

Embedding memory in coarse-grained Hamiltonian systems

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Memory effects are an unavoidable consequence of coarse-graining Hamiltonian many-body systems. Although Markovian embeddings with auxiliary variables are widely used to approximate such dynamics, their consistency with the exact projected microscopic evolution is rarely examined. Here, we analyze this consistency problem at the structural level. Starting from a general Markovian Fokker-Planck equation defined on an extended state space comprising coarse-grained variables and auxiliary degrees of freedom, we derive the exact non-Markovian evolution governing the marginal probability of the coarse-grained variables. We then identify the conditions under which this marginal equation reproduces the structural form of the generalized Fokker-Planck equation obtained from Zwanzig's projection formalism. These conditions follow from microscopic Hamiltonian dynamics and constrain the admissible form of Markovian embeddings, ensuring consistency with equilibrium structure, conservation laws, positivity, and microscopic reversibility. The resulting framework provides a systematic route for constructing microscopically consistent Markovian representations of non-Markovian coarse-grained dynamics. We illustrate the approach in coarse-grained particle models, ranging from isothermal dynamics to fully energy-conserving nonisothermal formulations.

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I. INTRODUCTION

Memory effects are a defining and unavoidable consequence of coarse graining. Whenever a high-dimensional Hamiltonian system is reduced to a closed description in terms of a limited set of coarse-grained (CG) variables, the resulting dynamics generically depends on the past history of those variables [1–3]. Representative examples include diffusion in liquid water [4] and methanol [5], dihedral dynamics of butane molecules [6], barrier crossing and rare-event dynamics [7–9], clusters of Lennard-Jones particles [10], star polymers [1,11,12], protein folding [13], crystalline solids [14], graphene [15], and passive microrheology [16]. In all these cases, effective dynamics cannot be described solely in terms of instantaneous state variables.

This structural non-Markovianity is formalized by the Mori-Zwanzig projection framework [17–19], which yields an *exact* generalized Fokker-Planck equation (GFPE) and an associated generalized Langevin equation (GLE) for the CG dynamics. Closure comes at the price of temporal nonlocality: The evolution involves memory kernels fully determined by the underlying microscopic Hamiltonian dynamics.

Despite this structural non-Markovianity, practical modeling and simulation frequently rely on *Markovian* descriptions. A common strategy is to augment the state space with auxil-

iary variables and construct a Markovian embedding whose marginal dynamics reproduces the observed memory. In most existing approaches, however, the embedding is introduced as a modeling ansatz, and its connection to the exact projected microscopic dynamics remains largely implicit.

This widespread practice raises a fundamental structural question: Under what conditions can a Markovian embedding faithfully reproduce the form of the exact projected dynamics? If the projected GFPE is fixed by microscopic Hamiltonian mechanics, then not every Markovian extension can be admissible. Consistency with microscopic reversibility, positivity, and equilibrium structure must impose nontrivial constraints on the drift and diffusion operators of the embedded dynamics. Clarifying these constraints is the central goal of this work.

Although the GFPE is formally exact, it is rarely usable in practice, as its evaluation requires the computation of projected microscopic dynamics [20] and high-dimensional conditional expectations, making direct implementation computationally challenging. Numerous approximation strategies have therefore been developed [1,3,21,22], including orthogonal-dynamics reconstruction [20,23–25], deconvolution approaches [9,10,26,27], and various embedding-based methods.

The idea of Markovian embedding itself has a long pedigree. A contraction of a Markovian stochastic differential equation (SDE) naturally produces non-Markovian dynamics [28,29]. The argument can be reversed: Suitably chosen auxiliary variables can convert non-Markovian dynamics into a Markovian process. Following Mori's original construction [18], this idea has been explored extensively [5,15,30–37]. Model coefficients are often related to static equilibrium quantities [15,18,33,34] or tuned to reproduce velocity

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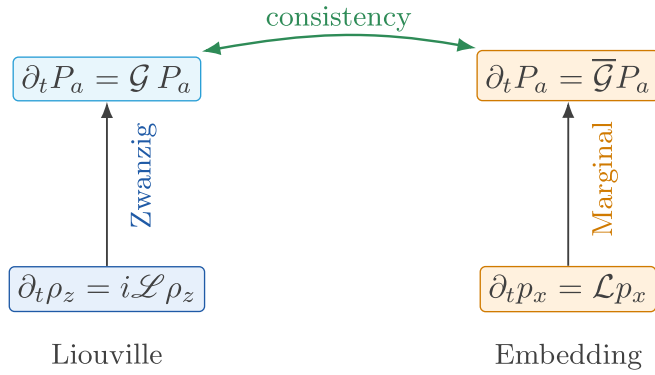


FIG. 1. Schematic roadmap: Two complementary routes to the GFPE. Zwanzig projection of the Liouville equation yields a microscopic partial-integro-differential operator $\mathcal{G}$, while marginalization of a Markovian embedding produces another operator $\bar{\mathcal{G}}$. Consistency requires $\bar{\mathcal{G}} \simeq \mathcal{G}$, which constrains the admissible form of the embedding.

autocorrelation functions [35,36]; likelihood-based estimation has been studied [38,39], data-driven auxiliary discovery is emerging [40], and efficient numerical integrators for GLEs have been developed [14,25,41,42]. On the mathematical side, finite-dimensional Markovian embeddings represent exactly only a restricted class of memory kernels, typically finite sums of exponentially damped modes and their oscillatory generalizations. For such kernels, properties such as ergodicity and convergence to equilibrium can be analyzed rigorously [43]. More general memory laws arise, for example, in Kac-Zwanzig heat-bath models [30], where suitable limits lead to power-law kernels. Power-law memory also appears naturally in fractional Langevin dynamics, where fluctuation-dissipation balance relates Caputo-type friction to fractional Brownian noise [44]. In general, the long-time diffusive behavior of a GLE is controlled by the tail of the memory kernel: Integrable kernels lead to normal diffusion, whereas power-law kernels may produce anomalous subdiffusion [45]. Direct simulation of GLEs with prescribed memory kernels is possible in important special cases, such as linear GLEs with Gaussian noise [22] or models with state-independent kernels [9]. The present work addresses the structurally richer case of state-dependent memory. Its purpose is not to provide an exact finite-dimensional realization of arbitrary kernels, but to derive the constraints that Markovian embeddings must satisfy in order to remain compatible with the microscopic Hamiltonian structure. Although any finite embedding generates only a restricted class of kernels, increasingly general memory laws may be approximated by enlarging the auxiliary space [30].

In this work, we formulate a general Markovian Fokker-Planck equation on an extended state space comprising the CG variables and auxiliary degrees of freedom. By eliminating the auxiliary variables, we derive the exact non-Markovian evolution equation governing the marginal probability of the CG variables. We then identify the precise conditions under which this marginal equation reproduces the structural form of the Zwanzig GFPE derived directly from the Liouville equation (Fig. 1). These conditions are not modeling assumptions but necessary consequences of underlying microscopic

Hamiltonian dynamics. While they do not uniquely determine the embedding FPE, they significantly constrain its admissible form. The remaining modeling choices are selected to maximize simplicity and computational tractability of the auxiliary dynamics.

A central outcome of our analysis is a sharp separation between quantities that are microscopically fixed and those that remain genuine modeling degrees of freedom. We show that the equilibrium distribution, the reversible drift, and the covariance structure coupling CG and auxiliary variables are completely determined by static conditional expectations of microscopic observables. Once these constraints are enforced, the remaining freedom resides in a relaxation matrix acting in the auxiliary sector, which may be tuned to reproduce dynamical information without violating microscopic consistency.

We illustrate the general methodology in two broad classes of CG particle models. First, for isothermal non-Markovian dissipative particle dynamics (DPD) systems, we recover recent results on fully nonlinear, state-dependent memory kernels proposed by Lei and coworkers [11,46]. Second, we formulate a non-Markovian, nonisothermal, energy-conserving DPD model that demonstrates the full scope of the approach, highlighting its capacity to systematically enforce thermodynamic consistency beyond the isothermal regime.

The paper is organized as follows. Section II reviews the exact projected GFPE obtained by Zwanzig and its structural microscopic constraints. Section III derives the marginal dynamics generated by a general Markovian embedding. Section IV establishes the consistency conditions linking the two constructions. Section V discusses admissible modeling simplifications, and Secs. VI and VII illustrate the framework in isothermal and nonisothermal CG particle models, respectively. We conclude in Sec. VIII.

II. ZWANZIG'S NON-MARKOVIAN CG DYNAMICS

Much of the literature on non-Markovian coarse-grained dynamics relies on the Mori projector [18], which produces linear evolution equations with state-independent memory kernels that are, in principle, simpler to approximate. In contrast, the Zwanzig projector [17] yields fully nonlinear dynamics. It is common practice to employ nonlinear drift terms—that capture potential of mean forces—together with linear state-independent memory kernels [6,7,30,31,33,35,36], a combination that has been shown to be structurally inconsistent in general [2,47–49]. Hybrid constructions combining both projectors have also been proposed [24]. A central advantage of the Zwanzig formulation is that when dynamical invariants are treated explicitly, the resulting Markovian approximation leads to a fully and explicit *thermodynamically consistent* description, known as the GENERIC framework [50,51]. For these structural reasons, the present work adopts the Zwanzig GFPE as the reference microscopic formulation.

In this section, we concentrate on the left column of the road map shown in Fig. 1. To streamline the notation, we write $P_a(t)$ for the probability density that the set of n CG variables $\hat{A}(z) \in \mathbb{R}^n$, defined on phase space $z \in \mathbb{R}^{6N}$, takes the value a at time t . Throughout, we adopt the convention that function arguments are indicated by subscripts, and we

use circumflexes to denote phase-space functions. The density $P_a(t)$ is the pushforward of the microscopic distribution under the mapping $z \mapsto \hat{A}(z)$:

$$P_a(t) = \int dz \rho_t(z) \delta(\hat{A}(z) - a), \quad (1)$$

where $\rho_t(z)$ is the solution of the Liouville equation $\partial_t \rho_t = i\mathcal{L}\rho_t$ with initial condition $\rho_0(z)$, and the integral is over the phase space. Here, the microstate z is the collection of positions and momenta of all atoms in the system. The time evolution of the probability density $P_a(t)$ associated with a set of coarse-grained variables is, in general, non-Markovian. The *exact* GFPE originally derived by Zwanzig [17,19,29] can be cast in the form

$$\partial_t P_a(t) = \mathcal{G}P_a(t), \quad (2)$$

where $\mathcal{G}$ is an integro-differential operator. Explicitly,

$$\begin{aligned} \partial_t P_a(t) = & -\partial_a^\top \cdot V_a P_a(t) \\ & + k_B \partial_a^\top \cdot \int_0^t dt' \int da' P_a^{\text{eq}} D_{aa'}(t-t') \cdot \partial_{a'} \frac{P_{a'}(t')}{P_a^{\text{eq}}}, \end{aligned} \quad (3)$$

where ∂_a denotes the partial derivative with respect to a , understood to act on all functions to its right. The superscript $\top$ denotes transpose, in such a way that $a^\top \cdot b$ is the scalar product of the two vectors a, b , while $a \cdot b^\top$ denotes the dyadic tensor. We present a derivation of Zwanzig GFPE in Appendix A, as a particular case of the general projection given in Ref. [52].

The only assumption used in deriving this GFPE is that the initial ensemble $\rho_0(z)$ is of the relevant form [17,19,53]

$$\rho_0(z) = \frac{1}{P_a^{\text{eq}}} \rho^{\text{eq}}(z) \delta(\hat{A}(z) - a), \quad (4)$$

where the equilibrium probability of macrostate a is

$$P_a^{\text{eq}} = \int dz \rho^{\text{eq}}(z) \delta(\hat{A}(z) - a). \quad (5)$$

The initial ensemble [Eq. (4)] reflects the statistical assumption that initially the macrostate is a and that all microstates corresponding to this initial macrostate are equiprobable.

The building blocks of the GFPE are the equilibrium probability P_a^{eq} , the drift V_a , and memory kernel $D_{aa'}(t)$. The drift is defined in microscopic terms as the conditional expectation of the action of the Liouville operator $i\mathcal{L}$ on the CG variables, i.e.,

$$V_a = \langle i\mathcal{L}\hat{A} \rangle^a = \frac{1}{P_a^{\text{eq}}} \int dz \rho^{\text{eq}}(z) \delta(\hat{A}(z) - a) i\mathcal{L}\hat{A}(z). \quad (6)$$

The microscopic definition of the memory kernel is

$$D_{aa'}(t-t') = \frac{P_a^{\text{eq}}}{k_B} \int dz \rho^{\text{eq}}(z) \hat{F}_a(z, t) \hat{F}_{a'}^\top(z, t'), \quad (7)$$

where the “projected force” is the following phase function:

$$\hat{F}_a(z, t) = e^{Q^Z i\mathcal{L}t} \left[\frac{\delta(\hat{A}(z) - a)}{P_a^{\text{eq}}} (i\mathcal{L}\hat{A}(z) - V_a) \right], \quad (8)$$

where Q^Z is Zwanzig’s projector [17,19].

For a mixing Hamiltonian system, the equilibrium measure depends on the microstate through the Hamiltonian of the system and, when appropriate, through additional dynamical invariants such as total linear or angular momentum [53]. In this way,

$$\rho^{\text{eq}}(z) = \Phi(\hat{H}(z)). \quad (9)$$

The function $\Phi(E)$ is fully determined by the probability distribution $P_0(E)$ of the energy at the initial time [53]:

$$\Phi(E) = \frac{P_0(E)}{\Omega_B(E)}, \quad (10)$$

where the measure of the energy shell

$$\Omega_B(E) = \int dz \delta(\hat{H}(z) - E) \quad (11)$$

ensures the proper normalization of the equilibrium ensemble. The function $\Phi(E)$ takes an exponential form for the canonical ensemble or a Dirac delta form for the microcanonical ensemble.

When the Hamiltonian can be expressed in terms of the rest of CG variables via a coarse-grained energy function $E(a)$ [50], namely,

$$\hat{H}(z) = E(\hat{A}(z)), \quad (12)$$

then a number of simplifications occur. The equilibrium distribution function P_a^{eq} takes the form

$$P_a^{\text{eq}} = \frac{P_0(E_a)}{\Omega(E_a)} e^{S_a/k_B}, \quad (13)$$

where the entropy is

$$S_a = k_B \ln \Omega_a, \quad (14)$$

where k_B is Boltzmann’s constant and the measure of the submanifold of constant CG variables is

$$\Omega_a = \int dz \delta(\hat{A}(z) - a). \quad (15)$$

Under the assumption (12), the drift [Eq. (6)] and the memory kernel [Eq. (7)] simplify, as cancellations between numerator and denominator amount to replacing $\rho^{\text{eq}}(z) \rightarrow 1$ and $P_a^{\text{eq}} \rightarrow \Omega_a$.

The assumption (12) entails no loss of generality: If the chosen set of coarse-grained variables $\hat{A}(z)$ does not allow for such a representation, the Hamiltonian itself should be included among the coarse-grained variables. When the Hamiltonian is included explicitly, the resulting reduced description is typically isothermal. Conversely, when the Hamiltonian is not included as a CG variable because the rest of CG variables already satisfy Eq. (12), the reduced dynamics can describe nonisothermal situation where energy is transported. In either case, this construction allows us to account explicitly for energy conservation, an aspect that is not explicitly addressed in Zwanzig’s original formulation but is fully incorporated in the GENERIC framework [51].

A. Properties of the building blocks

A number of properties arise from the fact that energy (and other dynamic invariants) is conserved by the dynamics,

implying

$$0 = i\mathcal{L}\hat{H}(z) \stackrel{(12)}{=} i\mathcal{L}\hat{A}(z) \cdot \partial_a E(\hat{A}(z)). \quad (16)$$

It is straightforward to show that, as a consequence, we have

$$\boxed{V_a^\top \cdot \partial_a E_a = 0}, \quad (17)$$

$$\boxed{D_{aa'}(t - t') \cdot \partial_a E_a = 0}. \quad (18)$$

These constraints ensure that the GFPE is consistent with energy conservation, as they imply invariance of the energy probability distribution,

$$\partial_t P_t(E) = 0, \quad P_t(E) = \int da P_a(t) \delta(E(a) - E). \quad (19)$$

Accordingly, the dynamics preserves the probability assigned to each energy shell.

In isothermal descriptions, where the microscopic Hamiltonian $\hat{H}(z)$ is included among the coarse-grained variables and fixed to a prescribed numerical value E [so that $E(a) = E$], the constraints (17) and (18) become trivial. The energy components of both the drift and diffusion vanish identically, and energy conservation is trivially accomplished. In contrast, in nonisothermal situations energy conservation is nontrivial and imposes stringent structural constraints on both the drift and the memory kernel, significantly restricting their admissible form.

Observe that the reversible drift [Eq. (6)] satisfies

$$\partial_a^\top \cdot V_a \Omega_a = 0, \quad (20)$$

which in terms of the coarse-grained entropy [Eq. (14)] reads

$$\boxed{V_a^\top \cdot \partial_a S_a + k_B \partial_a^\top \cdot V_a = 0}, \quad (21)$$

and leads to one of the degeneracy conditions of the GENERIC framework [51]. Together with energy conservation [Eq. (17)], Eq. (20) ensures that

$$\partial_a^\top \cdot V_a P_a^{\text{eq}} = 0, \quad (22)$$

so that P_a^{eq} is a stationary solution of the GFPE (3). The reversibility condition (21) constitutes a structural constraint that any admissible model for the drift V_a and entropy S_a must satisfy.

Observe that when $t = t'$ the kernel takes the diagonal form in the a, a' space:

$$D_{aa'}(0) = \delta_{aa'} \Gamma_a, \quad (23)$$

where the *kinetic matrix* Γ_a ,

$$\boxed{\Gamma_a \equiv \frac{1}{k_B} \langle [i\mathcal{L}\hat{A} - V_a][i\mathcal{L}\hat{A} - V_a]^\top \rangle^a \geq 0}, \quad (24)$$

is the covariance of the fluctuations of time derivatives of the CG variable. As such, it is manifestly symmetric and positive semidefinite. The semiproperty arises because the energy conservation identity [Eq. (16)] implies in Eq. (24) that

$$\Gamma_a \cdot \partial_a E_a = 0, \quad (25)$$

showing that the null space of Γ_a is not empty.

Any respectable model for S_a , V_a , $D_{aa'}(t)$ should satisfy the microscopic constraints (17), (18), (21), and (24).

Time reversibility and detailed balance give rise to additional properties, which are discussed in Appendix B.

B. Exact GLE

By using Zwanzig's projector, it is possible to obtain an exact projected equation for the phase functions $\hat{A}(z_t)$ along the Hamiltonian trajectory z_t . This equation may be written as [54,55]

$$\begin{aligned} \frac{d}{dt} \hat{A}(z_t) = & V(\hat{A}(z_t)) + \int_0^t du D(\hat{A}(z_u); t - u) \cdot \partial_a S(\hat{A}(z_u)) \\ & + k_B \int_0^t du \partial_a \cdot D(\hat{A}(z_u); t - u) + \hat{F}(t), \end{aligned} \quad (26)$$

where the tensor notation is schematic and the precise index structure is fixed by the corresponding GFPE. The projected force is, in standard compact notation,

$$\hat{F}(t) = \exp\{Q i \mathcal{L} t\} Q i \mathcal{L} \hat{A}. \quad (27)$$

The associated memory tensor is given by a conditional projected-force correlation,

$$D(a; t) = \frac{1}{k_B} \langle \hat{F}(t) \hat{F}(0)^T \rangle^a, \quad (28)$$

where $\langle \dots \rangle^a$ denotes an equilibrium conditional average at fixed value $\hat{A}(z) = a$.

The phase function $\hat{F}(t)$ is usually termed the random force, although at this stage it is a time-dependent phase function: The only stochastic ingredient is the sampling of the initial condition z_0 from the relevant ensemble. We may refer to Eq. (26) as a *mechanistic* GLE, to distinguish it from a stochastic GLE for the numerical values a_t of the CG variables $\hat{A}(z)$,

$$\begin{aligned} \frac{d}{dt} a_t = & V(a_t) + \int_0^t du D(a_u; t - u) \cdot \partial_a S(a_u) \\ & + k_B \int_0^t du \partial_a \cdot D(a_u; t - u) + \tilde{F}(t), \end{aligned} \quad (29)$$

where, in analogy with Eq. (28), one may impose the two-time fluctuation-dissipation relation

$$D(a; t) = \frac{1}{k_B} \langle \tilde{F}(t) \tilde{F}(0)^T \rangle^{a_0=a}. \quad (30)$$

Here, $\langle \dots \rangle^{a_0=a}$ denotes an average over realizations of the stochastic process initialized with $a_0 = a$. This conditional notation is essential: An unconditional average over realizations would not, in general, retain the state dependence of the kernel $D(a; t)$.

Equation (30) specifies only a two-time covariance. It therefore does not determine the full stochastic law of the fluctuating force unless additional assumptions are made. In particular, a general non-Markovian stochastic process is specified by a consistent hierarchy of multitime joint probability distributions. If the force is assumed to be Gaussian, this hierarchy is fixed by its mean and two-time covariance, and Eq. (30) is sufficient to determine its law. Without the Gaussian assumption, higher-order and multitime correlations remain part of the stochastic specification. Replacing the projected force by Gaussian colored noise with covariance

fixed by Eq. (30) is a questionable modeling approximation that does not derive from the projection formalism itself [23,26,54].

Many existing approaches start from a GLE of the form in Eq. (29) and introduce auxiliary variables to represent the memory term through Markovian dynamics in an enlarged state space. In Appendix D, we discuss the induced GLE obtained directly from an embedded SDE. When the memory is state dependent, this GLE is a nontrivial stochastic object, with multiplicative, history-dependent noise, which provides an additional motivation for imposing the consistency requirements at the GFPE level. This GFPE route avoids postulating a complete stochastic law for the colored force.

III. FROM MARKOVIAN EMBEDDING TO NON-MARKOVIAN MARGINALS

In this section, we show how a non-Markovian description emerges upon marginalization of a Markovian embedding. This corresponds to the right column of the road map in Fig. 1. We consider a set of n coarse-grained variables a . We introduce a set of m auxiliary variables b and the space $x = (a, b) \in \mathbb{R}^{n+m}$ will be referred to as the *enlarged or embedding CG space*. We introduce a joint probability distribution $p_{ab}(t)$ in this enlarged space such that its marginal over b reproduces the correct probability $P_a(t)$ of CG variables,

$$\int db p_{ab}(t) = P_a(t). \quad (31)$$

Here, lowercase $p_{ab}(t)$ denotes the probability density in the extended (detailed) space, while uppercase $P_a(t)$ denotes the probability of CG variables. We seek to construct an FPE in the embedded space governing the joint probability $p_{ab}(t)$ such that the induced closed evolution for the marginal $P_a(t)$ reproduces, as closely as possible, the GFPE (3) and satisfies the boxed microscopic identities in Sec II.

The general form of the FPE for the joint probability is

$$\partial_t p(t) = \mathcal{L}p(t), \quad (32)$$

where $\mathcal{L}$ is the Fokker-Planck second-order differential operator acting on functions in the enlarged space. This operator has the most general form

$$\mathcal{L} = -\partial_x^\top \cdot \mathbf{v} + \partial_x^\top \cdot \mathbf{d} \cdot \partial_x, \quad (33)$$

where the partial differential operators $\partial_x = (\partial_a, \partial_b)$ act on everything to its right. Note the placing of the diffusion matrix $\mathbf{d}$ in between partial derivatives. No particular requirement on the symmetry of $\mathbf{d}$ is imposed, and a skew-symmetric contribution may be valuable for modeling purposes. However, the symmetric part of $\mathbf{d}$ should be a positive semidefinite matrix to get a stable equilibrium solution p_{ab}^{eq} that satisfies

$$\mathcal{L}p_{ab}^{\text{eq}} = 0. \quad (34)$$

The Fokker-Planck operator satisfies

$$\int dadb \mathcal{L}f_{ab} = 0 \quad (35)$$

for arbitrary functions f_{ab} , under the assumption that boundary terms vanish.

Making explicit the two sectors in the embedding space corresponding to CG and auxiliary variables, respectively, the drift and diffusion have the block form

$$\mathbf{v} = \begin{pmatrix} \mathbf{A} \\ \mathbf{B} \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \mathbf{C} & \mathbf{E} \\ \mathbf{F} & \mathbf{H} \end{pmatrix}. \quad (36)$$

In terms of these blocks, the explicit form of the FPE (32) with the operator [Eq. (33)] is

$$\begin{aligned} \partial_t p(t) = & -\partial_a^\top \cdot \mathbf{A}p(t) - \partial_b \cdot \mathbf{B}p(t) \\ & + \partial_a^\top \cdot \mathbf{C} \cdot \partial_a p(t) + \partial_a^\top \cdot \mathbf{E} \cdot \partial_b p(t) \\ & + \partial_b^\top \cdot \mathbf{F} \cdot \partial_a p(t) + \partial_b^\top \cdot \mathbf{H} \cdot \partial_b p(t). \end{aligned} \quad (37)$$

The ultimate objective is to identify suitable expressions for the blocks $\mathbf{A}$ – $\mathbf{H}$. These blocks depend in general on both sets of variables a and b but this dependence is suppressed to keep the notation uncluttered.

Starting from the Fokker-Planck equation (37) defined in the enlarged state space (a, b) , our goal is to derive a closed evolution equation for the marginal probability $P_a(t)$. To this end, we specialize in Appendix A the general results of Refs. [52,56], where the GFPE for the probability of *arbitrary* CG variables is obtained from a more detailed FPE. In the present case, the selected CG variables are just a subset of the whole set of variables. The result is the following *exact* GFPE for $P_a(t)$:

$$\begin{aligned} \partial_t P_a(t) = & -\partial_a^\top \cdot \bar{\mathbf{V}}_a P_a(t) \\ & + k_B \partial_a^\top \cdot \int_0^t dt' \int da' P_{a'}^{\text{eq}} \bar{\mathbf{D}}_{aa'}(t-t') \cdot \partial_{a'} \frac{P_{a'}(t')}{P_{a'}^{\text{eq}}}, \end{aligned} \quad (38)$$

where all the building blocks in this equation are defined in terms of the building blocks $\mathbf{A}$ – $\mathbf{H}$ in the FPE (37) in the enlarged space. In particular, the *induced drift* $\bar{\mathbf{V}}_a$ and *induced memory kernel* $\bar{\mathbf{D}}_{aa'}(t-u)$ are given by

$$\bar{\mathbf{V}}_a = \left[v^+ \right]_a, \quad (39)$$

$$\bar{\mathbf{D}}_{aa'}(t-u) = \frac{1}{P_{a'}^{\text{eq}}} \int dx p_x^{\text{eq}} F_a^-(t) F_{a'}^+(u), \quad (40)$$

where the “projected forces” are

$$\begin{aligned} F_{a'}^+(u) &= \left[e^{\mathcal{Q}\mathcal{L}^-u} \left(v^+ - \left[v^+ \right]^{a'} \right) \Psi_{a'}(x) \right], \\ F_a^-(t) &= \left[e^{\mathcal{Q}\mathcal{L}^+t} \left(v^- - \left[v^- \right]^a \right) \Psi_a(x) \right]. \end{aligned} \quad (41)$$

The notation is condensed by using $x = (a'', b'')$ in Eq. (40) and $\Psi_a(x) = \delta(a - a'')$ in Eq. (41). To avoid confusion, we reserve the symbols $F_a^\pm(t)$ for projected-force-like objects entering the memory kernel; these should not be confused with the block $\mathbf{F}$ of the diffusion matrix in Eq. (36). The superscripts $+$ and $-$ indicate which of the adjoint projected generators, $\mathcal{L}^+$ or $\mathcal{L}^-$, is used in their definition. In addition,

$$v^+ = \mathbf{A} + \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2}, \quad (42)$$

$$v^- = \mathbf{A} - \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2} - (\mathbf{E} + \mathbf{F}^T) \cdot \partial_b \ln p_{ab}^{\text{eq}}, \quad (43)$$

with the understanding that $v^\pm$ are functions of $x = (a'', b'')$, and the average of an arbitrary function f_{ab} over b variables, conditional on a , is denoted as

$$\left[f \right]_a = \int db p_{b|a}^{\text{eq}} f_{ab}, \quad (44)$$

where the equilibrium probability of b conditional on a is defined in the usual way as

$$p_{b|a}^{\text{eq}} = \frac{p_{ab}^{\text{eq}}}{P_a^{\text{eq}}}. \quad (45)$$

Finally, the operators $\mathcal{L}^\pm$ in the “projected evolution” $e^{\mathcal{Q}\mathcal{L}^\pm t}$ within the projected forces are defined in Eqs. (A23) and (A24), while the projector $\mathcal{Q} = 1 - \mathcal{P}$, and $\mathcal{P}$ is the projector operator introduced in the enlarged space [see Eq. (A19)].

Only two assumptions enter the derivation from the FPE (37) of the exact marginal GFPE (38) in Appendix A. The first concerns the initial condition for the joint probability, which is taken to be of the relevant form $p_{ab}(0) = p_{b|a}^{\text{eq}} P_a(0)$. This assumption is entirely analogous to the standard requirement that the initial ensemble be of the relevant type [Eq. (4)] in the microscopic derivation of Eq. (3). The second, and crucial, assumption is

$$\boxed{\mathbf{C} = 0}, \quad (46)$$

which eliminates from the Fokker-Planck operator [Eq. (33)] the term accompanying two partial derivatives with respect to the CG variables a . Since the memory kernel arises as the correlation of two contributions, each involving an action of the operators $\mathcal{L}^\pm$, the presence of the $\mathbf{C}$ term would generate third- and fourth-order derivatives with respect to a in the resulting marginal equation [52,56]. In contrast, the microscopic GFPE (3) contains only second-order derivatives ∂_a , which provides the rationale for imposing the condition (46).

Equation (38) is the desired closed equation for the marginal probability $P_a(t)$. It is *formally identical* to the microscopically derived GFPE (3), establishing that the marginal distribution obtained from the joint Fokker-Planck equation (37) with $\mathbf{C} = 0$ evolves with the same structural form as the exact non-Markovian dynamics.

However, in order for $P_a(t)$ to exhibit the correct evolution, the induced coefficients $\bar{V}_a, \bar{D}_{aa'}(t - t')$ must be good approximations to the microscopic building blocks $V_a, D_{aa'}^+(t - t')$, ideally

$$\bar{V}_a = V_a, \quad (47)$$

$$\bar{D}_{aa'}(t - t') = D_{aa'}^+(t - t'). \quad (48)$$

While Eq. (47) can, in principle, be satisfied—since both $\bar{V}_a$ and V_a can be computed by suitable means—Eq. (48) is not directly amenable to evaluation. In practice, neither $\bar{D}_{aa'}(t - t')$ nor $D_{aa'}^+(t - t')$ can be computed explicitly, owing to the presence of projected time-evolution operators in both terms. The central question is therefore how to choose the blocks A–H in the Fokker-Planck equation (37) so as to enforce Eqs. (47) and (48), at least to a good approximation. A minimal and non-negotiable requirement is that the induced quantities $\bar{V}_a$ and $\bar{D}_{aa'}(t - t')$ obey the same microscopic constraints as the exact coefficients V_a and $D_{aa'}^+(t - t')$.

IV. MICROSCOPIC CONSTRAINTS ON $\bar{V}_a, \bar{D}_{aa'}$

We now examine whether the induced drift and memory kernel, $\bar{V}_a$ and $\bar{D}_{aa'}$, satisfy the microscopic constraints (17), (18), (21), and (24). This analysis allows us to identify the precise conditions under which these constraints are preserved by the induced non-Markovian dynamics.

We start with the microscopic constraint (23) as it has strong implications on the form of the FPE (37). The equal-time limit $t = t'$ of the kernel [Eq. (40)] is

$$\bar{D}_{aa'}(0) = \delta_{aa'} \frac{1}{k_B} \left[\left[v^+ - \left[v^+ \right]^a \right] \left[v^- - \left[v^- \right]^a \right]^T \right]^a. \quad (49)$$

According to Eq. (23), we should have

$$\Gamma_a = \frac{1}{k_B} \left[\left[v^+ - \left[v^+ \right]^a \right] \left[v^- - \left[v^- \right]^a \right]^T \right]^a, \quad (50)$$

where Γ_a is defined in microscopic terms in Eq. (24) and it is manifestly a symmetric positive matrix. For the right-hand side of Eq. (50) to be a symmetric positive matrix, we impose the sufficient structural condition

$$v^+ = v^- \equiv \mathbf{V}, \quad (51)$$

where

$$\mathbf{V} \stackrel{(42)}{=} \mathbf{A} + \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2}. \quad (52)$$

This condition is not the most general algebraic way of making the right-hand side of Eq. (50) symmetric and positive. It is the minimal choice adopted here because it makes the equal-time covariance a true conditional covariance and leads directly to the microscopic kinetic matrix structure used below. More general choices would introduce extra antisymmetric or solenoidal components and are not pursued in this minimal construction. The condition (51) implies, according to Eqs. (42) and (43),

$$\boxed{\partial_b(\mathbf{E}^T + \mathbf{F})p_{ab}^{\text{eq}} = 0}, \quad (53)$$

providing a first constraint on the building blocks of the FPE. When this constraint is satisfied, the kinetic matrix [Eq. (50)] takes the form

$$\Gamma_a = \frac{1}{k_B} \left[\left[\mathbf{V} - \left[\mathbf{V} \right]^a \right] \left[\mathbf{V} - \left[\mathbf{V} \right]^a \right]^T \right]^a \geq 0, \quad (54)$$

and the memory kernel [Eq. (40)] takes the form

$$\begin{aligned} \bar{D}_{aa'}(t) &= \frac{1}{k_B} \int db \left[\mathbf{V}_{ab} - \left[\mathbf{V} \right]^a \right] \\ &\times e^{\mathcal{Q}\mathcal{L}t} p_{b|a}^{\text{eq}} \left[\mathbf{V}_{ab} - \left[\mathbf{V} \right]^a \right]^T \delta_{aa'}. \end{aligned} \quad (55)$$

We now consider the remaining constraints. The identification of the drift [Eq. (47)] together with Eq. (22) requires

$$\partial_a^T \cdot \bar{V}_a p_a^{\text{eq}} = 0. \quad (56)$$

This constraint ensures that P_a^{eq} is the equilibrium solution of the induced GFPE (38). Substituting the form in Eq. (39) for

the drift into the equilibrium condition (56) leads to

$$\partial_a^\top \cdot \int db \, V_{ab} p_{ab}^{\text{eq}} = 0. \quad (57)$$

Therefore, to satisfy the microscopic constraint (22) any model for V should comply with Eq. (57).

The microscopic constraints ensuring energy conservation [Eqs. (17) and (18)] are satisfied provided that

$$V^\top \cdot \partial_a E_a = 0. \quad (58)$$

Similar constraints apply for any other dynamic invariant like, for example, total linear momentum.

V. MODELING ASSUMPTIONS ON THE FPE

Despite the structural constraints imposed on the building blocks A – H , and p_{ab}^{eq} of the FPE (37) (summarized in the boxed equations above), substantial modeling freedom remains in specifying their functional form. We now reduce this freedom by introducing additional *modeling assumptions* that define a minimal admissible subclass of the extended dynamics. The assumptions in this section are not necessary consequences of the microscopic theory; they are chosen to obtain the simplest explicit embedding compatible with the structural constraints derived above. While more elaborate constructions are certainly possible, the choices adopted here are guided by two principles: conceptual transparency and computational efficiency. Our strategy is to keep the auxiliary sector as simple as possible, while allowing for a general and flexible dependence of all building blocks on the coarse-grained variables.

The first modeling choice is to assume an auxiliary dynamics for which the equilibrium joint distribution factorizes in the form

$$p_{ab}^{\text{eq}} = G_b P_a^{\text{eq}}, \quad (59)$$

where G_b is a simple normalized Gaussian

$$G_b = \frac{e^{-b^\top \cdot b/2}}{(2\pi)^{m/2}} \quad (60)$$

that assumes that the auxiliary variables b are dimensionless, and the marginal equilibrium distribution P_a^{eq} is given in Eq. (5). Observe that the conditional probability [Eq. (45)] is given by the Gaussian

$$p_{b|a} = G_b. \quad (61)$$

Using Eq. (59) in the microscopic constraint (53) leads to a partial differential equation

$$\partial_b \cdot (E^\top + F) = (E^\top + F) \cdot b \quad (62)$$

that has as solution

$$E^\top + F = e^{b^2/2} J, \quad (63)$$

where J is any matrix with zero divergence: $\partial_b \cdot J = 0$. Given the superexponential growth in this equation, it seems natural to simply request $J = 0$, implying

$$F = -E^\top, \quad (64)$$

which implies in Eq. (52),

$$V = A. \quad (65)$$

With the conditions (46) and (64), the original Fokker-Planck equation (37) reduces to

$$\begin{aligned} \partial_t p_{ab}(t) = & -\partial_a \cdot A p_{ab}(t) - \partial_b \cdot B p_{ab}(t) + \partial_a \cdot E \cdot \partial_b p_{ab}(t) \\ & - \partial_b \cdot E^\top \cdot \partial_a p_{ab}(t) + \partial_b \cdot H \cdot \partial_b p_{ab}(t). \end{aligned} \quad (66)$$

In seeking minimal models, the most elementary approach would be to assume constant coefficients in the FPE (66). However, this choice is immediately seen to be incompatible with the required structure of the induced dynamics. Indeed, if A_{ab} in Eq. (52) was independent of b , we would have from Eq. (65) that $V = V_a$, and Eq. (55) would imply the trivial result $\bar{D}_{aa'}(t) = 0$, which is clearly inconsistent with a nonvanishing $D_{aa'}(t)$ in Zwanzig's GFPE. It follows that A_{ab} must depend explicitly on the auxiliary variables b .

Observe that if the matrix E_{ab} is independent of both a and b , the cross-diffusion terms in Eq. (66) vanish identically. The same conclusion holds if E_{ab} depends only on a or only on b . In the latter cases, the mixed second-order contributions reduce to divergence terms of the form $\partial_a^\top \cdot E_a$ or $\partial_b^\top \cdot E_b$, which can be absorbed into a redefinition of the drift operators A or B , respectively. Since such terms do not alter the structural content of the equation, it is natural, for simplicity, to set

$$E = 0. \quad (67)$$

With this modeling assumption, the FPE (66) simplifies to

$$\partial_t p_{ab}(t) = -\partial_a \cdot A p_{ab}(t) - \partial_b \cdot B p_{ab}(t) + \partial_b \cdot H \cdot \partial_b p_{ab}(t). \quad (68)$$

Next, by requiring that Eq. (59) is the equilibrium solution of Eq. (68) gives, after taking the derivatives of the Gaussian with respect to b ,

$$\begin{aligned} \frac{1}{P_a^{\text{eq}}} \partial_a^\top \cdot A_{ab} P_a^{\text{eq}} + \partial_b^\top \cdot B_{ab} - B_{ab} \cdot b \\ + b \partial_b^\top : H_{ab} + H_{ab} : (\mathbb{1} - b b^\top) = 0, \end{aligned} \quad (69)$$

where the colon denotes double contraction. The relation (69) constitutes a differential constraint on the functions A_{ab} , B_{ab} , and H_{ab} that any admissible model must satisfy in order for the factorized joint distribution [Eq. (59)] to be the stationary solution of the FPE (68). To proceed, we must further specify the functional forms of these building blocks.

We start with A and assume a simple linear ansatz given by

$$A_{ab} = V_a + W_a \cdot b, \quad (70)$$

where V_a is the microscopic drift [Eq. (6)] and the matrix $W_a \in \mathbb{R}^{n \times m}$ is to be determined. This ansatz is motivated by the fact that Eq. (70) with Eq. (65) automatically satisfies the reversibility condition (57) when the equilibrium joint distribution P_{ab}^{eq} factorizes as in Eq. (59) and uses Eq. (22).

The matrix W_a is further restricted by requirement [Eq. (54)] and the energy conservation property [Eq. (25)]. In fact, substituting Eq. (70) in Eq. (54) and performing the Gaussian average of the dyadic $b b^\top$, one obtains

$$W_a \cdot W_a^\top = \Gamma_a, \quad (71)$$

which enforces the matrix W_a to be the “square root” of the microscopic kinetic matrix. The energy conservation property [Eq. (25)] of Γ_a necessarily implies that

$$W_a^T \cdot \partial_a E_a = 0. \quad (72)$$

The requirement [Eq. (71)] does not fix entirely the matrix W_a . To see this, consider the principal square root matrix Σ_a , which is the *unique* symmetric positive matrix $\Sigma_a = \Sigma_a^T > 0$ that satisfies

$$\Sigma_a \cdot \Sigma_a^T = \Gamma_a. \quad (73)$$

Then, any matrix of the form

$$W_a = \Sigma_a \cdot U \quad (74)$$

satisfies Eq. (71) provided that U is an $n \times m$ matrix whose rows are orthonormal, i.e., $U \cdot U^T = \mathbb{1}_{m \times m}$. Because the covariance matrix Γ_a is an $n \times n$ matrix, with rank $n - k$ (where k is the number of dynamic invariants) for a matrix $W_a \in \mathbb{R}^{n \times m}$ to satisfy Eq. (71), it is necessary that $m \geq n - k$, implying that the number of auxiliary variables b must be equal to or exceed the number of coarse-grained variables a (minus the number of conserved quantities). In principle, U provides additional modeling degrees of freedom constrained by $U \cdot U^T = \mathbb{1}_m$ but unconstrained by the microscopic requirements.

Now, let us look at the consequences of the previous modeling assumptions on the form of B . Substitution of Eq. (70) in Eq. (69), and using the form in Eq. (13) for the equilibrium distribution, leads to

$$l_a^T \cdot b + \partial_b \cdot B_{ab} - B_{ab} \cdot b + b \partial_b : H_{ab} + H_{ab} : (\mathbb{1} - bb^T) = 0, \quad (75)$$

where we have introduced

$$l_a \equiv W_a^T \cdot \partial_a S_a + \partial_a \cdot W_a^T \quad (76)$$

and we have used

$$W_a^T \cdot \partial_a \ln P_a^{\text{eq}} \stackrel{(13)(72)}{=} W_a^T \cdot \partial_a S_a. \quad (77)$$

A natural first impulse is to simplify further and take the remaining two coefficients B_{ab} and H_{ab} appearing in the constraint (75) to be independent of b . This assumption, however, is overly restrictive. Under it, Eq. (75) reduces to a scalar polynomial in b that must vanish identically: The constant and linear coefficients are forced to zero, and the quadratic term must arise from a skew-symmetric matrix H_{ab} . However, this would imply that there is no diffusion term in the FPE (68), which is unacceptable. We therefore relax the assumption of constant coefficients and assume that B_{ab} retains an explicit dependence on a, b while, for simplicity, we assume

$$H_{ab} = H_a. \quad (78)$$

This leads to the differential equation for B_{ab} :

$$l_a^T \cdot b + \partial_b \cdot B_{ab} - B_{ab} \cdot b + H_a : (\mathbb{1} - bb^T) = 0. \quad (79)$$

This differential equation has the following solution, as discussed in Appendix C:

$$B_{ab} = -l_a - H_a \cdot b. \quad (80)$$

Inserting Eqs. (70), (76), and (80) into Eq. (68) gives the final form for the FPE in the enlarged space:

$$\begin{aligned} \partial_t p_{ab}(t) = & -\partial_a \cdot (V_a + W_a \cdot b) p_{ab}(t) \\ & - \partial_b \cdot (W_a^T \cdot \partial_a S_a + \partial_a \cdot W_a^T) p_{ab}(t) \\ & + \partial_b \cdot H_a \cdot b p_{ab}(t) + \partial_b \cdot H_a \cdot \partial_b p_{ab}(t). \end{aligned} \quad (81)$$

Observe that the FPE in the enlarged space is fully determined by the building blocks S_a, V_a, W_a , and H_a .

The corresponding Ito SDE is

$$\begin{aligned} da_t &= V_a dt + W_{a_t} \cdot b_t dt, \\ db_t &= W_{a_t}^T \cdot \partial_a S_{a_t} dt + \partial_a \cdot W_{a_t}^T dt \\ &\quad - H_{a_t} \cdot b_t dt + \sigma_{a_t} d\mathcal{W}_t, \end{aligned} \quad (82)$$

where $d\mathcal{W}_t$ denotes a vector of independent Wiener increments and the noise amplitude is given by the fluctuation-dissipation theorem

$$\sigma_a \cdot \sigma_a^T = H_a + H_a^T. \quad (83)$$

Observe that, for fixed a , the dynamics of b reduces to an Ornstein-Uhlenbeck (OU) process. It is therefore natural to refer to H as the *relaxation matrix*.

Equations (81) and (82) constitute the central results of this work. They provide an explicit and self-consistent characterization of the embedded Markovian dynamics, obtained by enforcing a set of exact microscopic constraints (given in the square-framed equations in Sec. IV) together with a minimal collection of modeling assumptions (given in the rounded-framed equations in the present Sec. V). Remarkably, these requirements are restrictive enough to determine, within the minimal ansatz adopted here, the structural form of the embedding. Upon marginalization, the resulting dynamics yields the generalized Fokker-Planck equation (38) for the coarse-grained variables, which is structurally identical to the exact, microscopically derived GFPE (3): The reversible drift is reproduced exactly, and the induced memory kernel satisfies all the fundamental microscopic properties of the exact kernel.

An important asset of the proposed strategy is the clear separation it provides between microscopically determined quantities and genuine modeling degrees of freedom. In particular, the entropy S_a , the reversible drift V_a , and the square root W_a of the kinetic matrix are entirely fixed by *static* information, which can, in principle, be extracted from equilibrium molecular-dynamics (MD) or Monte Carlo (MC) simulations. In contrast, all remaining modeling freedom is confined to the choice of the relaxation matrix H_a , whose entries may be treated as fitting parameters and tuned to reproduce the relevant *dynamical* information, without compromising microscopic consistency.

A few final remarks. First, we note that no symmetry has been imposed *a priori* on the matrix H . Its symmetric part determines the noise amplitude through the fluctuation-dissipation relation (83) and, when acting alone, gives rise to purely monotonic decay of the associated memory kernels. In contrast, any skew-symmetric component of H generates damped oscillatory behavior, thereby providing a natural mechanism for encoding underdamped relaxation within the embedding. Second, as discussed in Appendix B, microscopic

reversibility imposes that the functional dependence of the matrices W_a, H_a should satisfy

$$\begin{aligned} W_{\varepsilon \cdot a} &= -\varepsilon \cdot W_a \cdot \bar{\varepsilon}, \\ H_{\varepsilon \cdot a} &= \bar{\varepsilon} \cdot H_a \cdot \bar{\varepsilon}, \end{aligned} \quad (84)$$

where $\varepsilon \in \mathbb{R}^{n \times n}$ is a diagonal matrix with entries ± 1 specifying the time-reversal character of each CG variable and $\bar{\varepsilon} \in \mathbb{R}^{m \times m}$ is a diagonal matrix with entries ± 1 specifying the time-reversal character of each auxiliary variable. In general, the transformation of the square-root matrix W_a under time reversal is known, since its explicit form follows from the factorization of the kinetic matrix Γ_a . This information determines the structure of $\bar{\varepsilon}$, that is, the time-reversal parity of the auxiliary variables. Once $\bar{\varepsilon}$ has been identified, condition (84) imposes corresponding constraints on the relaxation matrix.

Finally, Appendix D derives the induced GLE obtained by eliminating b_t from the embedded SDE (82). This elimination is an exact rewriting of the joint Markov process in (a, b) , but it does not generally yield a closed GLE driven by an externally prescribed colored noise. Because a_t remains coupled to the auxiliary variables, the induced force is multiplicative, history dependent, and correlated with the CG trajectory. The familiar FDT form, in which the colored-force covariance is proportional to the memory kernel, is recovered only when the auxiliary variables relax fast enough that a_t can be treated as locally frozen. Thus, for state-dependent memory, the induced GLE is a nontrivial stochastic object; this is why we formulate the theory at the GFPE level.

VI. ISOTHERMAL CG PARTICLE MODELS

In this section, we illustrate the general methodology by applying it to CG particle models, in which each CG particle represents a group of underlying atoms. The set of CG variables consists of the positions and momenta of the centers of mass of each particle. Since the microscopic Hamiltonian cannot, in general, be expressed solely in terms of the position and momentum of the centers of mass of the objects, this choice leads naturally to an isothermal coarse-grained description.

The list of CG variables $\hat{A}(z)$ taking numerical values a is, therefore,

$$\begin{aligned} \hat{A}(z) \rightarrow (\hat{R}, \hat{P}) &= \{\hat{\mathbf{R}}_\mu(z), \hat{\mathbf{P}}_\mu(z), \mu = 1, \dots, M\}, \\ a \rightarrow (R, P) &= \{\mathbf{R}_\mu, \mathbf{P}_\mu, \mu = 1, \dots, M\}. \end{aligned} \quad (85)$$

The CG variables are defined in microscopic terms as

$$\begin{aligned} \hat{\mathbf{R}}_\mu(z) &= \frac{1}{M_\mu} \sum_i^N m_i \mathbf{q}_i \delta_\mu(i), \\ \hat{\mathbf{P}}_\mu(z) &= \sum_i^N \mathbf{p}_i \delta_\mu(i), \end{aligned} \quad (86)$$

where the mass of the CG particle is $M_\mu = \sum_i^N m_i \delta_\mu(i)$. The indicator symbol $\delta_\mu(i)$ takes the value 1 if the atom i belongs to the blob μ and zero otherwise. Because one atom can only be in one blob, this indicator satisfies

$$\delta_\mu(i) \delta_\nu(i) = \delta_{\mu\nu} \delta_\mu(i). \quad (87)$$

The action of the Liouville operator on each variable is

$$i\mathcal{L}\hat{A} \rightarrow \begin{pmatrix} i\mathcal{L}\hat{\mathbf{R}}_\mu \\ i\mathcal{L}\hat{\mathbf{P}}_\mu \end{pmatrix} = \begin{pmatrix} \hat{\mathbf{V}}_\mu \\ \hat{\mathbf{F}}_\mu \end{pmatrix}, \quad (88)$$

where $\hat{\mathbf{V}}_\mu(z) = \hat{\mathbf{P}}_\mu(z)/M_\mu$ is the velocity of the CG particle and $\hat{\mathbf{F}}_\mu$ is the total force on the μ th CG particle, which depends only on position variables.

Once we have specified the CG variables $\hat{A}(z)$ and their time derivatives $i\mathcal{L}\hat{A}(z)$, the construction of the embedded Markovian dynamics hinges on the calculation of the static quantities S_a, V_a , and Γ_a, W_a , and on the specification of the relaxation matrix H . Once these building blocks are given, one then constructs the FPE and SDE equations, Eqs. (81) and (82), respectively.

To obtain the entropy S_a , we look at the equilibrium probability, defined in this level of description as

$$P_a^{\text{eq}} \rightarrow P^{\text{eq}}(R, P) = \int dz \rho^{\text{eq}}(z) \prod_\mu^M \delta(\hat{\mathbf{R}}_\mu - \mathbf{R}_\mu) \delta(\hat{\mathbf{P}}_\mu - \mathbf{P}_\mu), \quad (89)$$

where $\rho^{\text{eq}}(z)$ denotes the equilibrium ensemble. For simplicity, we adopt the canonical ensemble, in which the momentum integrals in Eq. (89) can be carried out analytically. This leads to a factorization between position and momentum variables, substantially simplifying the resulting expressions. In particular, the probability takes the form

$$P^{\text{eq}}(R, P) = \frac{1}{Z} e^{-\beta \left(\sum_\mu^M \frac{\mathbf{P}_\mu^2}{2M_\mu} + V^{\text{MF}}(R) \right)}, \quad (90)$$

where $V^{\text{MF}}(R)$ is the potential of mean force and $\beta = (k_B T)^{-1}$, where T is the temperature. The entropy [Eq. (14)] in this description is, up to an irrelevant constant,

$$S_a \rightarrow S(R, P) = -\frac{1}{T} \left(\sum_\mu^M \frac{\mathbf{P}_\mu^2}{2M_\mu} + V^{\text{MF}}(R) \right), \quad (91)$$

with derivatives given by

$$\partial_a S_a \rightarrow \frac{1}{T} \begin{pmatrix} -\frac{\partial V^{\text{MF}}}{\partial \mathbf{R}_\mu} \\ -\frac{\mathbf{P}_\mu}{M_\mu} \end{pmatrix} = \frac{1}{T} \begin{pmatrix} \bar{\mathbf{F}}_\mu \\ -\mathbf{V}_\mu \end{pmatrix}, \quad (92)$$

where the mean force $\bar{\mathbf{F}}_\mu$ is defined as minus the gradient of the potential of mean force.

The reversible drift [Eq. (6)] requires conditional expectations that in this level of description are given by

$$\langle \dots \rangle^a \rightarrow \frac{1}{P^{\text{eq}}} \int dz \rho^{\text{eq}}(z) \prod_\mu^M \delta(\hat{\mathbf{R}}_\mu - \mathbf{R}_\mu) \delta(\hat{\mathbf{P}}_\mu - \mathbf{P}_\mu) \dots \quad (93)$$

The conditional expectation of Eq. (88) leads to a reversible drift with the form

$$V_a \rightarrow \begin{pmatrix} \frac{\mathbf{P}_\mu}{M_\mu} \\ \langle \hat{\mathbf{F}}_\mu \rangle^a \end{pmatrix}. \quad (94)$$

As shown in the Supplemental Material [57], the mean force depends only on the coarse-grained positions. Consequently,

the phase-space divergence of the reversible drift vanishes, i.e., $\partial_a^\top \cdot V_a = 0$. The reversibility condition (21) with Eqs. (92) and (94) implies the celebrated connection between the mean force and the conditional expectation of the microscopic force [58–60]:

$$\bar{\mathbf{F}}_\mu = \langle \hat{\mathbf{F}}_\mu \rangle^a. \quad (95)$$

It is apparent that the drift term V_a in this case is entirely determined by the entropy function S_a or, equivalently, by the potential of mean force $V^{\text{MF}}(R)$.

The kinetic matrix [Eq. (24)] now takes the block form

$$\Gamma_a \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & T\Theta(R) \end{pmatrix}, \quad (96)$$

where the four blocks are of size $3M \times 3M$. The vanishing of three of the blocks follows from the fact that $i\mathcal{L}\hat{\mathbf{R}}_\mu = \hat{\mathbf{V}}_\mu$ is identical for all microstates contributing to a given coarse-grained state, so that its conditional fluctuations vanish. The matrix $\Theta \in \mathbb{R}^{3M \times 3M}$ is made of 3×3 blocks with elements given by the force conditional covariance

$$\Theta_{\mu\nu}(R) = \frac{1}{k_B T} \langle (\hat{\mathbf{F}}_\mu - \bar{\mathbf{F}}_\mu)(\hat{\mathbf{F}}_\nu - \bar{\mathbf{F}}_\nu) \rangle^R, \quad (97)$$

with $\mu, \nu = 1, \dots, M$. Because the force depends only on the positions, the momentum integral in the conditional expectations can be carried out trivially so Θ depends only on the configuration R of positions of the CG particles but not on their momentum [57]. We introduce a rectangular matrix $\Xi \in \mathbb{R}^{3M \times 3K}$ that satisfies

$$\Xi \cdot \Xi^\top = \Theta. \quad (98)$$

The minimum number of columns $3K$ that this matrix may have is the rank of Θ that is $3M$ in general.

The following matrix

$$W(R) = \begin{pmatrix} 0 & 0 \\ 0 & \Xi(R) \end{pmatrix} \quad (99)$$

then satisfies Eq. (71) with $\Gamma(R)$ given by Eq. (96). Note that the term $\partial_a^\top \cdot W = 0$ in Eq. (82) vanishes:

$$\partial_a^\top \cdot W_a \rightarrow \begin{pmatrix} \partial_R^\top \cdot 0 + \partial_P^\top 0 \\ \partial_R^\top \cdot 0 + \partial_P^\top \cdot \Xi(R) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (100)$$

We have now all the microscopic information required to construct the SDE (82) in the enlarged space. Because of the particular block structure of Eq. (99), it makes sense to split the auxiliary variables in two sets $b = (\rho, \pi) = (\rho_1, \dots, \rho_K, \pi_1, \dots, \pi_K)$. In addition, we decompose the relaxation matrix in block form

$$H_a \rightarrow \begin{pmatrix} H_a^{\rho\rho} & H_a^{\rho\pi} \\ H_a^{\pi\rho} & H_a^{\pi\pi} \end{pmatrix}, \quad (101)$$

where each block is made of 3×3 matrices of the form $H_{\mu\nu}^{\rho\rho}$, etc.

The time-reversal parity $\bar{\varepsilon}$ of the auxiliary variables is determined from the first equation in Eq. (84). Because the matrix W_a depends on positions that are even functions under time reversal, we have $W_{\varepsilon \cdot a} = W_a$, implying, therefore, that the auxiliary variables ρ are even and π are odd. As a consequence, the second equation in Eq. (84) implies that

$H_{\varepsilon \cdot a}^{\rho\pi} = -H_a^{\rho\pi}$ and $H_{\varepsilon \cdot a}^{\pi\rho} = -H_a^{\pi\rho}$. If the dependence on the CG variables of H_a is only through positions (or it is just a constant matrix), this implies $H_{\varepsilon \cdot a}^{\rho\rho} = 0$ and $H_{\varepsilon \cdot a}^{\pi\pi} = 0$.

Particularizing the SDE (82) to the present case gives

$$\begin{aligned} d\mathbf{R}_\mu &= \mathbf{V}_\mu dt, \\ d\mathbf{P}_\mu &= \bar{\mathbf{F}}_\mu dt + \sum_i^K \Xi_{\mu i} \cdot \boldsymbol{\pi}_i dt, \\ d\rho_i &= - \sum_j^K H_{ij}^{\rho\rho} \cdot \rho_j dt + d\tilde{\rho}_i, \\ d\pi_i &= - \sum_v^M \Xi_{iv} \cdot \beta \mathbf{V}_v dt - \sum_j^K H_{ij}^{\pi\pi} \cdot \pi_j dt + d\tilde{\pi}_i. \end{aligned} \quad (102)$$

Here, $d\tilde{\rho}_i$ and $d\tilde{\pi}_i$ denote the corresponding components of $\sigma_a d\mathcal{W}_t$ after the block decomposition of the auxiliary variables. Their covariance is fixed by Eq. (83) or equivalently by the symmetric part of the relevant blocks of H , where $\mu = 1, \dots, M$ and $i = 1, \dots, K$. The auxiliary variables ρ do not affect the dynamics of the rest of variables and can be eliminated altogether. This yields the final SDE

$$\begin{aligned} d\mathbf{R}_\mu &= \mathbf{V}_\mu dt, \\ d\mathbf{P}_\mu &= \bar{\mathbf{F}}_\mu dt + \sum_i^K \Xi_{\mu i} \cdot \boldsymbol{\pi}_i dt, \\ d\pi_i &= - \sum_v^M \Xi_{iv} \cdot \beta \mathbf{V}_v dt - \sum_j^K H_{ij}^{\pi\pi} \cdot \pi_j dt + d\tilde{\pi}_i. \end{aligned} \quad (103)$$

These are the SDEs for the Markovian embedding of a non-Markovian isothermal CG particle model of an underlying Hamiltonian molecular system. They still require the specification of the potential of mean force giving rise to the mean forces $\bar{\mathbf{F}}$, the calculation of the square root Ξ of the force-force covariance, and the fitting of the relaxation matrix $H^{\pi\pi}$.

A model similar to Eq. (103) has been proposed by Lei and coworkers [11,12]. To the best of our knowledge, these works were the first to explicitly incorporate *state-dependent* many-body Markovian embeddings in coarse-grained particle models, thereby allowing the structure of the auxiliary dynamics to adapt to the instantaneous CG configuration—a physically essential feature for capturing configuration-dependent dissipation and fluctuations.

In our formulation, Ξ is defined in Eq. (98) as a matrix square root of the equilibrium conditional force-force covariance Θ , which is assumed to be known. In practice, however, Θ is not available in closed analytical form and must itself be modeled. A natural strategy is to adopt an equivariant ansatz whose parameters are fitted to MD or MC data, in a manner analogous to the modeling of the potential of mean force. Once a model for Θ has been specified, it can be factorized to obtain Ξ according to Eq. (98).

Computational cost

The calculation of the square root Ξ of the force-force covariance matrix Θ may be carried out by a Cholesky-type factorization, although this is not the only possible strategy. In high-dimensional problems, iterative Gaussian-sampling

methods or matrix-free approaches can be preferable when fast matrix-vector products or additional structure are available [61]. We expect Θ to be sparse—since force correlations vanish beyond a finite interaction range. For a sparse matrix whose sparsity arises from a finite cutoff distance, the associated fill-in in Cholesky factorization leads to a computational cost that typically scales quadratically with the number of particles. In addition, although Θ is sparse, locality does not automatically extend to its square root Ξ . As a consequence, the direct numerical implementation of Eq. (103) becomes computationally expensive.

However, when total momentum is conserved by the coarse-grained particles, a computationally feasible scaling can be achieved. Momentum conservation imposes a specific constraint on the force-force covariance matrix, endowing it with a structured form that allows its square root to be constructed at a cost that scales linearly with the number of CG particles. To elucidate this point, we recall that conservation of total momentum at the microscopic level—ultimately a consequence of Newton’s third Law—implies that the forces acting on the CG particles satisfy

$$\sum_{\mu} \hat{\mathbf{F}}_{\mu} = 0 \implies \sum_{\mu} \Theta_{\mu\nu} = 0. \quad (104)$$

This implies that we may express the diagonal elements in terms of the off-diagonal

$$\Theta_{\mu\mu} = - \sum_{\nu \neq \mu} \Theta_{\mu\nu}. \quad (105)$$

This structure is precisely that of a discrete Laplacian defined on the interaction graph, whose vertices correspond to the CG particles and whose edges represent interacting particle pairs. As discussed in Sec. VII and detailed in Ref. [57], this graph structure can be exploited by lifting the description from particle (node) space to pair (edge) space. In this lifted representation, the square-root factor of the discrete Laplacian admits a construction whose computational cost scales linearly with the number of CG particles. In addition, for a momentum conserving model, the resulting square-root matrix is also local.

Because in momentum-conserving coarse-grained particle models the square root matrix Ξ is local, one may bypass an explicit construction of Θ and instead model Ξ directly through an equivariant, many-body, local ansatz. The parameters of this ansatz can be determined via data-driven fitting of the SDE (103). A similar strategy is adopted in Refs. [11,12], where the model parameters of a many-body equivariant ansatz are chosen so that the resulting memory kernel approximates the Zwanzig memory kernel, evaluated with the constrained dynamics proposed in Ref. [60]. These approaches are expected to ensure, in a natural way, that the fitted Ξ satisfies Eq. (98). For this construction to be consistent, however, the number K of auxiliary variables must obey the rank condition $K \geq \text{rank}(\Theta)$.

VII. NONISOTHERMAL CG PARTICLE MODELS

No coarse-grained description can be expected to be universally accurate: even when memory effects are incorporated, a given choice of CG variables may remain intrinsically incapable of capturing essential physical processes. The

isothermal particle model considered in the previous section provides a clear illustration. No matter how accurately its non-Markovian dynamics is fitted, such a model is structurally unable to account for energy transport. This limitation is not a shortcoming of the embedding procedure but a direct consequence of the selected CG variables. By retaining only positions and momenta, the coarse-grained description is effectively blind to energy exchange between CG particles; the resulting dynamical lens exhibits a genuine *scotoma* for energy, and an entire class of phenomena lies outside its descriptive scope.

It is therefore natural to *physically enlarge* the set of CG variables by introducing an internal energy variable for each particle, leading to nonisothermal particle models such as those proposed in Refs. [62,63]. While this enriched description captures additional thermodynamic structure and may restore Markovianity in specific cases, it does not, in general, eliminate memory effects *per se*. Phenomena such as short-scale and transient energy transport, fast external forcing [64], or finite-time energy exchange between translational and internal modes, all involve conserved energy coupled to eliminated degrees of freedom on comparable timescales, thereby generating intrinsic memory effects.

The purpose of this section is to demonstrate how the general Markovian embedding strategy developed above can be applied systematically to nonisothermal particle models. In this setting, it is essential to account explicitly for dynamical invariants, most notably total energy and momentum, and to fully exploit the constraints that these invariants impose on the admissible form of the model building blocks. By doing so, we show how explicit enforcement of conservation laws and microscopic consistency can be combined with controlled memory modeling to obtain a thermodynamically consistent coarse-grained description of non-Markovian energy transport.

In this section, we consider systems composed of groups of atoms that are permanently bonded together and treated as coarse-grained units. A prototypical example is a melt of star polymers [11,12,60,65], although the framework applies more generally. Each group of atoms is represented by a *bead* or *blob*, which may correspond to an entire molecule when sufficient spherical symmetry is present, or to a subunit of a larger macromolecule when additional internal or shape information is required to capture the relevant structure.

For simplicity, we restrict attention to pairwise additive microscopic interactions; extensions to more general many-body forces are discussed in Ref. [62]. We further assume that all atoms in the system are uniquely assigned to coarse-grained blobs, with no implicit solvent. This assumption guarantees exact conservation of total momentum and energy at the microscopic level, which is inherited by the coarse-grained description.

The list of CG variables $\hat{A}(z)$ taking numerical values a is now

$$\begin{aligned} \hat{A}(z) &\rightarrow (\hat{R}, \hat{P}, \mathcal{E}) = \{\hat{\mathbf{R}}_{\mu}(z), \hat{\mathbf{P}}_{\mu}(z), \hat{\mathcal{E}}_{\mu}(z), \mu = 1, \dots, M\}, \\ a &\rightarrow (R, P, \mathcal{E}) = \{\mathbf{R}_{\mu}, \mathbf{P}_{\mu}, \mathcal{E}_{\mu}, \mu = 1, \dots, M\}, \end{aligned} \quad (106)$$

where $\hat{\mathbf{R}}_{\mu}$ is the position and $\hat{\mathbf{P}}_{\mu}$ the momentum of the center of mass, while $\hat{\mathcal{E}}_{\mu}$ is the internal energy of the blob, defined

microscopically as [62]

$$\hat{\mathcal{E}}_\mu(z) = \sum_i^N \frac{m_i}{2} (\mathbf{v}_i - \hat{\mathbf{V}}_\mu(z))^2 \delta_\mu(i) + \hat{\phi}_\mu(z). \quad (107)$$

The intrinsic potential energy of the μ th blob is defined as

$$\hat{\phi}_\mu(z) = \frac{1}{2} \sum_{ij}^N \hat{\phi}_{ij} \delta_\mu(j), \quad (108)$$

where $\hat{\phi}_{ij}$ is the potential energy of the pair of atoms i, j . Both the total energy and the total momentum of the system can be expressed explicitly in terms of the CG variables

$$\hat{H}(z) = E(\hat{A}(z)), \quad \hat{\mathbf{P}}(z) = \mathbf{P}(\hat{A}(z)),$$

where E and $\mathbf{P}$ denote the corresponding CG energy and momentum functions given by

$$E(a) = \sum_\mu^M \left[\frac{\mathbf{P}_\mu^2}{2M_\mu} + \mathcal{E}_\mu \right], \quad \mathbf{P}(a) = \sum_\mu^M \mathbf{P}_\mu. \quad (109)$$

The strategy for representing the non-Markovian dynamics through the Markovian embedding [Eq. (82)] follows the same logic as in the previous section. One first identifies the static building blocks S_a , V_a , and Γ_a , which are fully determined by the choice of coarse-grained variables and by their microscopic time derivatives under the Liouville operator. Once these quantities are specified, one constructs a square root W_a of the kinetic matrix Γ_a and selects a relaxation matrix $\mathbf{H}$ to complete the definition of the embedding SDE (82).

The detailed construction is presented in Ref. [57]. There we show that the structure of the square root W_a naturally leads to the introduction of two auxiliary variables per interacting pair of particles, $\Pi_{\mu\nu}$ and $\Lambda_{\mu\nu}$, which are skew symmetric under index exchange,

$$\begin{aligned} \Pi_{\mu\nu} &= -\Pi_{\nu\mu}, \\ \Lambda_{\mu\nu} &= -\Lambda_{\nu\mu}. \end{aligned} \quad (110)$$

With these variables, the embedding SDE governing the coupled dynamics of the coarse-grained and auxiliary degrees of freedom takes the form

$$d\mathbf{R}_\mu = \mathbf{V}_\mu dt, \quad (111)$$

$$d\mathbf{P}_\mu = \sum_\nu \mathbf{F}_{\mu\nu} dt + \frac{1}{\sqrt{2}} \sum_\nu \boldsymbol{\Theta}_{\mu\nu}^{1/2} \cdot \Pi_{\mu\nu} dt, \quad (112)$$

$$\begin{aligned} d\mathcal{E}_\mu &= -\frac{1}{2} \sum_\nu \mathbf{F}_{\mu\nu} \cdot \mathbf{V}_{\mu\nu} dt - \frac{1}{2\sqrt{2}} \sum_\nu \mathbf{V}_{\mu\nu} \cdot \boldsymbol{\Theta}_{\mu\nu}^{1/2} \Pi_{\mu\nu} dt \\ &\quad + \frac{1}{\sqrt{2}} \sum_\nu \kappa_{\mu\nu}^{1/2} \Lambda_{\mu\nu} dt, \end{aligned} \quad (113)$$

$$\begin{aligned} d\Pi_{\mu\nu} &= \frac{1}{\sqrt{2}} \boldsymbol{\Theta}_{\mu\nu}^{1/2} \cdot \mathbf{V}_{\mu\nu} \left[\frac{1}{T_\mu} + \frac{1}{T_\nu} \right] - \gamma_{\mu\nu}^\pi \Pi_{\mu\nu} dt \\ &\quad + 2\sqrt{2\gamma_{\mu\nu}^\pi} d\mathcal{W}_{\mu\nu}, \\ d\Lambda_{\mu\nu} &= \kappa_{\mu\nu}^{1/2} \left[\frac{1}{T_\mu} - \frac{1}{T_\nu} \right] dt - \gamma_{\mu\nu}^\lambda \Lambda_{\mu\nu} dt + \sqrt{2\gamma_{\mu\nu}^\lambda} d\mathcal{V}_{\mu\nu}. \end{aligned} \quad (114)$$

The derivation of these equations in Ref. [57] relies on several simplifying assumptions. The first is a *pair-independence* approximation for the microscopic pair forces [62]: The force $\hat{\mathbf{F}}_{\mu\mu'}$ exerted by particle μ' on μ is assumed to be statistically uncorrelated with the force $\hat{\mathbf{F}}_{\nu\nu'}$ exerted by ν' on ν , unless the pairs coincide, i.e., $\mu, \mu' = \nu, \nu'$. Correlations between distinct pairs are neglected in this approximation. In this way,

$$\langle \delta \hat{\mathbf{F}}_{\mu\mu'} \delta \hat{\mathbf{F}}_{\nu\nu'} \rangle^a \simeq (\delta_{\mu\nu} \delta_{\mu'\nu'} - \delta_{\mu\nu'} \delta_{\nu\mu'}) \boldsymbol{\Theta}_{\mu\mu'}, \quad (115)$$

where the pair covariance is

$$\boldsymbol{\Theta}_{\mu\mu'} \equiv \frac{1}{k_B} \langle \delta \hat{\mathbf{F}}_{\mu\mu'} \delta \hat{\mathbf{F}}_{\mu\mu'}^\top \rangle^a = \boldsymbol{\Theta}_{\mu'\mu}. \quad (116)$$

This pair covariance is a 3×3 matrix that is by construction positive definite and has, therefore, a 3×3 square root matrix $\boldsymbol{\Theta}_{\mu\nu}^{1/2}$ satisfying, for each μ, ν ,

$$\boldsymbol{\Theta}_{\mu\nu}^{1/2} \cdot \boldsymbol{\Theta}_{\mu\nu}^{1/2} = \boldsymbol{\Theta}_{\mu\nu}. \quad (117)$$

The scalar $\kappa_{\mu\nu}$ denotes the conditional covariance of the microscopic heat-transfer term, with $\kappa_{\mu\nu}^{1/2} = \sqrt{\kappa_{\mu\nu}}$. As shown in Ref. [57], both the force-force covariance $\boldsymbol{\Theta}_{\mu\mu'}$ and the heat-transfer covariance $\kappa_{\mu\nu}$ depend on the CG particle positions and internal energies, but not on their momenta. In writing Eq. (114), we further assume that the dependence of these covariances on the internal energies is weak, so that the corresponding conditional expectations at fixed $R, \mathcal{E}$ may be approximated as equilibrium averages at fixed R , that is, $\langle \dots \rangle^{R\mathcal{E}} \simeq \langle \dots \rangle^R$.

The relaxation matrix $\mathbf{H}$ in Eq. (82) has been simplified in order to have a minimum of fitting parameters, by taking two independent inverse relaxation times $\gamma_{\mu\nu}^\pi, \gamma_{\mu\nu}^\lambda$ for each auxiliary variable. The following symmetries of the relaxation times are assumed:

$$\begin{aligned} \gamma_{\mu\nu}^\pi &= \gamma_{\nu\mu}^\pi, \\ \gamma_{\mu\nu}^\lambda &= \gamma_{\nu\mu}^\lambda. \end{aligned} \quad (118)$$

If desired, the number of fitting parameters can be further reduced by imposing a common relaxation time for all interacting pairs. Alternatively, one may retain the full structure of $\mathbf{H}$, including its skew-symmetric components, thereby preserving maximal flexibility in the parametrization. These alternatives reflect modeling choices rather than fundamental constraints.

Finally, $d\mathcal{W}_{\mu\nu} = -d\mathcal{W}_{\nu\mu}$ and $d\mathcal{V}_{\mu\nu} = -d\mathcal{V}_{\nu\mu}$ are independent increments of the Wiener process.

The mean force $\mathbf{F}_{\mu\nu}$, the square-root force covariance $\boldsymbol{\Theta}$, and the heat-transfer covariance $\kappa_{\mu\nu}$ are many-body functions of the coarse-grained particle positions. These quantities are not available in closed analytical form and must therefore be represented by flexible parametric models, whose parameters should be estimated from molecular-dynamics or Monte Carlo simulation data.

It is a simple calculation relying on the symmetry properties of the building blocks that the SDE (114) conserve both total momentum and total energy given by Eq. (109).

Computational cost

As we have an auxiliary variable for each pair of particles, their number scales quadratically with the number M of coarse-grained particles. At first sight, this scaling may appear to constitute a severe computational limitation. In practice, this scaling is only nominal, since the force- and heat-transfer covariances are spatially local and supported solely on bead pairs whose separation lies within a finite cutoff distance. Therefore, the auxiliary variables do not live on the complete set of bead pairs, but only on the *instantaneous interaction graph* defined by the neighbor list. When a pair of beads no longer interacts, the corresponding auxiliary variables $\Pi_{\mu\nu}$, $\Lambda_{\mu\nu}$ cease to enter the equations for the coarse-grained variables and evolve independently according to an OU process:

$$\begin{aligned} d\Pi_{\mu\nu} &= -\gamma_{\mu\nu}^{\pi} \Pi_{\mu\nu} dt + 2\sqrt{2\gamma_{\mu\nu}^{\pi}} d\mathcal{W}_{\mu\nu}, \\ d\Lambda_{\mu\nu} &= -\gamma_{\mu\nu}^{\lambda} \Lambda_{\mu\nu} dt + \sqrt{2\gamma_{\mu\nu}^{\lambda}} d\mathcal{V}_{\mu\nu}. \end{aligned} \quad (119)$$

There is no need to numerically integrate this process, because the solution is known analytically. Once the pair exits the cutoff, the auxiliary variable is removed altogether, while its value $\Pi_{\mu\nu}^*$ and the removal time $t_{\mu\nu}^*$ are recorded for future use. If a previously noninteracting pair becomes active at time t upon entering the cutoff, a new auxiliary variable is created and initialized according to the transition probability of the OU process between times $t_{\mu\nu}^*$ and t , which is

$$\begin{aligned} p(\Pi_{\mu\nu}, t \mid \Pi_{\mu\nu}^*, t^*) &= \frac{1}{\sqrt{2\pi(1 - e^{-2\gamma_{\mu\nu}^{\pi}(t-t^*)})}} \\ &\times \exp\left[-\frac{(\Pi_{\mu\nu} - e^{-\gamma_{\mu\nu}^{\pi}(t-t^*)}\Pi_{\mu\nu}^*)^2}{2(1 - e^{-2\gamma_{\mu\nu}^{\pi}(t-t^*)})}\right]. \end{aligned} \quad (120)$$

Therefore, one needs to update only the auxiliary variables by looping over the interaction graph, while inactive pairs are removed and newly active pairs are sampled from Eq. (120).

VIII. CONCLUSIONS

In this work, we have investigated the structure of Markovian embeddings of Hamiltonian coarse-grained dynamics from a first-principles perspective. Starting from Zwanzig's exact GFPE, we have shown that Markovian embeddings are not arbitrary modeling devices: Once one requires that the marginal dynamics reproduces the structural form of the microscopic GFPE—its symmetry properties, positivity, equilibrium structure, and conservation laws—the admissible form of the embedded Markovian process becomes strongly constrained.

By working directly at the level of the generalized Fokker-Planck equation, rather than at the level of a generalized Langevin equation, we were able to identify the precise microscopic constraints that must be respected by any consistent embedding. These constraints fix the equilibrium distribution, the reversible drift, and the covariance governing the coupling between coarse-grained and auxiliary variables in terms of static conditional expectations of microscopic observables. In

particular, the square-root factorization of the kinetic matrix plays a central role, as it determines the structure of admissible couplings and enforces the correct null spaces associated with conserved quantities.

Within this constrained framework, we have derived a minimal and explicit form of the embedded Fokker-Planck equation and its associated stochastic differential equation. Remarkably, a small set of transparent modeling assumptions—chiefly the factorization of the equilibrium distribution in the auxiliary sector and the linearity of the coupling in the auxiliary variables—is sufficient to uniquely fix the structural form of the embedding. All remaining freedom is confined to the relaxation matrix governing the auxiliary dynamics, which may be tuned to reproduce dynamical information such as relaxation spectra or time-correlation functions without violating microscopic consistency.

We have further shown how these general results specialize to both isothermal and nonisothermal coarse-grained particle models. In the isothermal case, the formalism naturally recovers state-dependent Markovian embeddings closely related to recent non-Markovian DPD models [11,12], while clarifying their microscopic meaning: The coupling matrices are identified as square roots of force-force covariances rather than phenomenological friction operators. In the nonisothermal case, explicit treatment of internal energies and conservation laws leads to a structured kinetic matrix whose congruence factorization reveals a natural interpretation in terms of directed particle pairs and velocity differences. This representation not only preserves momentum and energy exactly but also provides a constructive route to efficient implementations based on local interaction graphs.

Beyond the specific models discussed here, the main contribution of this work is conceptual. Rather than proposing a new embedding scheme, we have identified the structural backbone that any admissible Markovian embedding of Hamiltonian coarse-grained dynamics must satisfy. This separation between microscopically dictated structure and genuine modeling degrees of freedom provides a principled basis for the construction, comparison, and assessment of coarse-grained models with memory. It also clarifies which approximations are structural and which are empirical, thereby offering a clearer path toward data-driven and systematically improvable non-Markovian coarse-grained descriptions.

Several directions for future research naturally emerge from the present framework. A particularly promising avenue is the integration of the embedding strategy with modern machine-learning techniques to represent the static quantities S_a , V_a , and Γ_a . Such a combination would enable the construction of quantitatively accurate and thermodynamically consistent coarse-grained models for complex many-body systems, while preserving the structural constraints imposed by microscopic reversibility and conservation laws. Potential applications include non-Markovian barrier-crossing processes [7–9] and conformational transitions in proteins [13,24,66,67], where memory effects play a central role in rare-event dynamics. A second promising direction concerns colloidal particles, macromolecules, and other mesoscopic structures suspended in a solvent, where long-ranged hydrodynamic memory may be captured through reduced Markovian embeddings involving only local auxiliary variables. Whether such

representations can provide accurate and computationally efficient alternatives to conventional hydrodynamic descriptions remains an open question for future work.

Finally, Markovian embeddings with state-dependent memory kernels remain much less understood than their state-independent counterparts, particularly regarding convergence properties and their ability to approximate memory laws beyond finite sums of exponentials. Developing such a theory is an important avenue for future research.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: GFPE FROM MARGINALIZED FPE AND ZWANGIG GFPE

The derivation of the GFPE for the marginal probability distribution $P_a(t)$, starting from the FPE for the joint density $P_{ab}(t)$, can be formulated within the projection-operator framework developed in Ref. [52]. That framework extends Zwanzig’s construction from deterministic Hamiltonian dynamics, governed by the Liouville equation, to stochastic detailed dynamics governed by an FPE. When the selected CG variables are a subset of the detailed variables, the projected equation reduces to the exact marginal evolution for $P_a(t)$. Since the Liouville equation is recovered as a special case of

the FPE, the same formalism also yields the standard Zwanzig GFPE for Hamiltonian microscopic dynamics.

This common framework allows the two routes shown in Fig. 1 to be compared in a single notation: projection of the microscopic Liouville dynamics on the one hand and marginalization of a Markovian embedding on the other.

The mesoscopic degrees of freedom of the system at the detailed level are denoted by $z = \{z_i, \quad i = 1, \dots, N\}$. The probability density $\rho_t(z)$ evolves according to an FPE

$$\partial_t \rho_t(z) = \mathcal{L} \rho_t(z), \quad (\text{A1})$$

where $\mathcal{L}$ is an evolution operator of the form

$$\mathcal{L} = -\partial_i v_i(z) + k_B \partial_i \partial_j d_{ij}(z), \quad (\text{A2})$$

where k_B is the Boltzmann constant, $d_{ij} = d_{ji}$ is a positive definite matrix, ∂_i denotes the partial derivative with respect to z_i , and summation over repeated indices is implied. Note that the derivatives act on every function on their right. The steady state solution of the FPE (A1) is denoted by $\rho^{\text{ss}}(z)$ and satisfies $\mathcal{L} \rho^{\text{ss}} = 0$.

At a coarse-grained level, the system is described by a collection of CG variables $A(z) = \{A^\mu(z), \quad \mu = 1, \dots, m\}$, where m is the number of CG variables, which in general is much smaller than the number N of variables z used to describe the system at the detailed level. Note the use of Greek indices for labeling variables at the coarse level and Latin indices for labeling those at the detailed level.

The probability density $p(\alpha, t)$ for the set of coarse functions $A(z)$ taking values α at time t is related to the actual probability density of z by the pushforward of the microscopic distribution under the mapping $z \mapsto A(z)$:

$$p(\alpha, t) = \int \rho_t(z) \delta(A(z) - \alpha) dz = \text{tr}[\rho_t \Psi_\alpha], \quad (\text{A3})$$

where $\Psi_\alpha(z) = \delta(A(z) - \alpha)$.

The probability density $p(\alpha, t)$ obeys the following *exact* GFPE [52]:

$$\begin{aligned} \partial_t p(\alpha, t) = & -\partial_\mu \langle v_+^\mu \rangle^\alpha p(\alpha, t) + k_B \partial_\mu \partial_\nu \langle d^{\mu\nu} \rangle^\alpha p(\alpha, t) \\ & + k_B \partial_\mu \int d\alpha' \int_0^t du D^{\mu\mu'}(\alpha, \alpha', t-u) P^{\text{ss}}(\alpha') \partial_{\mu'} \frac{p(\alpha', u)}{P^{\text{ss}}(\alpha')} \\ & - k_B^2 \partial_\mu \partial_\nu \int d\alpha' \int_0^t du K_-^{\mu\nu\mu'}(\alpha, \alpha', t-u) P^{\text{ss}}(\alpha') \partial_{\mu'} \frac{p(\alpha', u)}{P^{\text{ss}}(\alpha')} \\ & - k_B^2 \partial_\mu \int d\alpha' \int_0^t du K_+^{\mu\mu'\nu'}(\alpha, \alpha', t-u) P^{\text{ss}}(\alpha') \partial_{\mu'} \partial_{\nu'} \frac{p(\alpha', u)}{P^{\text{ss}}(\alpha')} \\ & + k_B^3 \partial_\mu \partial_\nu \int d\alpha' \int_0^t du K^{\mu\nu\mu'\nu'}(\alpha, \alpha', t-u) P^{\text{ss}}(\alpha') \partial_{\mu'} \partial_{\nu'} \frac{p(\alpha', u)}{P^{\text{ss}}(\alpha')}, \end{aligned} \quad (\text{A4})$$

where we have defined the following memory kernels:

$$\begin{aligned} D^{\mu\mu'}(\alpha, \alpha', t-u) &= \frac{1}{k_B} \frac{1}{P^{\text{ss}}(\alpha')} \text{tr}[\rho^{\text{ss}}(e^{\mathcal{Q}\mathcal{L}^{-u}}(v_-^{\mu'} - \langle v_-^{\mu'} \rangle^{\alpha'}) \Psi_{\alpha'}) (e^{\mathcal{Q}\mathcal{L}^{+t}}(v_+^\mu - \langle v_+^\mu \rangle^\alpha) \Psi_\alpha)], \\ K_-^{\mu\nu\mu'}(\alpha, \alpha', t-u) &= \frac{1}{k_B} \frac{1}{P^{\text{ss}}(\alpha')} \text{tr}[\rho^{\text{ss}}(e^{\mathcal{Q}\mathcal{L}^{-u}}(v_-^{\mu'} - \langle v_-^{\mu'} \rangle^{\alpha'}) \Psi_{\alpha'}) (e^{\mathcal{Q}\mathcal{L}^{+t}}(d^{\mu\nu} - \langle d^{\mu\nu} \rangle^\alpha) \Psi_\alpha)], \\ K_+^{\mu\mu'\nu'}(\alpha, \alpha', t-u) &= \frac{1}{k_B} \frac{1}{P^{\text{ss}}(\alpha')} \text{tr}[\rho^{\text{ss}}(e^{\mathcal{Q}\mathcal{L}^{-u}}(d^{\mu\nu'} - \langle d^{\mu\nu'} \rangle^{\alpha'}) \Psi_{\alpha'}) (e^{\mathcal{Q}\mathcal{L}^{+t}}(v_+^\mu - \langle v_+^\mu \rangle^\alpha) \Psi_\alpha)], \\ K^{\mu\nu\mu'\nu'}(\alpha, \alpha', t-u) &= \frac{1}{k_B} \frac{1}{P^{\text{ss}}(\alpha')} \text{tr}[\rho^{\text{ss}}(e^{\mathcal{Q}\mathcal{L}^{-u}}(d^{\mu\nu'} - \langle d^{\mu\nu'} \rangle^{\alpha'}) \Psi_{\alpha'}) (e^{\mathcal{Q}\mathcal{L}^{+t}}(d^{\mu\nu} - \langle d^{\mu\nu} \rangle^\alpha) \Psi_\alpha)]. \end{aligned} \quad (\text{A5})$$

We have introduced

$$\begin{aligned} v_{\pm}^{\mu} &= \mathcal{L}^{\pm} A^{\mu}, \\ d^{\mu\nu} &= d_{ij}(\partial_i A^{\mu})(\partial_j A^{\nu}). \end{aligned} \quad (\text{A6})$$

The dynamic operators $\mathcal{L}^+$ and $\mathcal{L}^-$ are

$$\mathcal{L}^+ = v_i(z)\partial_i + k_B d_{ij}(z)\partial_i\partial_j, \quad (\text{A7})$$

$$\mathcal{L}^- = \left[v_i(z) - \frac{2k_B}{\rho^{\text{ss}}(z)} \partial_j (d_{ij} \rho^{\text{ss}}(z)) \right] \partial_i - k_B d_{ij}(z)\partial_i\partial_j. \quad (\text{A8})$$

The constrained average over the submanifold $A(z) = \alpha$ is defined by

$$\langle F \rangle^{\alpha} = \int \rho_{\alpha}(z) F(z) dz, \quad (\text{A9})$$

where the constrained ensemble is

$$\rho_{\alpha}(z) = \frac{1}{P^{\text{ss}}(\alpha)} \rho^{\text{ss}}(z) \delta(A(z) - \alpha), \quad (\text{A10})$$

with normalization

$$P^{\text{ss}}(\alpha) = \int \rho^{\text{ss}}(z) \delta(A(z) - \alpha) dz. \quad (\text{A11})$$

Finally, the projector $\mathcal{Q} = 1 - \mathcal{P}$ is the complement of the projector $\mathcal{P}$:

$$\mathcal{P}F = \int \langle F \rangle^{\alpha} \Psi_{\alpha} d\alpha. \quad (\text{A12})$$

Observe that the time dependence of the memory kernels [Eq. (A5)] is through $t - u$, because

$$\text{tr}[\rho^{\text{ss}} F e^{\mathcal{Q}\mathcal{L}^+ t} G] = \text{tr}[\rho^{\text{ss}} G e^{-\mathcal{Q}\mathcal{L}^- t} F], \quad (\text{A13})$$

which can be proved by using the series expansion of the exponential operator and using

$$\text{tr}[\rho^{\text{ss}} F \mathcal{L}^+ G] = -\text{tr}[\rho^{\text{ss}} G \mathcal{L}^- F], \quad (\text{A14})$$

as can be seen by noting that each side of Eq. (A14) equals $\text{tr}[G \mathcal{L} \rho^{\text{ss}} F]$.

1. Zwanzig GFPE

When we set $d_{ij} = 0$ in Eq. (A2), we obtain a deterministic evolution. The Liouville equation $\partial_t \rho_t = i\mathcal{L} \rho_t$ of Classical Mechanics is then a special case of Eq. (A1) that, in addition, satisfies $\partial_i^{\text{T}} \cdot v_i = 0$ (Liouville's theorem). This last property ensures that the Liouville dynamical operator $i\mathcal{L} = v_i^{\text{T}} \cdot \partial_i$ is self-adjoint. Setting $d_{ij} = 0$ implies that $d^{\mu\nu} = 0$ and $\mathcal{L}^{\pm} = i\mathcal{L}$. The GFPE reduces to

$$\partial_t p(\alpha, t) = -\partial_{\mu} V^{\mu}(\alpha) p(\alpha, t) + k_B \partial_{\mu} \int d\alpha' \int_0^t du D^{\mu\mu'}(\alpha, \alpha', t - u) P^{\text{ss}}(\alpha') \partial_{\mu'} \frac{p(\alpha', u)}{P^{\text{ss}}(\alpha')}, \quad (\text{A15})$$

with

$$\begin{aligned} V(\alpha) &= \langle i\mathcal{L}\hat{A} \rangle^{\alpha}, \\ D^{\mu\mu'}(\alpha, \alpha', t - u) &= \frac{1}{k_B} \frac{1}{P^{\text{ss}}(\alpha')} \text{tr}[\rho^{\text{ss}}(e^{\mathcal{Q}i\mathcal{L}u} (i\mathcal{L}\hat{A}^{\mu'} - \langle i\mathcal{L}\hat{A}^{\mu'} \rangle^{\alpha'}) \Psi_{\alpha'}) (e^{\mathcal{Q}i\mathcal{L}t} (i\mathcal{L}\hat{A}^{\mu} - \langle i\mathcal{L}\hat{A}^{\mu} \rangle^{\alpha}) \Psi_{\alpha})]. \end{aligned} \quad (\text{A16})$$

This is the GFPE first obtained by Zwanzig [17]. In the notation of the present paper, we have

$$\begin{aligned} \alpha &\rightarrow a, \\ P^{\text{ss}}(\alpha) &\rightarrow P_a^{\text{eq}}, \\ V(\alpha) &\rightarrow V_a, \\ D(\alpha, \alpha', t - u) &\rightarrow D_{aa'}(t - u). \end{aligned} \quad (\text{A17})$$

Then, Eq. (A15) gives the GFPE (3) in the main text.

2. Marginalizing an FPE

In order to find the GFPE that governs the evolution of the marginal $P_a(t)$ of the joint probability $p_{ab}(t)$ given by Eq. (31), we may particularize the GFPE (A4) to the case that the selected CG variables are a subset of the FG variables. In other words, we write $z = (a, b)$, with $a \in \mathbb{R}^m$, $b \in \mathbb{R}^n$, and take the CG variables to be the identity function, $\hat{A}(z) = a$, selecting the first m components of z . This implies that

$$\partial_i A^{\mu} = \delta_{i\mu}. \quad (\text{A18})$$

Latin index goes over the components of z so $i = 1, \dots, m + n$, while Greek index μ goes over $1, \dots, m$ corresponding to the selected CG variables.

The correspondence of the different quantities introduced in Ref. [52] and those introduced in Sec. III is the following:

$$\begin{aligned} \Psi_{\alpha}(z) &\rightarrow \delta(a - \alpha), \\ \rho_t(z) &\rightarrow p_{ab}(t), \\ \rho^{\text{ss}}(z) &\rightarrow p_{ab}^{\text{eq}}(t), \\ p(\alpha, t) &\rightarrow P_a(t), \\ P^{\text{ss}}(\alpha) &\rightarrow P_a^{\text{eq}}, \\ \rho_{\alpha}(z) &\rightarrow p_{b|a}^{\text{eq}} \delta(a - \alpha), \\ \mathcal{P}^+ F(z) &\rightarrow p_{b|a}^{\text{eq}} \int db' F_{ab'}, \\ \langle F \rangle^{\alpha} &\rightarrow \int db p_{b|a}^{\text{eq}} F_{ab} \stackrel{(44)}{=} \left[F \right]^a, \\ \mathcal{P} F_{ab} &\rightarrow \int db p_{b|a}^{\text{eq}} F_{ab} \stackrel{(44)}{=} \left[F \right]^a. \end{aligned} \quad (\text{A19})$$

The operator $\mathcal{L}$ defined in Eq. (A2) differs from the operator introduced in Eq. (33) in the ordering of derivatives. A direct comparison yields

$$\begin{aligned}\mathcal{L} &\stackrel{(A2)}{=} -\partial_i(v_i - k_B \partial_j d_{ij}) + k_B \partial_i d_{ij} \partial_j \\ &\stackrel{(33)}{=} -\partial_i v_i + \partial_i \mathbf{d}_{ij}^S \partial_j.\end{aligned}\quad (\text{A20})$$

Matching the two representations leads to the identifications

$$\begin{aligned}k_B d_{ij} &\longrightarrow \mathbf{d}_{ij}^S, \\ v_i &\longrightarrow v_i + \partial_j \mathbf{d}_{ij}^S,\end{aligned}\quad (\text{A21})$$

where $\mathbf{d}_{ij}^S$ denotes the symmetric part of $\mathbf{d}_{ij}$,

$$\mathbf{d}_{ij}^S = \frac{1}{2}(\mathbf{d}_{ij} + \mathbf{d}_{ji}). \quad (\text{A22})$$

In Ref. [52], the tensor d_{ij} is assumed to be symmetric, whereas the tensor $\mathbf{d}_{ij}$ in Eq. (33) is not required to satisfy this constraint. Since only the symmetric part contributes to the second-order diffusion operator, the identification naturally involves $\mathbf{d}_{ij}^S$. The antisymmetric component, however, can be retained as a modeling degree of freedom. Such skew-symmetric contributions do not generate diffusion but instead modify the effective drift, and they are often responsible for oscillatory behavior that may be required in certain applications.

On the other hand, the operator $\mathcal{L}^+$ introduced in Eq. (A7) takes the form

$$\mathcal{L}^+ \stackrel{(A21)}{=} (v_i + (\partial_j \mathbf{d}_{ij}^S)) \partial_i + \mathbf{d}_{ij}^S \partial_i \partial_j, \quad (\text{A23})$$

while the operator $\mathcal{L}^-$ introduced in Eq. (A8) takes the form

$$\mathcal{L}^- \stackrel{(A21)}{=} [v_i - \partial_j \mathbf{d}_{ij}^S - 2(\mathbf{d}_{ij}^S \partial_j \ln \rho^{ss})] \partial_i - \mathbf{d}_{ij}^S \partial_i \partial_j. \quad (\text{A24})$$

Once we use Eq. (A18), the quantities defined in Eq. (A6) take the form

$$\begin{aligned}v_+^\mu &\stackrel{(A23)}{=} (v_i + (\partial_j \mathbf{d}_{ij}^S)) \partial_i A^\mu + \mathbf{d}_{ij}^S \partial_i \partial_j A^\mu \\ &\stackrel{(36)}{=} \left[\mathbf{A} + \partial_a \cdot \frac{\mathbf{C} + \mathbf{C}^T}{2} + \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2} \right]^\mu, \\ v_-^\mu &\stackrel{(A23)}{=} \left[\mathbf{A} - \partial_a \cdot \frac{\mathbf{C} + \mathbf{C}^T}{2} - \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2} \right]^\mu \\ &\quad - 2 \left[\frac{\mathbf{C} + \mathbf{C}^T}{2} \cdot \partial_a k_B \ln P_{ab}^{\text{eq}} + \frac{\mathbf{E} + \mathbf{F}^T}{2} \cdot \partial_b k_B \ln P_{ab}^{\text{eq}} \right]^\mu, \\ k_B d^{\mu\nu} &\stackrel{(A6)}{=} \mathbf{d}_{ij}^S (\partial_i A^\mu) (\partial_j A^\nu) \stackrel{(36)}{=} \left[\frac{\mathbf{C} + \mathbf{C}^T}{2} \right]^{\mu\nu}.\end{aligned}\quad (\text{A25})$$

A crucial observation is that the Zwanzig GFPE (A15) contains at most second-order partial derivatives, whereas the marginalized GFPE (A4) generally involves third- and fourth-order derivatives. These higher-order contributions originate from the tensor $d^{\mu\nu}$. To ensure that the marginalized equation retains the same structural form as the Zwanzig GFPE, the third- and fourth-order derivative terms must vanish. This requirement is satisfied by imposing $d^{\mu\nu} = 0$ or, equivalently,

$$\mathbf{C} = 0, \quad (\text{A26})$$

in such a way that Eq. (A25) simplifies to

$$\begin{aligned}v_+^\mu &= \left[\mathbf{A} + \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2} \right]^\mu, \\ v_-^\mu &= \left[\mathbf{A} - \partial_b \cdot \frac{\mathbf{E} + \mathbf{F}^T}{2} \right]^\mu - [(\mathbf{E} + \mathbf{F}^T) \cdot \partial_b \ln P_{ab}^{\text{eq}}]^\mu, \\ k_B d^{\mu\nu} &= 0,\end{aligned}\quad (\text{A27})$$

and, consequently, the GFPE (A4) becomes

$$\begin{aligned}\partial_t P_a(t) &= -\partial_a \cdot \bar{V}_a P_a(t) \\ &\quad + k_B \partial_a \int da' \int_0^t du \bar{D}_{aa'}(t-u) P_{a'}^{\text{eq}} \partial_{a'} \frac{P_{a'}(u)}{P_{a'}^{\text{eq}}},\end{aligned}\quad (\text{A28})$$

where

$$\begin{aligned}\bar{V}_a &= \left[v^+ \right]^a, \\ \bar{D}_{aa'}(t-u) &= \frac{1}{P_{a'}^{\text{eq}}} \int dx p_x^{\text{eq}} \\ &\quad \times \left[e^{\mathcal{Q} \mathcal{L}^- u} \left(v_x^+ - \left[v^+ \right]^{a'} \right) \Psi_{a'}(x) \right] \\ &\quad \times \left[e^{\mathcal{Q} \mathcal{L}^+ t} \left(v_x^- - \left[v^- \right]^a \right) \Psi_a(x) \right],\end{aligned}\quad (\text{A29})$$

Here, $x = (a'', b'')$ and $\Psi_a(x) = \delta(a - a'')$.

By using the property in Eq. (A13), the memory kernel takes the form

$$\begin{aligned}\bar{D}_{aa'}(t-u) &= \frac{1}{P_{a'}^{\text{eq}}} \int db p_{a'b}^{\text{eq}} \left(v_{a'b}^+ - \left[v^+ \right]^{a'} \right) \\ &\quad \times \left[e^{\mathcal{Q} \mathcal{L}^+(t-u)} \left(v_{ab}^- - \left[v^- \right]^a \right) \delta_{aa'} \right]\end{aligned}\quad (\text{A30})$$

that implies

$$\begin{aligned}\bar{D}_{aa'}(0) &= \delta_{aa'} \frac{1}{P_{a'}^{\text{eq}}} \int db p_{a'b}^{\text{eq}} \\ &\quad \times \left(v_{a'b}^+ - \left[v^+ \right]^{a'} \right) \left(v_{ab}^- - \left[v^- \right]^a \right),\end{aligned}\quad (\text{A31})$$

which leads to Eq. (23) with Eq. (24).

APPENDIX B: MICROSCOPIC REVERSIBILITY AND DETAILED BALANCE

In this Appendix, we demonstrate that microscopic reversibility of Hamilton's equations imposes specific symmetry properties on both the drift and the memory kernel of Zwanzig's GFPE. We then show that these same symmetries are inherited by the drift and memory kernel of the marginalized GFPE, provided that the FPE in the embedded space satisfies the necessary and sufficient conditions for detailed balance. Finally, we analyze how detailed balance constrains the fundamental building blocks of the embedding FPE.

1. Microscopic reversibility in Zwanzig's GFPE

Microscopic reversibility of the underlying Hamiltonian dynamics imposes important symmetry properties on the

fundamental building blocks of the theory. Let the CG variables $\hat{A}(z)$ possess a well-defined parity under time reversal, i.e.,

$$\hat{A}(\epsilon z) = \epsilon \hat{A}(z), \quad (\text{B1})$$

where $\epsilon \in \mathbb{R}^{6N \times 6N}$ is a diagonal matrix with entries ± 1 implementing the microscopic time-reversal transformation $q \rightarrow q$, $p \rightarrow -p$, and $\epsilon \in \mathbb{R}^{n \times n}$ is a diagonal matrix with entries ± 1 specifying the time-reversal character of each CG variable.

Then, microscopic reversibility implies [19,51]

$$\begin{aligned} E_{\epsilon \cdot a} &= E_a, \\ S_{\epsilon \cdot a} &= S_a, \\ P_{\epsilon \cdot a}^{\text{eq}} &= P_a^{\text{eq}}, \\ V_{\epsilon \cdot a} &= -\epsilon \cdot V_a, \\ \Omega_{a'} D_{\epsilon \cdot a \epsilon \cdot a'}(t) &= \Omega_a \epsilon \cdot D_{a'}^T(-t) \cdot \epsilon. \end{aligned} \quad (\text{B2})$$

In the Markovian approximation of the GFPE, the last identity leads to the celebrated Onsager reciprocity relations. Finally, at $t = 0$ and using Eq. (23) the microscopic reversibility condition (B2) implies

$$\Gamma_{\epsilon \cdot a} = \epsilon \cdot \Gamma_a \cdot \epsilon. \quad (\text{B3})$$

We want to show that the same properties [Eq. (B2)] are satisfied by the induced building blocks. In particular,

$$\begin{aligned} \bar{V}_{\epsilon \cdot a} &= -\epsilon \cdot \bar{V}_a, \\ \Omega_{a'} \bar{D}_{\epsilon \cdot a \epsilon \cdot a'}(t) &= \Omega_a \epsilon \cdot \bar{D}_{a'}^T(-t) \cdot \epsilon. \end{aligned} \quad (\text{B4})$$

This can be proved if the FPE for the joint probability satisfies the property of detailed balance. The proof follows closely the steps given in Sec. IV of Ref. [52], where we have proved that in the Markovian limit the induced FPE equations do satisfy the detailed balance conditions.

2. Detailed balance in marginalized GFPE

Detailed balance is not a property tied to a particular CG level of description, but a structural consequence of microscopic time-reversal invariance [52]. Since the underlying Hamiltonian dynamics satisfies detailed balance with respect to the equilibrium measure, any consistent CG description of the same equilibrium system must inherit this property. In particular, it is natural to impose detailed balance at the level of the Fokker-Planck equation defined in the embedded space. With this choice, the marginalized GFPE (38) preserves microscopic reversibility—reflected in Eq. (B4), and its corresponding Markovian limit would yield an FPE satisfying detailed balance by construction.

To impose detailed balance on the FPE in the embedded space, we assume that the variables $x = (a, b)$ have a well-defined parity $\bar{\epsilon} \cdot x$, where $\bar{\epsilon} = \epsilon \oplus \bar{\epsilon} \in \mathbb{R}^{(n+m) \times (n+m)}$ is a diagonal matrix with ± 1 entries depending on the time-reversal character of each variable. The time-reversal character ϵ of the CG variables a is determined by the CG mapping $\hat{A}(z)$, whereas the time-reversal character $\bar{\epsilon}$ of the auxiliary variables b is, in principle, a modeling choice. We will see later that imposing detailed balance constraints $\bar{\epsilon}$.

From the FPE (32) with (33), we construct the reversible and irreversible drifts according to

$$\begin{aligned} \mathbf{v}^{\text{rev}}(x) &= \frac{1}{2}[\mathbf{V}(x) - \bar{\epsilon} \cdot \mathbf{V}(\bar{\epsilon} \cdot x)], \\ \mathbf{v}^{\text{irr}}(x) &= \frac{1}{2}[\mathbf{V}(x) + \bar{\epsilon} \cdot \mathbf{V}(\bar{\epsilon} \cdot x)]. \end{aligned} \quad (\text{B5})$$

The necessary and sufficient conditions for the FPE (37) to satisfy detailed balance are [68]

$$p^{\text{eq}}(\bar{\epsilon} \cdot x) = p^{\text{eq}}(x), \quad (\text{B6})$$

$$\mathbf{d}(\bar{\epsilon} \cdot x) = \bar{\epsilon} \cdot \mathbf{d}(x) \cdot \bar{\epsilon}, \quad (\text{B7})$$

$$\mathbf{v}^{\text{irr}}(x) = \mathbf{d}(x) \cdot \partial_x \ln p^{\text{eq}}(x). \quad (\text{B8})$$

In terms of $\mathbf{A}_x, \mathbf{B}_x$, we have

$$\mathbf{v}^{\text{rev}} = \frac{1}{2} \begin{pmatrix} \mathbf{A}_x - \epsilon \cdot \mathbf{A}_{\bar{\epsilon} \cdot x} \\ \mathbf{B}_x - \bar{\epsilon} \cdot \mathbf{B}_{\bar{\epsilon} \cdot x} \end{pmatrix}, \quad (\text{B9})$$

$$\mathbf{v}^{\text{irr}} = \frac{1}{2} \begin{pmatrix} \mathbf{A}_x + \epsilon \cdot \mathbf{A}_{\bar{\epsilon} \cdot x} \\ \mathbf{B}_x + \bar{\epsilon} \cdot \mathbf{B}_{\bar{\epsilon} \cdot x} \end{pmatrix}. \quad (\text{B10})$$

The second condition (B7) implies

$$\begin{aligned} \mathbf{C}_{\bar{\epsilon} \cdot x} &= \epsilon \cdot \mathbf{C}_x \cdot \epsilon, \\ \mathbf{E}_{\bar{\epsilon} \cdot x} &= \epsilon \cdot \mathbf{E}_x \cdot \bar{\epsilon}, \\ \mathbf{F}_{\bar{\epsilon} \cdot x} &= \bar{\epsilon} \cdot \mathbf{F}_x \cdot \epsilon, \\ \mathbf{H}_{\bar{\epsilon} \cdot x} &= \bar{\epsilon} \cdot \mathbf{H}_x \cdot \bar{\epsilon}. \end{aligned} \quad (\text{B11})$$

The third condition (B8) reads in matrix form

$$\frac{1}{2} \begin{pmatrix} \mathbf{A}_x + \epsilon \cdot \mathbf{A}_{\bar{\epsilon} \cdot x} \\ \mathbf{B}_x + \bar{\epsilon} \cdot \mathbf{B}_{\bar{\epsilon} \cdot x} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_x & \mathbf{E}_x \\ \mathbf{F}_x & \mathbf{H}_x \end{pmatrix} \cdot \begin{pmatrix} \partial_a \ln p_x^{\text{eq}} \\ \partial_b \ln p_x^{\text{eq}} \end{pmatrix}, \quad (\text{B12})$$

that is,

$$\begin{aligned} \frac{1}{2}(\mathbf{A}_x + \epsilon \cdot \mathbf{A}_{\bar{\epsilon} \cdot x}) &= \mathbf{C}_x \cdot \partial_a \ln p_x^{\text{eq}} + \mathbf{E}_x \cdot \partial_b \ln p_x^{\text{eq}}, \\ \frac{1}{2}(\mathbf{B}_x + \bar{\epsilon} \cdot \mathbf{B}_{\bar{\epsilon} \cdot x}) &= \mathbf{F}_x \cdot \partial_a \ln p_x^{\text{eq}} + \mathbf{H}_x \cdot \partial_b \ln p_x^{\text{eq}}. \end{aligned} \quad (\text{B13})$$

3. Implications of detailed balance for the FPE (81)

The final FPE (81) is obtained under the modeling assumptions, $\mathbf{C} = 0$, $\mathbf{E} = 0$, $\mathbf{F} = 0$, with the ansatz [Eq. (59)]. In this case, the detailed balance conditions (B13) become

$$\begin{aligned} \mathbf{A}_{\bar{\epsilon} \cdot x} &= -\epsilon \cdot \mathbf{A}_x, \\ \frac{1}{2}(\mathbf{B}_x + \bar{\epsilon} \cdot \mathbf{B}_{\bar{\epsilon} \cdot x}) &= -\mathbf{H} \cdot b. \end{aligned} \quad (\text{B14})$$

Using Eq. (80),

$$\frac{1}{2}[-\mathbf{I}_a - \mathbf{H}_a \cdot b + \bar{\epsilon} \cdot (-\mathbf{I}_{\epsilon \cdot a} - \mathbf{H}_{\epsilon \cdot a} \cdot \bar{\epsilon} b)] = -\mathbf{H} \cdot b. \quad (\text{B15})$$

Using the last equation in Eq. (B11), this condition reduces to

$$\mathbf{I}_{\epsilon \cdot a} = -\bar{\epsilon} \cdot \mathbf{I}_a. \quad (\text{B16})$$

From the definition (76), we may satisfy Eq. (B16) provided that $\mathbf{W}_{\epsilon \cdot a} = -\epsilon \cdot \mathbf{W}_a \cdot \bar{\epsilon}$.

In summary, detailed balance in the enlarged state space is automatically satisfied by the Fokker-Planck equation

provided that

$$W_{\epsilon \cdot a} = -\epsilon \cdot W_a \cdot \bar{\epsilon}, \quad (\text{B17})$$

$$H_{\epsilon \cdot a} = \bar{\epsilon} \cdot H_a \cdot \bar{\epsilon}. \quad (\text{B18})$$

These relations express the compatibility of the Markovian embedding with time reversal. Once a factorization W_a of the friction matrix Γ_a has been constructed, condition (B17) can be enforced by assigning an appropriate time-reversal parity, represented by $\bar{\epsilon}$, to the auxiliary variables. Equation (B18) then becomes a structural constraint on the admissible functional form of H_a .

APPENDIX C: SOLUTION OF EQ. (79)

We write Eq. (79) in the form

$$\partial_b \cdot i_{ab} - i_{ab} \cdot b + H_a : (\mathbb{1} - bb^T) = 0, \quad (\text{C1})$$

where

$$i_{ab} \equiv i_a + B_{ab}. \quad (\text{C2})$$

This is a divergence equation for the vector field i_{ab} . It constrains the admissible functional forms of this field but does not determine it uniquely, since infinitely many solutions exist: any solenoidal (divergence-free) vector field may be added without violating the equation. In fact, the general solution is

$$i_{ab} = -H_a \cdot b + e^{b^2/4} C_b, \quad (\text{C3})$$

where C_b is any divergence-free vector field $\partial_b \cdot C_b = 0$, as can be verified by simple substitution. Due to the explosive Gaussian prefactor, it seems natural to choose $C_b = 0$, and we obtain a particularly simple solution

$$i_{ab} = -H_a \cdot b. \quad (\text{C4})$$

With Eqs. (C2) and (C4), this implies Eq. (80).

APPENDIX D: ELIMINATION OF THE AUXILIARY VARIABLES AND INDUCED GLE

In this Appendix, we discuss the GLE induced by eliminating the auxiliary variables from the embedded dynamics. This elimination is the standard route in Markovian embeddings with state-independent memory kernels, but it becomes more subtle when the memory is state dependent. For this reason, the main text follows the GFPE route, where the consistency requirements between the embedding and the microscopically exact GFPE can be imposed directly.

The embedded dynamics [Eq. (82)] defines a Markov process in the enlarged space (a, b) . Therefore, the fundamental stochastic process is the joint process (a_t, b_t) , not a closed equation for a_t alone. Still, because the equation for the auxiliary variables is linear in b_t , one may eliminate b_t explicitly and obtain an exact self-consistent non-Markovian representation for the CG variables.

Starting from Eq. (82), we write the auxiliary equation as

$$db_t = \eta_{a_t} dt - H_{a_t} \cdot b_t dt + \sigma_{a_t} d\mathcal{W}_t, \quad (\text{D1})$$

where

$$\eta_a \equiv W_a^T \cdot \partial_a S_a + \partial_a \cdot W_a^T. \quad (\text{D2})$$

The divergence term in Eq. (D2) is defined componentwise by

$$(\partial_a \cdot W_a^T)_i \equiv \partial_{a_\mu} (W_a^T)_{i\mu}, \quad (\text{D3})$$

where μ labels CG components and i labels auxiliary components.

For each realization of the joint process, define the random propagator $G_a(t, s)$ by

$$\partial_t G_a(t, s) = -H_{a_t} \cdot G_a(t, s), \quad G_a(s, s) = \mathbf{1}. \quad (\text{D4})$$

The subscript a emphasizes that $G_a(t, s)$ is a functional of the trajectory $a(\cdot)$. The solution of Eq. (D1) is then

$$b_t = G_a(t, 0) \cdot b_0 + \int_0^t ds G_a(t, s) \cdot \eta_{a_s} + \int_0^t G_a(t, s) \cdot \sigma_{a_s} d\mathcal{W}_s. \quad (\text{D5})$$

Substitution into the equation for a_t gives

$$\frac{da_t}{dt} = V_{a_t} + \int_0^t ds W_{a_t} \cdot G_a(t, s) \cdot \eta_{a_s} + \mathcal{F}_t, \quad (\text{D6})$$

where the induced force is

$$\mathcal{F}_t = W_{a_t} \cdot G_a(t, 0) \cdot b_0 + W_{a_t} \cdot \int_0^t G_a(t, s) \cdot \sigma_{a_s} d\mathcal{W}_s. \quad (\text{D7})$$

Equivalently, using Eq. (D2), the deterministic memory contribution may be written as

$$\frac{da_t}{dt} = V_{a_t} + \int_0^t ds W_{a_t} \cdot G_a(t, s) \cdot W_{a_s}^T \cdot \partial_a S_{a_s} + \int_0^t ds W_{a_t} \cdot G_a(t, s) \cdot \partial_a \cdot W_{a_s}^T + \mathcal{F}_t. \quad (\text{D8})$$

Equations (D6) and (D7) define the induced GLE associated with the Markovian embedding. This equation is an exact rewriting of the same stochastic process, but it should not be interpreted as a GLE driven by an externally prescribed colored noise. The reason is that a_t is itself driven by b_t , while b_t is driven by the Wiener process. Consequently, the propagator $G_a(t, s)$, the coupling W_{a_t} , and the noise amplitude σ_{a_t} are random functionals of the same trajectory and of the same noise that generate $\mathcal{F}_t$. The induced force is therefore multiplicative, history dependent, and in general correlated with the CG trajectory.

The formal elimination identifies the trajectory-dependent memory tensor generated by the embedding,

$$D_a(t, s) = W_{a_t} \cdot G_a(t, s) \cdot W_{a_s}^T, \quad t \geq s. \quad (\text{D9})$$

This object is the memory tensor induced by the chosen embedding. Its agreement with the microscopic Zwanzig memory kernel is not automatic; it is an additional consistency requirement on the model.

We now discuss the statistics of the induced force. For a prescribed coarse trajectory $a(\cdot)$, the force $\mathcal{F}_t$ is Gaussian whenever b_0 is Gaussian, because it is linear in b_0 and in the Wiener increments. This prescribed-path statement is useful for identifying the local colored-noise structure of the embedding, but it does not define the statistics of the full coupled process. In the full process, the coefficients entering $\mathcal{F}_t$ are themselves stochastic and correlated with the force.

Assume that the auxiliary variables are initially distributed according to their stationary conditional distribution,

$$\langle b_0 \rangle = 0, \quad \langle b_0 b_0^\top \rangle = \mathbf{1}, \quad (\text{D10})$$

and that b_0 is independent of the Wiener increments. For a prescribed path $a(\cdot)$, the induced force has zero mean,

$$\langle \mathcal{F}_t \rangle_{b_0, \mathcal{W}|a(\cdot)} = 0, \quad (\text{D11})$$

and covariance

$$\begin{aligned} \langle \mathcal{F}_t \mathcal{F}_{t'}^\top \rangle_{b_0, \mathcal{W}|a(\cdot)} &= W_{a_t} \cdot G_a(t, 0) \cdot G_a(t', 0)^\top \\ &+ W_{a_t} \cdot \int_0^{\min(t, t')} ds G_a(t, s) \cdot \sigma_{a_s} \cdot \sigma_{a_s}^\top \cdot G_a(t', s)^\top \cdot W_{a_{t'}}^\top. \end{aligned} \quad (\text{D12})$$

Using Eq. (83), this expression gives the colored-noise covariance associated with the embedding along the prescribed path.

The covariance in the full coupled process is obtained by averaging also over the random trajectories $a(\cdot)$.

Formally,

$$\begin{aligned} \langle \mathcal{F}_t \mathcal{F}_{t'}^\top \rangle &= \langle W_{a_t} \cdot G_a(t, 0) \cdot b_0 b_0^\top \cdot G_a(t', 0)^\top \rangle \\ &+ \left\langle W_{a_t} \cdot \int_0^{\min(t, t')} ds G_a(t, s) \cdot \sigma_{a_s} \cdot \sigma_{a_s}^\top \right. \\ &\quad \left. \cdot G_a(t', s)^\top \cdot W_{a_{t'}}^\top \right\rangle, \end{aligned} \quad (\text{D13})$$

where the outer average is taken with respect to the joint Markov process (a_t, b_t) . In general, this covariance is not stationary and does not reduce to a function of $t - t'$ alone. It also need not be Gaussian, even if the prescribed-path force is Gaussian, because the coefficients are random and correlated with the noise.

The familiar FDT form is recovered in the simpler case in which the coefficients are frozen at a fixed value of a . With the stationary auxiliary initial condition (D10), the propagator becomes

$$G_a(t, t') = \exp[-H_a(t - t')], \quad t \geq t', \quad (\text{D14})$$

and Eq. (D12) reduces to

$$\langle \mathcal{F}_t \mathcal{F}_{t'}^\top \rangle_a = W_a \cdot e^{-H_a(t - t')} \cdot W_a^\top, \quad t \geq t'. \quad (\text{D15})$$

Thus, in the frozen-coefficient limit, the induced colored force has covariance equal to the memory kernel generated by the embedding,

$$D_a(t - t') = W_a \cdot e^{-H_a(t - t')} \cdot W_a^\top. \quad (\text{D16})$$

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