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Quantum Brownian motion for embedded system

Meng Xu[a] and Joachim Ankerhold[b]

Institute for Complex Quantum Systems and IQST, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm, Germany

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Abstract Conventional derivations of the Wigner phase-space Fokker–Planck equation for open quantum systems often rely on heuristic coarse-graining of system-bath interactions. We present quantum dissipation in a minimally extended state space (QD-MESS), a unified framework that systematically models Gaussian bath dynamics in Wigner phase space with controllable numerical accuracy, yields a transparent quantum-classical picture for arbitrary noise spectra, and recovers the quantum-optical, Caldeira–Leggett, and quantum Smoluchowski limits.

1 Introduction

A small quantum subsystem linearly coupled to a Gaussian thermal bath is typically modeled as an open quantum system. Over the past decades, numerous approaches have been developed to simulate such dynamics, including the generalized Langevin equation, the stochastic Schrödinger equation, the stochastic Liouville–von Neumann equation, the quasi-adiabatic propagator path integral, the hierarchical equations of motion, and the hierarchy of pure states, among others. These methods have found widespread application in quantum transport, quantum thermodynamics, decoherence dynamics, and chemical reaction rates.

The phase-space representation offers a unified view of quantum-classical correspondence via a quasiprobability distribution evolving under a Fokker–Planck equation. This partial differential equation can be solved efficiently with finite-difference schemes and, more recently, physics-informed neural networks [1]. For harmonic reservoirs, the second-order Fokker–Planck equation is formally exact, with the fluctuation–dissipation relation encoded directly in the drift and diffusion coefficients [2]. In this representation, the phase-space equation facilitates a microscopic interpretation in terms of a generalized Langevin equation [2] and support asymptotic analyses, such as the derivation of Smoluchowski limits [3, 4].

However, the computational cost of exact simulations of open quantum systems grows exponentially with the dimension of the combined system-environment Hilbert space, rendering brute-force approaches feasible only for a few system degrees of freedom. While tensor-network methods can dramatically reduce memory, the computational effort per time step still grows roughly linearly with the number of effective bath modes. Model-order reduction offers an alternative by reducing the state space of the effective bath modes: one projects the Fokker–Planck dynamics onto a subspace spanned by dominant modes, yielding a computationally efficient reduced model equation, however, conservation laws are not guaranteed *a priori* without tailored constraints. In certain asymptotic limits, the Fokker–Planck equation simplifies further. A paradigmatic example is the reaction-coordinate (RC) mapping, wherein an Ohmic bath at high temperature can be replaced by a single Brownian-oscillator coordinate whose reduced dynamics obeys the Caldeira–Leggett master equation, thereby capturing the leading environmental influence with minimal added complexity. Despite its successes, the RC approach relies on coarse-grained approximations and is rigorously justified only for specific spectral densities and temperature regimes, limiting its general applicability. This raises the question of how to formulate a formally exact yet tractable Fokker–Planck description of system-bath dynamics within a minimal state space.

To derive a minimal state space Fokker–Planck equation for open quantum system, we first decompose a general Gaussian environment into a minimal set of effective modes with complex-valued frequencies and couplings that exactly reproduce the bath two-point correlation function. The Feynman–Vernon influence functional with these

[a] e-mail: meng.xu@uni-ulm.de (corresponding author)
[b] e-mail: joachim.ankerhold@uni-ulm.de (corresponding author)

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effective modes representation is then unraveled into a set of time-local ordinary differential equations (QD-MESS) via a Hubbard–Stratonovich transformation. Introducing squeezed-boson ladder operators for the effective modes maps QD-MESS onto a hybrid Liouville–phase-space equation of motion, i.e., Fokker–Planck equation description of an extended system.

For particular bath correlation functions (or, equivalently, noise spectra), the system-bath dynamics can be modeled as an embedded system governed by a quantum Brownian motion master equation, e.g., Caldeira–Leggett, quantum-optical, or Smoluchowski-type forms. Deviations from these canonical structures indicate genuinely nonclassical or unphysical effects and motivate alternative nonperturbative modeling strategies for open quantum systems.

2 Modeling of open quantum systems

The standard approach to modeling open quantum systems employs a system-plus-bath model [5–7]. The total Hamiltonian (with natural units $\hbar = k_B = m = 1$) is given by

$$\hat{H} = \hat{H}_s + \hat{H}_{\rm sb} + \hat{H}_b, \tag{1}$$

where the intrinsic dynamics of the system of interest is governed by the Hamiltonian

$$\hat{H}_s = \frac{\hat{p}_s^2}{2} + V(\hat{s},\, t), \tag{2}$$

while $\hat{H}_b$ governs the free fluctuations of the reservoir (typically a heat bath with many degrees of freedom). The system-bath interaction is assumed to be linear and separable,

$$\hat{H}_{\rm sb} = \hat{s} \otimes \hat{X}_b. \tag{3}$$

By eliminating bath degrees of freedom via Heisenberg equations of motion, one obtains a reduced system dynamics governed by the generalized quantum Langevin equation [7–11]. However, numerically propagating the quantum Langevin equation, especially in the presence of non-Markovian memory effects and over long timescales, poses significant challenges.

Another particularly powerful method for addressing Gaussian quantum dissipation nonperturbatively is provided by the path integral formalism pioneered by Feynman and Vernon [12] and subsequently developed in Refs. [5, 6, 13, 14]. Assuming an initially factorized state between the system and the bath, the reduced density operator $\hat{\rho}_s(t)$ can be expressed as a functional integral over paths defined on a Keldysh contour:

$$\rho_{\rm s}^{\pm}(t) = \int \mathcal{D}[s_+,\, s_-]\, \mathcal{A}_s[s_+,\, s_-]\, {\rm e}^{-iF[s_+,\, s_-]}\, \rho_{\rm s}^{\pm}(0). \tag{4}$$

Here, the bare action factor

$$\mathcal{A}_s[s_+,\, s_-] = \exp\{iS[s_+] - iS[s_-]\} \tag{5}$$

encapsulates the system's intrinsic quantum dynamics in the absence of the bath, with $S[s_+]$ and $S[s_-]$ denoting the actions along the forward $s_+(t)$ and backward $s_-(t)$ system paths, respectively. The explicit dependence on the endpoints of these paths (typically taken in the position representation) is indicated by the superscripts $\pm$, where $\langle \rho_{\rm s}^{\pm} \rangle = \langle s_- | \hat{\rho}_{\rm s} | s_+ \rangle$.

The environmental influence is introduced via the Feynman–Vernon influence functional [12]. By defining the classical and quantum coordinates,

$$s_c = \frac{s_+ + s_-}{\sqrt{2}}, \quad s_q = \frac{s_+ - s_-}{\sqrt{2}}, \tag{6}$$

the influence functional can be cast in the form

$$F = \int_0^t {\rm d}\tau \int_0^t {\rm d}\tau' \big[s_q(\tau)\; s_c(\tau) \big] \Sigma(\tau - \tau') \begin{bmatrix} s_q(\tau') \\ s_c(\tau') \end{bmatrix}. \tag{7}$$

The self-energy matrix in real time is given by

$$\Sigma(t) = -2i\,\theta(t)\left[\mathrm{Re}\,C(t)\begin{bmatrix}1&0\\0&0\end{bmatrix} + \mathrm{Im}\;C(t)\begin{bmatrix}0&i\\0&0\end{bmatrix}\right],$$

where the Heaviside step function $\theta(t)$ ensures proper time ordering of the double integral in Eq. (7). The reservoir correlation function,

$$C(t) = \mathrm{tr_b}\Big\{\hat{X}_\mathrm{b}(t)\,\hat{X}_\mathrm{b}(0)\,\rho_\mathrm{b}\Big\} \tag{8}$$

describes the free thermal fluctuations of the bath observable $\hat{X}_\mathrm{b}$, with ρ_b denoting the equilibrium density operator of the bath.

Since thermal fluctuations follow the fluctuation–dissipation theorem [5, 15], the reservoir's fluctuation spectrum

$$S_\beta(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{i\omega t}\,C(t), \tag{9}$$

can be obtained from the inverse reservoir temperature $\beta = 1/T$ and the dissipative response of the reservoir, i.e.

$$S_\beta(\omega) = \frac{J(\omega)}{1-\mathrm{e}^{-\beta\omega}}. \tag{10}$$

Here, $J(\omega)$ is defined as an antisymmetric function. Transforming Eq. (10) back to the time domain yields

$$C(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\,S_\beta(\omega)\,\mathrm{e}^{-i\omega t}. \tag{11}$$

Thus, the only information required about thermal environments are the bath spectral density $J(\omega)$ and temperature T. Knowledge about actual microscopic degrees of freedom is not necessary, which implies wide applicability. In essence, in the reduced framework (4), the reservoir correlation $C(t)$ induces self-interactions during the system's time evolution. Depending on temperature and spectral bath distribution, these can be very long-ranged, which implies that, in general, a simple time-local equation of motion for the reduced density operator does not exist.

3 Quantum dissipation with minimally extended state space

We introduce an operator space spanned by single-particle Green's functions. In this representation, the retarded Green's function obeys the equation of motion

$$(i\mathbb{1}\partial_t - \vec{\mathcal{E}})\vec{\mathcal{G}}^R(t) = \delta(t)\mathbb{1}. \tag{12}$$

The matrix $\vec{\mathcal{E}}$ is chosen such that its eigenvalues are confined to the lower half of the complex plane. $\mathbb{1}$ denotes the identity matrix, and $\delta(t)$ represents the boundary condition delta function.

In the sequel, we decompose the real and imaginary parts of the Gaussian bath correlation function as

$$\mathrm{Re}\{C(t\geq 0)\} = i\,\vec{\kappa}^\dagger\vec{\mathcal{G}}^R(t)\,\vec{\eta}', \tag{13a}$$

$$\mathrm{Im}\,\{C(t\geq 0)\} = \;\vec{\kappa}^\dagger\vec{\mathcal{G}}^R(t)\,\vec{\eta}''. \tag{13b}$$

For alternative decompositions, see Refs. [16, 17]. For practical simulations, a coarse-grained dynamics permits the selection of a minimal rank K for $\vec{\mathcal{E}}\in\mathbb{C}^{K\times K}$, along with the associated column vectors $\vec{\kappa}$, $\vec{\eta}'$, and $\vec{\eta}''\in\mathbb{C}^{K\times 1}$.

Accordingly, the Feynman–Vernon influence functional action [Eq. (7)] can be expressed as

$$F = -2i\int_0^t \mathrm{d}\tau\mathrm{d}\tau' s_\mathrm{q}(\tau)\vec{\kappa}^\dagger\vec{\mathcal{G}}^R(\tau-\tau')\Big[\vec{\eta}'\,s_\mathrm{q}(\tau') + \vec{\eta}''\,s_\mathrm{c}(\tau')\Big].$$

The time-nonlocality in the influence functional is unraveled by means of a Hubbard–Stratonovich transformation in path integral [18–20], introducing Gaussian auxiliary fields $\vec{\phi}(t) = [\phi_1(t) \quad \phi_2(t) \quad \dots \quad \phi_K(t)]^T$. The elements of reduced density operator [Eq. (4)] are then represented as $\rho_s^{\pm}(t) = \int_{-\infty}^{\infty} \mathrm{d}\phi^*(0)\mathrm{d}\phi(0)\mathrm{d}\phi^*(t)\mathrm{d}\phi(t)\, \rho_w[s_+, s_-; \vec{\phi}^\dagger, \vec{\phi}; t]$ with

$$\rho_w(t) = \int \mathcal{D}[s_+, s_-; \vec{\phi}^\dagger, \vec{\phi}]\, w[\vec{\phi}^\dagger, \vec{\phi}]\mathcal{A}[s_u^\dagger, s_v; \vec{\phi}^\dagger, \vec{\phi}]\, \rho_s^{\pm}(0). \tag{14}$$

Here, $\mathcal{A}$ denotes the amplitude

$$\mathcal{A} = \mathcal{A}_s \exp\left\{ i \int_0^t \mathrm{d}\tau [\vec{\phi}^\dagger(\tau)\vec{s}_v(\tau) + \vec{s}_u^\dagger(\tau)\vec{\phi}(\tau)] \right\} \tag{15}$$

with $s_u^\dagger(t) = \sqrt{2}s_q(t)\vec{\kappa}^\dagger$ and $s_v(t) = \sqrt{2}[\vec{\eta}' s_q(t) + \vec{\eta}'' s_c(t)]$. The effective mode path measure is

$$w[\vec{\phi}^\dagger, \vec{\phi}] = \exp\left\{ i \int_0^t \mathrm{d}\tau \left[\vec{\phi}^\dagger(\tau)(i\partial_\tau - \vec{\mathcal{E}})\vec{\phi}(\tau) \right] \right\}, \tag{16}$$

corresponding to the "free-field" action of bosonic excitations from the vacuum with Green's functions $\vec{\mathcal{G}}^R(t)$ truncated to K modes. The complex weights of the effective mode paths in Eq. (16), properly identify it as coherent-state path integrals for bosonic modes subject to *vacuum-state boundary conditions* [19, 20], i.e.,

$$\phi_k(0) = \phi_k^*(t) = 0, \quad k = 1, 2, \dots, K \tag{17}$$

Assigning raising and lowering operators $a_k^\dagger$, a_k to the pure-state modes described by the coherent-state paths ϕ_k^*, ϕ_k, the extended density operator $\hat{\rho}_w(t)$ (the hat here indicates that $\hat{\rho}_w(t)$ acts as a density matrix in the full system-bath Hilbert space) that evolves according to

$$\dot{\hat{\rho}}_w(t) = -i\,[\hat{H}_s,\ \hat{\rho}_w(t)] - i\,\vec{\hat{a}}^\dagger\,\vec{\mathcal{E}}\,\vec{\hat{a}}\,\rho_w(t) + i[\hat{s},\ (\vec{\kappa}^\dagger\,\vec{\hat{a}} + \vec{\hat{a}}^\dagger\,\vec{\eta}')\,\hat{\rho}_w(t)] + i\{\hat{s},\ \vec{\hat{a}}^\dagger\,\vec{\eta}''\,\hat{\rho}_w(t)\}. \tag{18}$$

In practice, the equation can be efficiently propagated using tensor network methods under the time-dependent variational principle (TDVP) [21, 22].

We introduce the number basis of the effective modes, defined by $\hat{a}_k^\dagger\hat{a}_k|n_k\rangle = n_k|n_k\rangle$, $n_k \in \mathbb{N}$ and denote the multi-mode basis as $|\vec{n}\rangle = \otimes_{k=1}^K |n_k\rangle$. In this basis, the $\hat{\rho}_w$ can be expanded as

$$\hat{\rho}_w(t) = \sum_{\vec{n}} \hat{\rho}_{\vec{n}}(t)|\vec{n}\rangle, \tag{19}$$

which leads to the hierarchical equations of motion [23]:

$$\dot{\hat{\rho}}_{\mathbf{n}}(t) = -i[H_s, \hat{\rho}_{\mathbf{n}}] - i\sum_{j,k=1}^{K} \sqrt{n_j}\sqrt{n_k+1}\,\mathcal{E}_{jk}\hat{\rho}_{\mathbf{n}_{jk}^{-+}} + i\sum_{j=1}^{K}\left[s,\ \kappa_j^*\sqrt{n_j+1}\rho_{\mathbf{n}_j^+} + \eta_j'\sqrt{n_j}\hat{\rho}_{\mathbf{n}_j^-}\right] + i\sum_{j=1}^{K}\left\{s,\ \eta_j''\sqrt{n_j}\hat{\rho}_{\mathbf{n}_j^-}\right\}. \tag{20}$$

The multi-index $\vec{n}_k^{\pm}$ is obtained from $\vec{n}$ by raising (lowering) its k-th component by one. The multi-index $\vec{n}_{jk}^{-+}$ denotes the j-th element is lowered by one, while the k-th element is raised by one, relative to $\vec{n}$.

4 Continuous variable representation

The retarded Green's function may be interpreted as the linear-response kernel of a Langevin equation (Ornstein–Uhlenbeck process) [2, 24], where the free effective modes satisfy the Langevin equation

$$\dot{x}_j(t) = -i\sum_{k=1}^{K} \mathcal{E}_{jk}\, x_k(t) + \xi_j(t), \tag{21}$$

where $\xi_j(t)$ denotes zero-mean Gaussian white noise with covariance $\langle \xi_j(t)\, \xi_k(u)\rangle = i\mathcal{E}_{jk}\delta(t-u)$. The stationary state correlation of the generalized coordinates $\vec{x}(t) = [x_1(t),\ x_2(t),\ \ldots,\ x_K(t)]^T$ upon ensemble averaging reads

$$\lim_{u\to\infty} \big\langle \vec{x}(t+u)\, \vec{x}^{\dagger}(u)\big\rangle = \vec{\mathcal{G}}^R(t)\, \vec{C}_{\infty} \tag{22}$$

with the $K \times K$ dimensional stationary covariance matrix $\vec{C}_{\infty} = \lim_{u\to\infty}\langle \vec{x}(u)\, \vec{x}^{\dagger}(u)\rangle$. Regardless of the effective interacting structure between quantum subsystem and the effective modes, any Gaussian bath can be represented on coarse-grained timescales by the stochastic differential equation Eq. (21).

We now define $x_j = \sigma_j\, q_j$ with σ_j the scaling parameter to be detailed in the sequel, the quasi-distribution $f(\vec{q},\, t)$ for effective modes obeys the Fokker–Planck equation [2]

$$\dot{f}(\vec{q},\, t) = i\sum_{j,\,k} \mathcal{E}_{jk}\, \frac{1}{\sigma_j}\frac{\partial}{\partial q_j}\bigg(\sigma_k q_k + \frac{1}{2\sigma_k}\frac{\partial}{\partial q_k}\bigg) f(\vec{q},\, t). \tag{23}$$

Consider a system S whose evolution is governed by the Liouville–von Neumann equation, while an external Gaussian bath B is described by a quasiprobability distribution obeying a Fokker–Planck equation as in Eq. (23). A key issue is to formulate a unified description of the coupled system-bath dynamics, $\hat{\rho}_w(t) = \hat{\rho}_{\vec{q}}(t)\, f(\vec{q},\, t)$, where $\hat{\rho}_{\vec{q}}(t)$ is the subsystem density operator conditioned on the bath distribution $f(\vec{q},\, t)$. One convenient route maps the bosonic creation and annihilation operators in QD-MESS onto c-number variables, representing the bath by a quasiprobability distribution while retaining the subsystem in Hilbert space. This hybrid formulation streamlines numerical implementation and clarifies the correspondence between quantum and classical environmental descriptions [25].

4.1 Squeezed ladder operators

For the effective bosonic modes in the QD-MESS framework, we define squeezed ladder operators for $\hat{a}_j$ and its Hermitian conjugate $\hat{a}_j^{\dagger}$ through

$$\hat{a}_j = \sqrt{2}\sigma_j q_j + \frac{1}{\sqrt{2}\sigma_j}\frac{\partial}{\partial q_j}, \tag{24a}$$

$$\hat{a}_j^{\dagger} = -\frac{1}{\sqrt{2}\sigma_j}\frac{\partial}{\partial q_j}, \tag{24b}$$

where q_j denotes a generalized variable corresponding to the quantum counterpart $\hat{q}_j$ in Hilbert space; σ_j is a nonzero scaling factor and σ_j^2 denotes the equilibrium variance of q_j, whose explicit form is dependent on the system to be described.

These differential operators preserve the usual bosonic commutation relations, i.e., $[\hat{a}_i,\, \hat{a}_j^{\dagger}] = \delta_{ij}$, although the uncertainty relation depends on σ_j reflecting the effective space resolution. Given the specific choice $\sigma_j = (m_j\omega_j/\hbar)^{1/2}$, one recovers the standard definition of harmonic ladder operators

$$\mathcal{S}\, \hat{a}_j^{(\dagger)}\, \mathcal{S}^{-1} = \frac{1}{\sqrt{2}}\bigg(\sigma_j q_j \pm \frac{1}{\sigma_j}\frac{\partial}{\partial q_j}\bigg), \tag{25}$$

via transformation $\mathcal{S}^{(-1)} = \exp\{\pm\frac{1}{2}\sum_j \sigma_j^2 q_j^2\}$.

4.2 Complete eigenfunctions

The right normalized eigenfunctions of the number operators $\hat{a}_j^{\dagger}\hat{a}_j$ in configuration space are denoted by $\psi_{\mathbf{n}}^{\beta}(\vec{q}) = \prod_j \psi_{n_j}^{\beta}(q_j)$ where

$$\psi_{n_j}^{\beta}(q_j) = \pi^{-\frac{1}{4}}\sigma_j^{\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}\sigma_j^2 q_j^2}\, \psi_{n_j}(q_j), \tag{26}$$

and the Hermite-Gaussian functions are defined as:

$$\psi_{n_j}(q_j) = \sqrt{\frac{\sigma_j}{\sqrt{\pi}\, 2^{n_j}\, n_j!}}\, \mathrm{e}^{-\frac{1}{2}\sigma_j^2 q_j^2}\, H_{n_j}(\sigma_j q_j), \tag{27}$$

with $H_n(\cdot)$ being the nth Hermite polynomial. The set of eigenfunctions $\psi^{\beta}_{\mathbf{n}}(\vec{q})$ form a complete and orthogonal basis

$$\int_{-\infty}^{\infty} \mathrm{d}\mu(\vec{q})\, \psi^{\beta}_{\mathbf{m}}(\vec{q})\, \psi^{\beta}_{\mathbf{n}}(\vec{q}) = \delta_{\mathbf{m},\mathbf{n}}, \tag{28}$$

where we have introduced the measure $\mathrm{d}\mu(\vec{q}) = \prod_j w_j^{-1}(q_j) dq_j$ with $w_j(q_j) = (\sigma_j/\sqrt{\pi})\exp\{-\sigma_j^2 q_j^2\}$ being the stationary distribution of the process.

In $\vec{q}$ representation, we expand the extended density operator in Liouville–Fock space $\hat{\rho}_w(\vec{q}, t)$ in terms of a complete orthogonal set of basis functions $\{\psi^{\beta}_{\mathbf{n}}(\vec{q})\}$,

$$\hat{\rho}_w(\vec{q}, t) = \sum_{\mathbf{n}} \hat{\rho}_{\mathbf{n}}(t)\psi^{\beta}_{\mathbf{n}}(\vec{q}), \tag{29}$$

where the hat denotes density matrix acting in the subsystem Hilbert space, and $\hat{\rho}_{\mathbf{n}}(t)$ evolves according to the HEOM as Eq. (20). The reduced density operator obtained by integrating over the entire $\vec{q}$-space reads

$$\hat{\rho}_s(t) = \sum_{\mathbf{n}} \hat{\rho}_{\mathbf{n}}(t) \int_{-\infty}^{\infty} \mathrm{d}\vec{q}\, \psi^{\beta}_{\mathbf{n}}(\vec{q}) = \hat{\rho}_{\mathbf{0}}(t). \tag{30}$$

This result is consistent with the vacuum boundary conditions inherent as Eq. (17) in the coherent-state path integral formulation.

However, in practical simulations, the system-bath coupling can shift the equilibrium position of q_j. Larger displacements typically require an increased number of basis functions $\psi^{\beta}_{n_j}(q_j)$ to represent the displaced state with high fidelity, resulting in extended computational resources during propagation of $\hat{\rho}_{\mathbf{n}}(t)$ according to Eq. (20). A way to mitigate this overhead is to switch to the continuous $\vec{q}$-space and to adopt a discrete-variable representation (DVR) [26, 27] with a grid-like structure that captures displaced wave packets more efficiently.

4.3 Fokker–Planck type structure of QD-MESS

Inserting the squeezed ladder operators of Eq. (24) into Eq. (18) yields a hybrid operator-valued diffusion equation of the form

$$\begin{aligned}\dot{\hat{\rho}}_w = &-i[\hat{H}_s, \hat{\rho}_w] + i\sum_{j,k} \mathcal{E}_{jk}\frac{1}{\sigma_j}\frac{\partial}{\partial q_j}\left(\sigma_k q_k + \frac{1}{2\sigma_k}\frac{\partial}{\partial q_k}\right)\hat{\rho}_w + i\sum_j \left(\sqrt{2}\kappa_j^* \sigma_j q_j + \frac{\kappa_j^* - \eta_j'}{\sqrt{2}\sigma_j}\frac{\partial}{\partial q_j}\right)[\hat{s}, \hat{\rho}_w] \\ &- i\sum_j \frac{\eta_j''}{\sqrt{2}\sigma_j}\frac{\partial}{\partial q_j}\{\hat{s}, \hat{\rho}_w\},\end{aligned} \tag{31}$$

where $\hat{\rho}_w \equiv \hat{\rho}_w(\vec{q}, t)$. Before we proceed, let us summarize the structure of the above equation: (i) The first line shows that, in the absence of coupling, the bare subsystem follows the Liouville–von Neumann equation, whereas the Gaussian bath state evolves under a Fokker–Planck operator whose drift and diffusion coefficients are collected in the matrix $\vec{\mathcal{E}}$. (ii) The second and third lines describe the linear system-bath interaction: the subsystem operator $\hat{s}$couples not only to the phase-space coordinate $q_j$but also to its conjugate tangent operator $\partial/\partial q_j$. (iii) If quantum fluctuations of the bath are neglected by setting $\eta'' = 0$ in Eq. (13), the model collapses to a quantum subsystem interacting with a purely classical environment. (iv) Finally, the reduced dynamics of the subsystem is unchanged under any similarity transformation of $\vec{\mathcal{E}}$, $\vec{\kappa}$, $\vec{\eta}'$, and $\vec{\eta}''$ that preserves the relations in Eq. (13) and keeps all $\sigma_j \neq 0$. (v) Coupling these effective modes to the quantum subsystem substantially complicates the joint evolution, see Eq. (31), which is the trade-off for using complex-valued couplings $\vec{\kappa}$, $\vec{\eta}'$, and $\vec{\eta}''$ in Eq. (13) to minimize the effective-mode state space. In what follows, we focus on three Fokker–Planck equations arising from the decompositions [Eq. (13)] that are particularly relevant to quantum optics, condensed-matter physics, and chemical dynamics, derived from this general framework.

5 Quantum Brownian motion equation

The above canonical transformation naturally maps the QD-MESS onto Fokker–Planck type equations for the density operator. By choosing a suitable set of basis functions to decompose the bath correlation function, we recover well-known types of quantum Brownian motion master equations, e.g., extended quantum optical master equation, extended Caldeira–Leggett master equation, and the Smoluchowski-type equation.

5.1 Extended Caldeira–Leggett master equation

We consider a bath with the Brownian-oscillator spectral density [28]

$$J(\omega) = \frac{2\,c^2\gamma\omega}{(\omega^2-\omega_0^2)^2+4\gamma^2\omega^2}, \tag{32}$$

which serves as the effective spectral density for the reaction-coordinate linearly coupling to the Ohmic residual bath [28]. In the high-temperature limit, $\beta|\zeta|\ll 1$ with $\zeta=\sqrt{\omega_0^2-\gamma^2}$, the bath correlation function admits the representation

$$\begin{aligned} C(t\geq 0) &= \frac{c^2}{\beta\omega_0^2}\phi_q(t) + i\frac{c^2}{2\omega_0}\phi_p(t) \\ &= i\vec{\kappa}^\dagger\vec{\mathcal{G}}^R(\tau,\,\tau')(\vec{\eta}'+\vec{\eta}'') \end{aligned} \tag{33}$$

with basis functions $\phi_q(t)=\mathrm{e}^{-\gamma t}[\cos\zeta t+(\gamma/\zeta)\sin\zeta t]$ and $\phi_p(t)=-(\omega_0/\zeta)\,\mathrm{e}^{-\gamma t}\sin\zeta t$ which are equivalent to the position and momentum response of a damped oscillator [24, Sec. 7], respectively. The coefficient matrices in the second line read

$$\vec{\kappa}=\vec{\eta}'=\begin{bmatrix}\frac{c}{\omega_0}\beta^{-\frac{1}{2}}\\ 0\end{bmatrix},\quad \vec{\eta}''=\begin{bmatrix}0\\ -\frac{c}{2}\beta^{\frac{1}{2}}\end{bmatrix},\quad \vec{\mathcal{E}}=i\begin{bmatrix}0 & \omega_0\\ -\omega_0 & -2\gamma\end{bmatrix}.$$

Choosing the scaling factors $\sigma_x=\omega_0(\beta/2)^{\frac{1}{2}}$ and $\sigma_p=(\beta/2)^{\frac{1}{2}}$, Eq. (31) reduces to the Kramers-type Fokker–Planck equation when identifying phase-space variables $\{q_1,\,q_2\}\to\{x,\,p\}$ [28], i.e.

$$\begin{aligned} \dot{\hat{\rho}}_w(x,\,p,\,t) = &-i[H_0,\,\rho_w] + ic\left([\hat{s},\,x\hat{\rho}_w]+\frac{i}{2}\left\{\hat{s},\,\frac{\partial}{\partial p}\hat{\rho}_w\right\}\right) \\ &+\left(\omega_0^2 x\frac{\partial}{\partial p}-p\frac{\partial}{\partial x}+2\gamma\frac{\partial}{\partial p}p+2\gamma T\frac{\partial^2}{\partial p^2}\right)\hat{\rho}_w\,. \end{aligned} \tag{34}$$

This equation describes a quantum subsystem bilinearly coupled to an oscillator subject to friction and Gaussian white noise. In the undamped limit, $\gamma=0$, the equation reduces to the results of Refs. [29, 30].

Defining $\hat{\rho}_w(x,\,p,\,t)$ as the partial Wigner transformation for $\hat{\rho}(t)$ via

$$\hat{\rho}_w(x,\,p,\,t)=\int \mathrm{d}y\,\mathrm{e}^{ipy}\langle x-y/2|\hat{\rho}(t)|x+y/2\rangle \tag{35}$$

an inverse partial Wigner transformation maps Eq. (34) to a type of Caldeira–Leggett master equation [28, 31] of an embedded system:

$$\dot{\hat{\rho}}(t) = -i[\hat{H}_0,\,\hat{\rho}] - i\gamma[\hat{x},\,\{\hat{p},\,\hat{\rho}\}] - 2\gamma T[\hat{x},\,[\hat{x},\,\hat{\rho}]]\,. \tag{36}$$

Here, the extended state space Hamiltonian is obtained as

$$\hat{H}_0 = \hat{H}_s + \frac{1}{2}(\hat{p}^2+\omega_0^2\hat{x}^2) - c\hat{s}\hat{x}. \tag{37}$$

5.2 Extended quantum optical master equation

The Brownian-oscillator spectral density can be decomposed into two Lorentzian contributions:

$$J(\omega) = \frac{1}{2\zeta}\left[\frac{\gamma\, c^2}{(\omega-\zeta)^2+\gamma^2} - \frac{\gamma\, c^2}{(\omega+\zeta)^2+\gamma^2}\right] \equiv J_+(\omega) - J_-(\omega). \tag{38}$$

In the strongly underdamped regime ($\omega_0 \gg \gamma$), when the Lorentzian distributions are sufficiently narrow ($\gamma \ll \zeta$), then $J_+(\omega) = J_-(-\omega) \approx 0$ for $\omega < 0$, and one may approximate

$$J(\omega) \approx J_+(\omega) = \frac{\gamma\, g^2}{(\omega-\zeta)^2+\gamma^2}, \quad g^2 = \frac{c^2}{2\,\zeta}. \tag{39}$$

This Lorentzian noise spectrum is commonly employed to model a single quantized mode of the electromagnetic field in a cavity [32–38], where ζ denotes the cavity-mode resonance frequency and γ its linewidth, corresponding to the photon-leakage rate through the cavity mirrors. Although $J_+(\omega)$ is, strictly speaking, not an odd function in ω as it should be, the negative frequency part is assumed to be negligible in this parameter domain. In the low-temperature limit, where thermal broadening is negligible compared to γ ($\beta\zeta \gg \beta\gamma \gg 1$), one has $\coth(\beta\zeta/2) \approx 1$, so that the power noise spectrum reduces to

$$S_\beta(\omega) \approx J_+(\omega). \tag{40}$$

The corresponding correlation function in Green's function representation reads

$$C(t \geq 0) = g^2 \mathrm{e}^{-i(\zeta - i\gamma)t} \tag{41}$$

$$= i\,\vec{\kappa}^\dagger\, \vec{\mathcal{G}}^R(\tau)\,(\vec{\eta}' + \vec{\eta}''), \tag{42}$$

where matrices

$$\vec{\kappa} = \vec{\eta}' = \begin{bmatrix} g \\ 0 \end{bmatrix}, \quad \vec{\eta}'' = \begin{bmatrix} 0 \\ -ig \end{bmatrix}, \quad \vec{\mathcal{E}} = -i\begin{bmatrix} \gamma & -\zeta \\ \zeta & \gamma \end{bmatrix}.$$

We choose the scaling factors $\sigma_x = \zeta^{\frac{1}{2}}$ and $\sigma_p = \zeta^{-\frac{1}{2}}$. Equation (31) then maps to

$$\dot{\hat{\rho}}_w(x,\, p;t) = -i[\hat{H}_s,\, \hat{\rho}_w] - ic([\hat{s},\, x\hat{\rho}_w] + \frac{i}{2}\{\hat{s},\, \partial_p\hat{\rho}_w\}) + (\zeta^2 x\partial_p - p\partial_x)\hat{\rho}_w + \gamma(\partial_x x + \partial_p p)\hat{\rho}_w + \frac{\gamma}{2}(\zeta\partial_p^2 + \frac{1}{\zeta}\partial_x^2)\hat{\rho}_w. \tag{43}$$

This equation describes a quantum subsystem coupled to a harmonic oscillator in the low temperature limit where the latter experiences friction and stochastic Gaussian noise through position and momentum.

Performing the inverse partial Wigner transformation for the harmonic part, we arrive at the quantum optical master equation for an embedded system in Hilbert space

$$\partial_t\hat{\rho}(t) = -i[\hat{H}_0,\, \hat{\rho}] - \frac{i\gamma}{2}([\hat{x},\, \{\hat{p},\, \hat{\rho}\}] - [\hat{p},\, \{\hat{x},\, \hat{\rho}\}]) - \frac{\gamma}{2}(\zeta[\hat{x},\, [\hat{x},\, \hat{\rho}]] + \frac{1}{\zeta}[\hat{p},\, [\hat{p},\, \hat{\rho}]]), \tag{44}$$

where the embedded system Hamiltonian reads

$$\hat{H}_0 = \hat{H}_s + \frac{1}{2}(\hat{p}^2 + \zeta^2\hat{x}^2) - c\,\hat{s}\hat{x}. \tag{45}$$

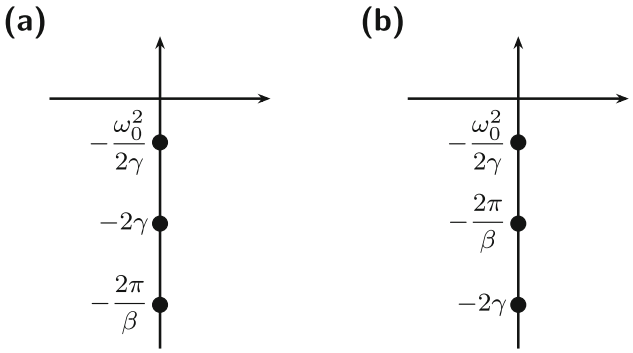

Fig. 1 Smoluchowski range $2\gamma/\omega_0^2 \gg \beta/2\pi,\ 1/\gamma$ comprises two particular subsets: **a** one is the known classical range $\gamma \ll 2\pi/\beta$; **b** the other is a quantum mechanical region with $\gamma \gg 2\pi/\beta$

5.3 Smoluchowski-type description

The strong friction limit, commonly referred to as the Smoluchowski limit [3, 39–42], is characterized by a distinct separation of timescales: rapid equilibration of momentum compared to the slower equilibration of position. This separation enables the adiabatic elimination of momentum from the phase-space Fokker–Planck equation, resulting in a simplified time evolution equation for the position distribution, known as the Smoluchowski equation. In this regime, the environment-induced linewidth significantly exceeds both the bare line separation and thermal excitation, and the dynamics of the harmonic oscillator system exhibit nearly classical behavior, but quantum fluctuations still play a crucial role.

In the strong friction limit $\gamma \gg \omega_0$, the bath correlation function for the spectral density in Eq. (32) at inverse temperature β can be approximated as:

$$C(t) \approx d_+ \mathrm{e}^{-\frac{\omega_0^2}{2\gamma}t} + d_- \mathrm{e}^{-2\gamma t} + \sum_{k=1}^{\infty} d_k \, \mathrm{e}^{-\nu_k t}, \tag{46}$$

with Matsubara frequencies $\nu_k = 2\pi k/\beta$ and

$$d_\pm = \frac{c^2}{4\zeta}\left[\coth\frac{\beta(\zeta \mp i\gamma)}{2} \pm 1\right], \tag{47a}$$

$$d_k = -\frac{4\,c^2\gamma}{\beta}\frac{\nu_k}{(\omega_0^2+\nu_k^2)^2 - 4\gamma^2\nu_k^2}. \tag{47b}$$

The quantum Smoluchowski range $2\gamma/\omega_0^2 \gg \beta/2\pi,\ 1/2\gamma$ comprises two particular scales: one is the known classical time scale separation $\gamma/\omega_0 \gg 1$, the other is a quantum mechanical separation $2\gamma/\omega_0^2 \gg \beta/2\pi$ [40–43].

At sufficiently elevated temperatures $\beta \ll 2\gamma/\omega_0^2$, cf. Fig. 1a, the position and momentum response function in Eq. (33) can be approximated under a coarse-grained timescale $t \geq 2\gamma/\omega_0^2 \gg \beta,\ \gamma^{-1}$ as

$$\phi_p(t) \approx -\frac{\omega_0}{2\gamma}\exp\left\{-\frac{\omega_0^2}{2\gamma}t\right\} \tag{48a}$$

$$\phi_q(t) \approx \exp\left\{-\frac{\omega_0^2}{2\gamma}t\right\}. \tag{48b}$$

The bath correlation function Eq. (33) then turns into

$$C(t \geq 0) = \left(\frac{c^2}{\beta\omega_0^2} - i\frac{c^2}{4\gamma}\right)\mathrm{e}^{-\frac{\omega_0^2}{2\gamma}t} = i\kappa^\dagger \mathcal{G}^R(\tau,\tau')(\eta' + \eta'') \tag{49}$$

with $\kappa = \eta' = c/\omega_0\sqrt{\beta}$, $\eta'' = -i\omega_0 c\sqrt{\beta}/4\gamma$, and $\mathcal{E} = -i\omega_0^2/2\gamma$, and a scaling factor $\sigma_x = -\omega_0\sqrt{\beta/2}$. This leads to a classical Smoluchowski equation [4, 28, 43–45] for the extended mode so that the time evolution of the embedded density reads

$$\dot{\hat{\rho}}_{\mathrm{S}}(x;t) = -i[\hat{H}_s,\, \hat{\rho}_{\mathrm{S}}] - ic[\hat{s},\, x\hat{\rho}_{\mathrm{S}}] + \frac{c}{4\gamma}\left\{\hat{s},\, \frac{\partial}{\partial x}\hat{\rho}_{\mathrm{S}}\right\} + \frac{\omega_0^2}{2\gamma}\frac{\partial}{\partial x}\left(x + \frac{1}{\beta\omega_0^2}\frac{\partial}{\partial x}\right)\hat{\rho}_{\mathrm{S}}. \tag{50}$$

In the quantum Smoluchowski regime, $2\gamma/\omega_0^2 \gg \beta/2\pi \gg 1/2\gamma$, cf. Fig. 1b, the bath correlation function is approximated as

$$C(t) \approx \left(\frac{c^2}{\beta\omega_0^2} - i\frac{c^2}{4\gamma}\right) \mathrm{e}^{-\frac{\omega_0^2}{2\gamma}t} + d_1\, \mathrm{e}^{-\nu_1 t} \tag{51}$$

keeping the leading-order contribution from the Matsubara sum. The dynamics of the mode then follow a quantum Smoluchowski dynamics so that in the extended state one arrives at

$$\begin{aligned}\dot{\hat{\rho}}_{\mathrm{qS}} = &-i[\hat{H}_s,\, \hat{\rho}_{\mathrm{qS}}] - ic[\hat{s},\, x\hat{\rho}_{\mathrm{qS}}] + \frac{c}{4\gamma}\left\{\hat{s},\, \frac{\partial}{\partial x}\hat{\rho}_{\mathrm{qS}}\right\} \\ &+ \frac{\omega_0^2}{2\gamma}\frac{\partial}{\partial x}\left(x + \frac{1}{\beta\omega_0^2}\frac{\partial}{\partial x}\right)\hat{\rho}_{\mathrm{qS}} + \nu_1\frac{\partial}{\partial q_1}\left(q_1 + \frac{1}{2}\frac{\partial}{\partial q_1}\right)\hat{\rho}_{\mathrm{qS}} + i\sqrt{2d_1}[\hat{s},\, q_1\hat{\rho}_{\mathrm{qS}}].\end{aligned} \tag{52}$$

In case of a two-level subsystem, such as a model of donor-acceptor electron transfer in a Debye solvent at high temperatures, the above equation reduces to the Zusman equation [4, 28, 44, 45]. In the low-temperature regime, however, generalized Zusman equations have been derived by [40, 43, 46, 47], capturing the effects of quantum fluctuations more accurately.

6 Summary

We have presented a constructive decomposition of the Gaussian bath correlation function $C(t)$ into a minimal set of single-particle Green's functions, thereby mapping a Gaussian reservoir onto an equally minimal ensemble of effective harmonic modes that exactly reproduces the bath two-point statistics. Applying a Hubbard–Stratonovich transformation to the Feynman–Vernon influence functional yields a time-local, nonperturbative formulation of quantum dissipation in a minimally extended state space (QD-MESS). For both computational efficiency and a transparent quantum-classical correspondence, we developed QD-MESS in complementary Fock-space and Wigner phase-space representations.

To demonstrate the versatility of the phase-space QD-MESS approach, we introduced squeezed-mode operators and showed how appropriate decompositions of $C(t)$ recover several well-known quantum Brownian-motion master equations for embedded systems: an extended quantum-optical master equation, an extended Caldeira–Leggett equation, and a quantum Smoluchowski-type equation. This unified framework naturally yields Wigner-space Fokker–Planck equations and enables classical partial differential equation methods to propagate open-system dynamics.

Under strong system-bath coupling, the auxiliary modes are effectively displaced from equilibrium, which increases the required local basis and enforces smaller time steps; this can dominate the computational cost. A promising direction is the design of adaptive basis strategies, especially in the strong-coupling regime, to optimize QD-MESS propagation while preserving accuracy with minimal overhead.

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