case of a system made of a two-level system with $s = \sigma_z$, the effective Hamiltonian for the dephasing is zero because $\sigma_z^2 = 1$, and Eq. [\(D60\)](#page-38-11) becomes

$$
\rho_S(t) = e^{\Gamma_{\text{deph}}(t)[2\sigma_z \cdot \sigma_z - 2 \cdot]} \rho_S(0), \tag{D64}
$$

which leaves the diagonal elements invariant, while causing a decay $exp[-4\Gamma_{\text{deph}}(t)]$ of the off-diagonal coherences. For the Ohmic spectral density in Eq. [\(D55\)](#page-37-4) and in the $\beta \to \infty$ limit, the decay rate can be further simplified to

$$
\Gamma_{\text{deph}}^{\text{Ohmic}}(t) \to \frac{\alpha}{2} \log \left(1 + \omega_c^2 t^2 \right). \tag{D65}
$$

- [1] H.-P. Breuer and F. Petruccione, *The Theory Of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
- [2] C. Gardiner and P. Zoller, *Quantum Noise: A Handbook of Markovian and Non-Markovian Quantum Stochastic Methods with Applications to Quantum Optics, Springer Series in Synergetics* (Springer, Berlin, 2004).
- [3] G. Lindblad, On the generators of quantum dynamical semigroups, [Commun. Math. Phys.](https://doi.org/10.1007/BF01608499) **48**, 119 (1976).
- [4] V. Gorini, A. Kossakowski, and E. Sudarshan, Completely positive dynamical semigroups of N-level systems, [J. Math. Phys.](https://doi.org/10.1063/1.522979) **17**, 821 (1976).
- [5] [A. G. Redfield, The theory of relaxation processes,](https://doi.org/10.1016/B978-1-4832-3114-3.50007-6) Adv. Magn. Opt. Reson. **1**, 1 (1965).
- [6] A. Ishizaki and G. R. Fleming, On the adequacy of the Redfield equation and related approaches to the study of

[quantum dynamics in electronic energy transfer,](https://doi.org/10.1063/1.3155214) J. Chem. Phys. **130**, 234110 (2009).

- [7] A. Dodin, T. V. Tscherbul, and P. Brumer, Quantum dynamics of incoherently driven V-type systems: Ana[lytic solutions beyond the secular approximation,](https://doi.org/10.1063/1.4954243) J. Chem. Phys. **144**, 244108 (2016).
- [8] P. R. Eastham, P. Kirton, H. M. Cammack, B. W. Lovett, and J. Keeling, Bath-induced coherence and the secular approximation, Phys. Rev. A **94**[, 012110 \(2016\).](https://doi.org/10.1103/PhysRevA.94.012110)
- [9] A. Trushechkin, Unified Gorini-Kossakowski-Lindblad-Sudarshan quantum master equation beyond the secular approximation, Phys. Rev. A **103**[, 062226 \(2021\).](https://doi.org/10.1103/PhysRevA.103.062226)
- [10] A. Fruchtman, N. Lambert, and E. Gauger, When do perturbative approaches accurately capture the dynamics of complex quantum systems?, Sci. Rep. **6**[, 28204 \(2016\).](https://doi.org/10.1038/srep28204)
- [11] I. de Vega and D. Alonso, Dynamics of non-Markovian [open quantum systems,](https://doi.org/10.1103/RevModPhys.89.015001) Rev. Mod. Phys. **89**, 015001 (2017).
- [12] H.-B. Chen, C. Gneiting, P.-Y. Lo, Y.-N. Chen, and F. Nori, Simulating Open Quantum Systems with Hamiltonian Ensembles and the Nonclassicality of the Dynamics, Phys. Rev. Lett. **120**[, 030403 \(2018\).](https://doi.org/10.1103/PhysRevLett.120.030403)
- [13] H.-B. Chen, P.-Y. Lo, C. Gneiting, J. Bae, Y.-N. Chen, and F. Nori, Quantifying the nonclassicality of pure dephasing, [Nat. Commun.](https://doi.org/10.1038/s41467-019-11502-4) **10**, 3794 (2019).
- [14] G. T. Landi, D. Poletti, and G. Schaller, Nonequilibrium boundary-driven quantum systems: Models, methods, and properties, Rev. Mod. Phys. **94**[, 045006 \(2022\).](https://doi.org/10.1103/RevModPhys.94.045006)
- [15] R. Feynman and F. Vernon, The theory of a general quantum system interacting with a linear dissipative system, Ann. Phys. **24**[, 118 \(1963\).](https://doi.org/10.1016/0003-4916(63)90068-X)
- [16] A. Caldeira and A. Leggett, Path integral approach to quantum Brownian motion, Phys. A **121**[, 587 \(1983\).](https://doi.org/10.1016/0378-4371(83)90013-4)
- [17] A. Caldeira and A. Leggett, Quantum tunnelling in a dissipative system, Ann. Phys. **149**[, 374 \(1983\).](https://doi.org/10.1016/0003-4916(83)90202-6)
- [18] P. Hedegård and A. O. Caldeira, Quantum dynamics of [a particle in a fermionic environment,](https://doi.org/10.1088/0031-8949/35/5/001) Phys. Scr. **35**, 609 (1987).
- [19] L. Bönig, K. Schönhammer, and W. Zwerger, Influence[functional theory for a heavy particle in a Fermi gas,](https://doi.org/10.1103/PhysRevB.46.855) Phys. Rev. B **46**, 855 (1992).
- [20] M. W. Y. Tu and W.-M. Zhang, Non-Markovian decoher[ence theory for a double-dot charge qubit,](https://doi.org/10.1103/PhysRevB.78.235311) Phys. Rev. B **78**, 235311 (2008).
- [21] J. Jin, M. W. Y. Tu, W.-M. Zhang, and Y. Yan, Nonequilibrium quantum theory for nanodevices based on the [Feynman–Vernon influence functional,](https://doi.org/10.1088/1367-2630/12/8/083013) New J. Phys. **12**, 083013 (2010).
- [22] W.-M. Zhang, P.-Y. Lo, H.-N. Xiong, M. W.-Y. Tu, and F. Nori, General Non-Markovian Dynamics of Open Quantum Systems, Phys. Rev. Lett. **109**[, 170402 \(2012\).](https://doi.org/10.1103/PhysRevLett.109.170402)
- [23] H.-N. Xiong, P.-Y. Lo, W.-M. Zhang, D. H. Feng, and F. Nori, Non-Markovian complexity in the quantum-toclassical transition, Sci. Rep. **5**[, 13353 \(2015\).](https://doi.org/10.1038/srep13353)
- [24] Y. Tanimura and R. Kubo, Time evolution of a quantum system in contact with a nearly Gaussian-Markoffian noise bath, [J. Phys. Soc. Jpn.](https://doi.org/10.1143/JPSJ.58.101) **58**, 101 (1989).
- [25] Y. Tanimura, Nonperturbative expansion method for a quantum system coupled to a harmonic-oscillator bath, Phys. Rev. A **41**[, 6676 \(1990\).](https://doi.org/10.1103/PhysRevA.41.6676)
- [26] A. Ishizaki and Y. Tanimura, Quantum dynamics of system strongly coupled to low-temperature colored noise [bath: Reduced hierarchy equations approach,](https://doi.org/10.1143/JPSJ.74.3131) J. Phys. Soc. Jpn. **74**, 3131 (2005).
- [27] Y. Tanimura, Stochastic Liouville, Langevin, Fokker– Planck, and master equation approaches to quantum dissipative systems, [J. Phys. Soc. Jpn.](https://doi.org/10.1143/JPSJ.75.082001) **75**, 082001 (2006).
- [28] A. Ishizaki and G. R. Fleming, Unified treatment of quantum coherent and incoherent hopping dynamics in electronic energy transfer: Reduced hierarchy equation approach, J. Chem. Phys. **130**[, 234111 \(2009\).](https://doi.org/10.1063/1.3155372)
- [29] A. G. Dijkstra and Y. Tanimura, Non-Markovian Entanglement Dynamics in the Presence of System-Bath Coherence, Phys. Rev. Lett. **104**[, 250401 \(2010\).](https://doi.org/10.1103/PhysRevLett.104.250401)
- [30] A. G. Dijkstra and Y. Tanimura, System bath correlations [and the nonlinear response of qubits,](https://doi.org/10.1143/JPSJ.81.063301) J. Phys. Soc. Jpn. **81**, 063301 (2012).
- [31] Y. Tanimura, Reduced hierarchical equations of motion in real and imaginary time: Correlated initial states and [thermodynamic quantities,](https://doi.org/10.1063/1.4890441) J. Chem. Phys. **141**, 044114 (2014).
- [32] N. Lambert, T. Raheja, S. Cross, P. Menczel, S. Ahmed, A. Pitchford, D. Burgarth, and F. Nori, QuTiP-BoFiN: A bosonic and fermionic numerical hierarchical-equationsof-motion library with applications in light-harvesting, quantum control, and single-molecule electronics, (2020), [ArXiv:2010.10806.](https://arxiv.org/abs/2010.10806)
- [33] Y. Tanimura, Numerically "exact" approach to open quantum dynamics: The hierarchical equations of motion (HEOM), J. Chem. Phys. **153**[, 020901 \(2020\).](https://doi.org/10.1063/5.0011599)
- [34] K. Nakamura and Y. Tanimura, Optical response of laser-driven charge-transfer complex described by Holstein–Hubbard model coupled to heat baths: Hierarchi[cal equations of motion approach,](https://doi.org/10.1063/5.0060208) J. Chem. Phys. **155**, 064106 (2021).
- [35] A. Garg, J. N. Onuchic, and V. Ambegaokar, Effect of fric[tion on electron transfer in biomolecules,](https://doi.org/10.1063/1.449017) J. Chem. Phys. **83**, 4491 (1985).
- [36] R. Martinazzo, B. Vacchini, K. H. Hughes, and I. Burghardt, Communication: Universal Markovian reduc[tion of Brownian particle dynamics,](https://doi.org/10.1063/1.3532408) J. Chem. Phys. **134**, 011101 (2011).
- [37] J. Iles-Smith, N. Lambert, and A. Nazir, Environmental dynamics, correlations, and the emergence of noncanon[ical equilibrium states in open quantum systems,](https://doi.org/10.1103/physreva.90.032114) Phys. Rev. A **90**, 032114 (2014).
- [38] M. P. Woods, R. Groux, A. W. Chin, S. F. Huelga, and M. B. Plenio, Mappings of open quantum systems [onto chain representations and Markovian embeddings,](https://doi.org/10.1063/1.4866769) J. Math. Phys. **55**, 032101 (2014).
- [39] P. Strasberg, G. Schaller, T. L. Schmidt, and M. Esposito, Fermionic reaction coordinates and their application to an autonomous Maxwell demon in the strong-coupling regime, Phys. Rev. B **97**[, 205405 \(2018\).](https://doi.org/10.1103/PhysRevB.97.205405)
- [40] M. Wertnik, A. Chin, F. Nori, and N. Lambert, Optimizing co-operative multi-environment dynamics in a dark-state[enhanced photosynthetic heat engine,](https://doi.org/10.1063/1.5040898) J. Chem. Phys. **149**, 084112 (2018).
- [41] T. Holstein, Studies of polaron motion: Part I. The molecular-crystal model, [Ann. Phys. \(N. Y\)](https://doi.org/10.1016/0003-4916(59)90002-8) **8**, 325 (1959).
- [42] T. Holstein, Studies of polaron motion: Part II. The "small" polaron, [Ann. Phys. \(N. Y\)](https://doi.org/10.1016/0003-4916(59)90003-X) **8**, 343 (1959).
- [43] B. Jackson and R. Silbey, On the calculation of transfer [rates between impurity states in solids,](https://doi.org/10.1063/1.445096) J. Chem. Phys. **78**, 4193 (1983).
- [44] R. Silbey and R. A. Harris, Variational calculation of the [dynamics of a two level system interacting with a bath,](https://doi.org/10.1063/1.447055) J. Chem. Phys. **80**, 2615 (1984).
- [45] R. A. Harris and R. Silbey, Variational calculation of the tunneling system interacting with a heat bath. II. Dynam[ics of an asymmetric tunneling system,](https://doi.org/10.1063/1.449469) J. Chem. Phys. **83**, 1069 (1985).
- [46] U. Weiss, *Quantum Dissipative Systems* (World Scientific Publishing Co. Pvt. Ltd, Singapore, 2008).
- [47] S. Jang, Y.-C. Cheng, D. R. Reichman, and J. D. Eaves, [Theory of coherent resonance energy transfer,](https://doi.org/10.1063/1.2977974) J. Chem. Phys. **129**, 101104 (2008).
- [48] S. Jang, Theory of coherent resonance energy transfer for [coherent initial condition.,](https://doi.org/10.1063/1.3247899) J. Chem. Phys. **131**, 164101 (2009).
- [49] A. Nazir, Correlation-Dependent Coherent to Incoherent [Transitions in Resonant Energy Transfer Dynamics,](https://doi.org/10.1103/PhysRevLett.103.146404) Phys. Rev. Lett. **103**, 146404 (2009).
- [50] D. P. S. McCutcheon and A. Nazir, On the calculation of [transfer rates between impurity states in solids,](https://doi.org/10.1063/1.445096) New J. Phys. **12**, 113042 (2010).
- [51] S. Jang, Theory of multichromophoric coherent resonance energy transfer: A polaronic quantum master equation approach, J. Chem. Phys. **135**[, 034105 \(2011\).](https://doi.org/10.1063/1.3608914)
- [52] D. P. S. McCutcheon and A. Nazir, Coherent and incoherent dynamics in excitonic energy transfer: Correlated [fluctuations and off-resonance effects,](https://doi.org/10.1103/PhysRevB.83.165101) Phys. Rev. B **83**, 165101 (2011).
- [53] A. Kolli, A. Nazir, and A. Olaya-Castro, Electronic excitation dynamics in multichromophoric systems described [via a polaron-representation master equation,](https://doi.org/10.1063/1.3652227) J. Chem. Phys. **135**, 034105 (2011).
- [54] F. Pollock, *Energy transport in open quantum systems*, Ph.D. thesis, Oxford University, UK (2014).
- [55] F. A. Pollock, D. P. S. McCutcheon, E. M. Lovett, B. W. Gauger, and A. Nazir, A multi-site variational master [equation approach to dissipative energy transfer.,](https://doi.org/10.1088/1367-2630/15/7/075018) New J. Phys. **15**, 075018 (2013).
- [56] D. Xu and J. Cao, Non-canonical distribution and nonequilibrium transport beyond weak system-bath coupling [regime: A polaron transformation approach,](https://doi.org/10.1007/s11467-016-0540-2) Front. Phys. **11**, 110308 (2016).
- [57] J. Rau, Relaxation phenomena in spin and harmonic oscillator systems, Phys. Rev. **129**[, 1880 \(1963\).](https://doi.org/10.1103/PhysRev.129.1880)
- [58] V. Scarani, M. Ziman, P. Štelmachovič, N. Gisin, and V. Bužek, Thermalizing Quantum Machines: Dissipation and Entanglement, Phys. Rev. Lett. **88**[, 097905 \(2002\).](https://doi.org/10.1103/PhysRevLett.88.097905)
- [59] M. Ziman, P. Štelmachovič, V. Bužek, M. Hillery, V. Scarani, and N. Gisin, Diluting quantum information: An analysis of information transfer in system-reservoir interactions, Phys. Rev. A **65**[, 042105 \(2002\).](https://doi.org/10.1103/PhysRevA.65.042105)
- [60] A. Purkayastha, G. Guarnieri, S. Campbell, J. Prior, and J. Goold, Periodically refreshed baths to simulate open [quantum many-body dynamics,](https://doi.org/10.1103/PhysRevB.104.045417) Phys. Rev. B **104**, 045417 (2021).
- [61] R. L. Hudson and K. R. Parthasarathy, Quantum Ito's for[mula and stochastic evolutions,](https://doi.org/10.1007/BF01258530) Commun. Math. Phys. **93**, 301 (1984).
- [62] C. W. Gardiner and M. J. Collett, Input and output in damped quantum systems: Quantum stochastic differen[tial equations and the master equation,](https://doi.org/10.1103/PhysRevA.31.3761) Phys. Rev. A **31**, 3761 (1985).
- [63] H. J. Carmichael, Quantum Trajectory Theory for Cascaded Open Systems, [Phys. Rev. Lett.](https://doi.org/10.1103/PhysRevLett.70.2273) **70**, 2273 (1993).
- [64] J. Zhang, Y.-x. Liu, R.-B. Wu, K. Jacobs, and F. Nori, [Non-Markovian quantum input-output networks,](https://doi.org/10.1103/PhysRevA.87.032117) Phys. Rev. A **87**, 032117 (2013).
- [65] J. E. Gough, Non-Markovian quantum feedback networks I: Quantum transmission lines, lossless bounded real prop[erty and limit Markovian channels,](https://doi.org/10.1063/1.4968817) J. Math. Phys. **57**, 122101 (2016).
- [66] J. Gough and M. R. James, The series product and its application to quantum feedforward and feedback networks, [IEEE Trans. Automat. Contr.](https://doi.org/10.1109/TAC.2009.2031205) **54**, 2530 (2009).
- [67] H. Mabuchi, Nonlinear interferometry approach to pho[tonic sequential logic,](https://doi.org/10.1063/1.3650250) Appl. Phys. Lett. **99**, 153103 (2011).
- [68] J. Zhang, Y.-x. Liu, R.-B. Wu, K. Jacobs, and F. Nori, Quantum feedback: Theory, experiments, and applications, [Phys. Rep.](https://doi.org/10.1016/j.physrep.2017.02.003) **679**, 1 (2017).
- [69] J. Combes, J. Kerckhoff, and M. Sarovar, The SLH frame[work for modeling quantum input-output networks,](https://doi.org/10.1080/23746149.2017.1343097) Adv. Phys. X **2**, 784 (2017).
- [70] A. Imamoglu, Stochastic wave-function approach to non-Markovian systems, Phys. Rev. A **50**[, 3650 \(1994\).](https://doi.org/10.1103/PhysRevA.50.3650)
- [71] B. M. Garraway, Nonperturbative decay of an atomic system in a cavity, Phys. Rev. A **55**[, 2290 \(1997\).](https://doi.org/10.1103/PhysRevA.55.2290)
- [72] E. Arrigoni, M. Knap, and W. von der Linden, Nonequilibrium Dynamical Mean-Field Theory: An Auxiliary Quan[tum Master Equation Approach,](https://doi.org/10.1103/PhysRevLett.110.086403) Phys. Rev. Lett. **110**, 086403 (2013).
- [73] A. Dorda, M. Nuss, W. von der Linden, and E. Arrigoni, Auxiliary master equation approach to nonequilibrium correlated impurities, Phys. Rev. B **89**[, 165105 \(2014\).](https://doi.org/10.1103/PhysRevB.89.165105)
- [74] I. Titvinidze, A. Dorda, W. von der Linden, and E. Arrigoni, Transport through a correlated interface: Aux[iliary master equation approach,](https://doi.org/10.1103/PhysRevB.92.245125) Phys. Rev. B **92**, 245125 (2015).
- [75] F. Schwarz, M. Goldstein, A. Dorda, E. Arrigoni, A. Weichselbaum, and J. von Delft, Lindblad-driven discretized leads for nonequilibrium steady-state transport in quantum impurity models: Recovering the continuum limit, Phys. Rev. B **94**[, 155142 \(2016\).](https://doi.org/10.1103/PhysRevB.94.155142)
- [76] A. Dorda, M. Sorantin, W. von der Linden, and E. Arrigoni, Optimized auxiliary representation of non-Markovian impurity problems by a Lindblad equation, New J. Phys. **19**[, 063005 \(2017\).](https://doi.org/10.1088/1367-2630/aa6ccc)
- [77] F. Mascherpa, A. Smirne, S. F. Huelga, and M. B. Plenio, Open Systems with Error Bounds: Spin-Boson Model [with Spectral Density Variations,](https://doi.org/10.1103/PhysRevLett.118.100401) Phys. Rev. Lett. **118**, 100401 (2017).
- [78] A. Lemmer, C. Cormick, D. Tamascelli, T. Schaetz, S. F. Huelga, and M. B. Plenio, A trapped-ion simulator for [spin-boson models with structured environments,](https://doi.org/10.1088/1367-2630/aac87d) New J. Phys. **20**, 073002 (2018).
- [79] D. Tamascelli, A. Smirne, S. F. Huelga, and M. B. Plenio, Nonperturbative Treatment of Non-Markovian Dynamics [of Open Quantum Systems,](https://doi.org/10.1103/PhysRevLett.120.030402) Phys. Rev. Lett. **120**, 030402 (2018).
- [80] N. Lambert, S. Ahmed, M. Cirio, and F. Nori, Modelling the ultra-strongly coupled spin-boson model with unphysical modes, [Nat. Commun.](https://doi.org/10.1038/s41467-019-11656-1) **10**, 3721 (2019).
- [81] D. Tamascelli, A. Smirne, J. Lim, S. F. Huelga, and M. B. Plenio, Efficient Simulation of Finite-Temperature [Open Quantum Systems,](https://doi.org/10.1103/PhysRevLett.123.090402) Phys. Rev. Lett. **123**, 090402 (2019).
- [82] G. Pleasance, B. M. Garraway, and F. Petruccione, Generalized theory of pseudomodes for exact descriptions of [non-Markovian quantum processes,](https://doi.org/10.1103/PhysRevResearch.2.043058) Phys. Rev. Res. **2**, 043058 (2020).
- [83] F. Mascherpa, A. Smirne, A. D. Somoza, P. Fernández-Acebal, S. Donadi, D. Tamascelli, S. F. Huelga, and M. B. Plenio, Optimized auxiliary oscillators for the simula[tion of general open quantum systems,](https://doi.org/10.1103/PhysRevA.101.052108) Phys. Rev. A **101**, 052108 (2020).
- [84] M. Cirio, N. Lambert, P.-C. Kuo, Y.-N. Chen, P. Menczel, K. Funo, and F. Nori, A pseudo-fermion method for the exact description of fermionic environments: From single-molecule electronics to Kondo resonance, (2022) , [ArXiv:2207.05780.](https://arxiv.org/abs/2207.05780)
- [85] Z. Tang, X. Ouyang, Z. Gong, H. Wang, and J. Wu, Extended hierarchy equation of motion for the spin-boson model, J. Chem. Phys. **143**[, 224112 \(2015\).](https://doi.org/10.1063/1.4936924)
- [86] C. Duan, Z. Tang, J. Cao, and J. Wu, Zero-temperature localization in a sub-Ohmic spin-boson model investi[gated by an extended hierarchy equation of motion,](https://doi.org/10.1103/PhysRevB.95.214308) Phys. Rev. B **95**, 214308 (2017).
- [87] J. Dalibard, Y. Castin, and K. Mølmer, Wave-Function Approach to Dissipative Processes in Quantum Optics, [Phys. Rev. Lett.](https://doi.org/10.1103/PhysRevLett.68.580) **68**, 580 (1992).
- [88] R. Dum, P. Zoller, and H. Ritsch, Monte Carlo simulation of the atomic master equation for spontaneous emission, Phys. Rev. A **45**[, 4879 \(1992\).](https://doi.org/10.1103/PhysRevA.45.4879)
- [89] H.-P. Breuer and F. Petruccione, Stochastic dynamics of quantum jumps, Phys. Rev. E **52**[, 428 \(1995\).](https://doi.org/10.1103/PhysRevE.52.428)
- [90] N. Gisin and I. C. Percival, The quantum-state diffusion [model applied to open systems,](https://doi.org/10.1088/0305-4470/25/21/023) J. Phys. A Math. Gen. **52**, 5677 (1992).
- [91] I. Percival, *Quantum State Diffusion* (Cambridge University Press, Cambridge (U.K.), 1998).
- [92] C. Gneiting, A. V. Rozhkov, and F. Nori, Jump-time [unraveling of Markovian open quantum systems,](https://doi.org/10.1103/PhysRevA.104.062212) Phys. Rev. A **104**, 062212 (2021).
- [93] C. Gneiting, A. Koottandavida, A. V. Rozhkov, and F. Nori, Unraveling the topology of dissipative quantum systems, Phys. Rev. Res. **4**[, 023036 \(2022\).](https://doi.org/10.1103/PhysRevResearch.4.023036)
- [94] W. T. Strunz, L. Diósi, and N. Gisin, Open System Dynamics with Non-Markovian Quantum Trajectories, [Phys. Rev. Lett.](https://doi.org/10.1103/PhysRevLett.82.1801) **82**, 1801 (1999).
- [95] L. Diósi, N. Gisin, and W. T. Strunz, Non-Markovian quantum state diffusion, Phys. Rev. A **58**[, 1699 \(1998\).](https://doi.org/10.1103/PhysRevA.58.1699)
- [96] L. Diósi, Exact semiclassical wave equation for stochastic quantum optics, [Quantum Semiclass. Opt.](https://doi.org/10.1088/1355-5111/8/1/023) **8**, 309 (1996).
- [97] L. Diósi and W. T. Strunz, The non-Markovian stochastic [Schrödinger equation for open systems,](https://doi.org/10.1016/S0375-9601) Phys. Lett. A **235**, 569 (1997).
- [98] J. T. Stockburger and H. Grabert, Exact *c*-Number Repre[sentation of Non-Markovian Quantum Dissipation,](https://doi.org/10.1103/PhysRevLett.88.170407) *Phys.* Rev. Lett. **88**, 170407 (2002).
- [99] J. Shao, Decoupling quantum dissipation interaction via stochastic fields, [J. Chem. Phys.](https://doi.org/10.1063/1.1647528) **120**, 5053 (2004).
- [100] J. T. Stockburger, Simulating spin-boson dynamics with [stochastic Liouville–von Neumann equations,](https://doi.org/10.1016/j.chemphys.2003.09.014) Chem. Phys. **296**, 159 (2004).
- [101] J. T. Stockburger and C. H. Mak, Stochastic Liouvillian algorithm to simulate dissipative quantum dynamics with arbitrary precision, [J. Chem. Phys.](https://doi.org/10.1063/1.478396) **110**, 4983 (1999).
- [102] J. T. Stockburger and H. Grabert, Non-Markovian quantum state diffusion, Chem. Phys. **268**[, 249 \(2001\).](https://doi.org/10.1016/S0301-0104(01)00307-X)
- [103] L. Han, A. Ullah, Y.-A. Yan, X. Zheng, Y. Yan, and V. Chernyak, Stochastic equation of motion approach to [fermionic dissipative dynamics. I. Formalism,](https://doi.org/10.1063/1.5142164) J. Chem. Phys. **152**, 204105 (2020).
- [104] A. Ullah, L. Han, Y.-A. Yan, X. Zheng, Y. Yan, and V. Chernyak, Stochastic equation of motion approach to fermionic dissipative dynamics. II. Numerical implementation, J. Chem. Phys. **152**[, 204106 \(2020\).](https://doi.org/10.1063/1.5142166)
- [105] L. Han, V. Chernyak, Y.-A. Yan, X. Zheng, and Y. Yan, Stochastic Representation of Non-Markovian Fermionic [Quantum Dissipation,](https://doi.org/10.1103/PhysRevLett.123.050601) Phys. Rev. Lett. **123**, 050601 (2019).
- [106] C. Y. Hsieh and J. Cao, A unified stochastic formulation of dissipative quantum dynamics. I. Generalized hierarchical equations., J. Chem. Phys. **148**[, 014103 \(2018\).](https://doi.org/10.1063/1.5018725)
- [107] C. Y. Hsieh and J. Cao, A unified stochastic formulation of dissipative quantum dynamics. II. Beyond linear response of spin baths., J. Chem. Phys. **148**[, 014104 \(2018\).](https://doi.org/10.1063/1.5018726)
- [108] J. Shao and Y.-A. Yan, Stochastic description of quantum Brownian dynamics, Front. Phys. **11**[, 110309 \(2016\).](https://doi.org/10.1007/s11467-016-0570-9)
- [109] J. M. Moix and J. Cao, A hybrid stochastic hierarchy equations of motion approach to treat the low temperature dynamics of non-Markovian open quantum systems, J. Chem. Phys. **139**[, 134106 \(2013\).](https://doi.org/10.1063/1.4822043)
- [110] Y. an Yan, F. Yang, Y. Liu, and J. Shao, Hierarchical approach based on stochastic decoupling to dissipative systems, [Chem. Phys. Lett.](https://doi.org/10.1016/j.cplett.2004.07.036) **395**, 216 (2004).
- [111] W. Koch, F. Großmann, J. T. Stockburger, and J. Ankerhold, Non-Markovian Dissipative Semiclassical Dynamics, Phys. Rev. Lett. **100**[, 230402 \(2008\).](https://doi.org/10.1103/PhysRevLett.100.230402)
- [112] J. T. Stockburger, Exact propagation of open quantum sys[tems in a system-reservoir context,](https://doi.org/10.1209/0295-5075/115/40010) Europhys. Lett. **115**, 40010 (2016).
- [113] D. Matos, M. A. Lane, I. J. Ford, and L. Kantorovich, Efficient choice of colored noise in the stochastic dynamics of open quantum systems, Phys. Rev. E **102**[, 062134 \(2020\).](https://doi.org/10.1103/PhysRevE.102.062134)
- [114] Y. Yun-An, Z. Xiao, and S. Jiushu, Piecewise ensemble averaging stochastic Liouville equations for simulat[ing non-Markovian quantum dynamics,](https://doi.org/10.1088/1367-2630/ac94f1/meta) New J. Phys. **24**, 103012 (2022).
- [115] C. M. Bender and S. Boettcher, Real Spectra in Non-[Hermitian Hamiltonians Having PT Symmetry,](https://doi.org/10.1103/PhysRevLett.80.5243) Phys. Rev. Lett. **80**, 5243 (1998).
- [116] C. M. Bender, Making sense of non-Hermitian Hamiltonians, [Rep. Prog. Phys.](https://doi.org/10.1088/0034-4885/70/6/R03) **70**, 947 (2007).
- [117] A. Mostafazadeh, Pseudo-Hermiticity versus PT symmetry: The necessary condition for the reality of the spectrum [of a non-Hermitian Hamiltonian,](https://doi.org/10.1063/1.1418246) J. Math. Phys. **43**, 205 (2002).
- [118] S. K. Özdemir, S. Rotter, F. Nori, and L. Yang, Parity—time symmetry and exceptional points in photonics, Nat. Mater. **18**[, 783 \(2019\).](https://doi.org/10.1038/s41563-019-0304-9)
- [119] We explicitly note that the constraint in Eq. (8) needs to hold for both positive and negative times; see Ref. [\[141\]](#page-42-18) for more details. We further comment on the fact that proving Eq. [\(8\)](#page-3-1) for positive times only and extending the result using the general identity $C(t) = C(-t)$ might require some extra care. When the parameters on the right-hand side are analytically continued, complex conjugation is, in general, no longer associated with the sign of time. The parameters of the pseudomode model have specific even (for λ_i , Ω_i , and n_i) and odd (for Γ_i) symmetries under time reversal irrespective of their complex nature.
- [120] T. Brandes, *Lectures on Background to Quantum Information: chapter 7 (quantum dissipation)* (2003).
- [121] J. R. Johansson, P. D. Nation, and F. Nori, QuTiP: An open-source Python framework for the dynamics of open quantum systems, [Comput. Phys. Commun.](https://doi.org/10.1016/j.cpc.2012.02.021) **183**, 1760 (2012).
- [122] J. R. Johansson, P. D. Nation, and F. Nori, QuTiP 2: A Python framework for the dynamics of open quantum systems, [Comput. Phys. Commun.](https://doi.org/10.1016/j.cpc.2012.11.019) **184**, 1234 (2013).
- [123] N. Shammah, S. Ahmed, N. Lambert, S. De Liberato, and F. Nori, Open quantum systems with local and collective incoherent processes: Efficient numerical simulations [using permutational invariance,](https://doi.org/10.1103/PhysRevA.98.063815) Phys. Rev. A **98**, 063815 (2018).
- [124] B. Li, S. Ahmed, S. Saraogi, N. Lambert, F. Nori, A. Pitchford, and N. Shammah, Pulse-level noisy quantum circuits with QuTiP, Quantum **6**[, 630 \(2022\).](https://doi.org/10.22331/q-2022-01-24-630)
- [125] An alternative representation that uses $2 + N_{\text{Mats}}$ is possible by introducing complex temperatures [\[141\]](#page-42-18).
- [126] A. J. Dunnett and A. W. Chin, Matrix product state simulations of non-equilibrium steady states and transient heat flows in the two-bath spin-boson model at finite temperatures, Entropy **23**[, 77 \(2021\).](https://doi.org/10.3390/e23010077)
- [127] P. Calabrese, Entanglement and thermodynamics in non[equilibrium isolated quantum systems,](https://doi.org/10.1016/j.physa.2017.10.011) Phys. A Stat. Mech. Appl. **504**, 31 (2018).
- [128] F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso, *Thermodynamics in the Quantum Regime* (Springer Nature Switzerland AG 2018, Cham (Switzerland), 2018).
- [129] C. Brif, R. Chakrabarti, and H. Rabitz, Control of quan[tum phenomena: past, present and future,](https://doi.org/10.1088/1367-2630/12/7/075008) New J. Phys. **12**, 075008 (2010).
- [130] E. Mangaud, R. Puthumpally-Joseph, D. Sugny, C. Meier, O. Atabek, and M. Desouter-Lecomte, Non-Markovianity in the optimal control of an open quantum system [described by hierarchical equations of motion,](https://doi.org/10.1088/1367-2630/aab651) New J. Phys. **20**, 043050 (2018).
- [131] M. B. Plenio and S. F. Huelga, Dephasing-assisted trans[port: quantum networks and biomolecules,](https://doi.org/10.1088/1367-2630/10/11/113019) New J. Phys. **10**, 113019 (2008).
- [132] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd, and A. Aspuru-Guzik, Environment-assisted quantum transport, New J. Phys. **11**[, 033003 \(2009\).](https://doi.org/10.1088/1367-2630/11/3/033003)
- [133] G. D. Scholes, G. R. Fleming, A. Olaya-Castro, and R. van Grondelle, Lessons from nature about solar light harvesting, Nat. Chem. **3**[, 763 \(2011\).](https://doi.org/10.1038/nchem.1145)
- [134] N. Lambert, Y.-N. Chen, Y.-C. Cheng, G.-Y. Li, C.-M. [Chen, and F. Nori, Quantum biology,](https://doi.org/10.1038/nphys2474) Nat. Phys. **9**, 10 (2013).
- [135] J. Ma, Z. Sun, X. Wang, and F. Nori, Entanglement [dynamics of two qubits in a common bath,](https://doi.org/10.1103/PhysRevA.85.062323) Phys. Rev. A **85**, 062323 (2012).
- [136] E. Aurell, R. Kawai, and K. Goyal, An operator derivation of the Feynman–Vernon theory, with applications to the generating function of bath energy changes and to an-harmonic baths, [J. Phys. A Math. Theor.](https://doi.org/10.1088/1751-8121/ab9274) **53**, 275303 (2020).
- [137] M. Cirio, P.-C. Kuo, Y.-N. Chen, F. Nori, and N. Lambert, Canonical derivation of the fermionic influence superoperator, Phys. Rev. B **105**[, 035121 \(2022\).](https://doi.org/10.1103/PhysRevB.105.035121)
- [138] J. Rammer, *Quantum Transport Theory* (Perseus Group, Reading, 1998).
- [139] A. Rastegin, Relations for certain symmetric norms and [anti-norms before and after partial trace,](https://doi.org/10.1007/s10955-012-0569-8) J. Stat. Phys. **148**, 1040 (2012).
- [140] R. Bhatia, *Matrix Analysis* (Springer, New York, 2012).
- [141] P. Menczel, *et al.*, In preparation, (2023).