Einstein-Helfand form for transport coefficients from coarse-grained descriptions

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We revisit the statistical mechanics problem of coarse-graining a system that at a detailed level is described by an already coarse-grained dynamics. The dynamics at the more detailed level is described by a Fokker-Planck equation instead of the Liouville equation. The method generalizes Zwanzig theory of projection operators and produces a friction matrix in terms of a correlation function that is not manifestly an autocorrelation. Therefore, from this expression, it is not obvious that the friction matrix is definite positive. We show that the Green-Kubo transport matrix can be written in the Einstein-Helfand form, which is manifestly positive definite. We also discuss the role of time reversal and detailed balance in the coarse-grained dynamics.

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I. INTRODUCTION

The theory of coarse-graining deals with the art of representing the dynamics of a system with a number of variables much smaller that the actual degrees of freedom of its molecular constituents. This is the central theme of Statistical Mechanics. In order to *understand* the general features of the dynamics of the very large number of molecules involved in any macroscopic system, it is clearly necessary to identify gross features of the dynamics and concentrate our attention on those. In that sense, coarse-graining is the art of pattern recognition. Previous experience, intuition, and trial and error are crucial in the process of selecting the few *relevant variables* that will capture the gross features that are of our interest. The good news is that if the relevant variables are "good" ones, in the sense of being "slow," then the theory of coarse-graining acts as a black box by providing the general dynamic equation for these variables.

The theory of coarse-graining is also known as nonequilibrium statistical mechanics and was formulated in the midst of the last century by Kirkwood [1,2], Green [3], Zwanzig [4], Mori [5], and many others [6]. In our opinion, its most elegant and general formulation is that of Zwanzig [4] who, with the aid of a projection operator technique, derived from the Liouville equation of the microscopic system the Fokker-Planck equation (FPE) governing the probability distribution of the coarse variables. The Fokker-Planck equation was previously obtained by Green by using stochastic arguments [3]. The textbook by Grabert presents in great detail this formulation [7] (see also [6,8]).

The problem we address in this paper is the formulation of a FPE for a set of gross variables, when the detailed dynamics of the system is not governed by a Liouville equation but rather by a detailed FPE. This detailed level will be in general an already coarse-grained description from the actual molecular dynamics of the system. Instances where the coarse-graining of a coarse grained description is necessary are numerous. For example, a polymer molecule in a solvent that at a detailed level is described by a FPE with hydrodynamic interactions may be described at a coarser level with coarse-grained variables like blobs containing many monomer [9] or other variables describing the overall shape and orientation. A colloidal suspension described at the level of fluctuating hydrodynamics [10] needs to be described at the level of the positions of the colloidal particles alone. A colloidal suspension described at the level of Brownian dynamics may be coarsened to the Fickian level of the concentration field [11]. Very recently, coarse-grained potentials and frictions have been introduced to describe complex macromolecular systems [12] and lipid molecules [13] able to self-assembly into membranes. One may want to further coarse-grain these descriptions in favor of hydrodynamics or membrane elasticity, respectively.

The problem of coarse-graining from a coarse-grained description has been considered in [11], and, within the GENERIC framework in [6,14,15]. In the present paper, we give a look to the derivation of [11] in order to prove that the friction matrix is positive definite. The phase space expression that is obtained in the projection operator framework for the friction matrix has two contributions, a first one that captures the fluctuations at the detailed stochastic level while the second contribution has the form of a Green-Kubo formula [6]. The first contribution is easily seen to be positive definite but the Green-Kubo expression is not manifestly positive definite as it is not the time integral of an *auto*correlation for which the Wiener-Kinchine theorem ensures positiveness of its time integral. This is clearly an issue of concern and our motivation to revisit the problem. Very recently, Ernst and Brito have presented general Green-Kubo expressions for transport coefficients in systems with nonconservative dynamics [16,17]. One particular case studied by these authors is when the system is governed at a detailed level by Langevin equations [17]. In that particular case, the Green-Kubo expression is an example of those obtained in the general theory presented in [6,11] and are, therefore, also subject to the question of whether the transport coefficients are positive. In the present paper, we show that the friction matrix admits a representation in terms of the "mean square displacements" of the relevant variables, in a formula that generalizes the Einstein-Helfand expression for the transport coefficients [18]. Being a mean square, the Einstein-Helfand expression is clearly definite positive.

Finally, we also study what are the consequences on the coarse FPE of the fact that the underlying dynamics satisfies detailed balance. One interesting thing about detailed bal-

ance is that it is a property of the system and not of the level of description. Therefore, the coarse FPE should satisfy the usual necessary and sufficient conditions for detailed balance. The proof that the obtained coarse FPE does indeed satisfies these conditions gives strong support to the *asymmetric* structure of the Green-Kubo expression [6,11,17], as opposed to the symmetric structure of some other candidates [15].

II. DERIVATION OF THE COARSE-GRAINED DYNAMIC EQUATION

The coarse FPE when the detailed level is stochastic has been obtained in Ref. [14,11] For the sake of setting up the notation, we present in this section a derivation of the coarse FPE.

A. Dynamics at the detailed level

Let us denote the mesoscopic degrees of freedom of the system at the detailed level by $z=\{z_i,\ i=1,\ldots,N\}$. We assume that the one time probability density $\rho_t(z)$ evolves according to a FPE

$$\partial_t \rho_t(z) = L\rho_t(z), \tag{1}$$

where L is an evolution operator of the form

$$L = -\frac{\partial}{\partial z_i} v_i(z) + k_B \frac{\partial}{\partial z_i}\frac{\partial}{\partial z_j} d_{ij}(z) \equiv -\partial_i v_i(z) + k_B \partial_i \partial_j d_{ij}(z), \tag{2}$$

where k_B is the Boltzmann constant, $d_{ij}=d_{ji}$ is a positive definite matrix, and summation over repeated indices is implied. Note that the derivatives act on every function on its right. The case $d_{ij}=0$ corresponds to a deterministic evolution. The Liouville equation of Classical Mechanics is then a special case of Eq. (1), which, in addition, satisfies $\partial_i v_i=0$ (Liouville's theorem). This last property ensures that the Liouville dynamical operator is self-adjoint. We pursue in this paper a generalization for not self-adjoint dynamical operators.

We assume that the FPE (1) has a steady state solution $\rho^{ss}(z)$ that satisfies $L\rho^{ss}=0$. We will write this steady state solution in the form

$$\rho^{ss}(z) = \exp\{\mathcal{S}(z)/k_B\}, \tag{3}$$

where $\mathcal{S}(z)$ will be an "entropy," a "free energy," or an "energy" (Hamiltonian) depending on the context.

B. Adjoint operators

In this subsection, we present the two dynamic operators L^+ and L^- that play a crucial role in what follows. The operator L^+ is the adjoint operator of L with respect to the unit measure, this is,

$$L^+ \equiv v_i(z)\partial_i + k_B d_{ij}(z)\partial_i\partial_j, \tag{4}$$

which satisfies

$$\mathrm{tr}[FLG] = \mathrm{tr}[GL^+F], \tag{5}$$

where F,G are arbitrary functions and $\mathrm{tr}[\cdots]$ denotes an integration over the space of detailed variables z. The operator L^- is defined as

$$L^- \equiv \left\{ v_i(z) - \frac{2k_B}{\rho^{ss}(z)}\partial_j[d_{ij}\rho^{ss}(z)] \right\}\partial_i - k_B d_{ij}(z)\partial_i\partial_j, \tag{6}$$

and it satisfies

$$LF\rho^{ss} = -\rho^{ss}L^-F, \tag{7}$$

as can be shown by an explicit calculation that uses $L\rho^{ss}=0$. The property in Eq. (7) allows one to "drag" the steady state ensemble to the left in the following calculations. Note that, the operators L^+,L^- are antiadjoint of each other with respect to the steady state measure, in the following sense:

$$\mathrm{tr}[\rho^{ss}FL^+G] = -\mathrm{tr}[\rho^{ss}GL^-F], \tag{8}$$

as can be seen by noting that each side of Eq. (8) equals $\mathrm{tr}[GL\rho^{ss}F]$. For future reference, we note that Eq. (8) implies the following identity:

$$\mathrm{tr}[\rho^{ss}F\ \exp\{L^+t\}G] = \mathrm{tr}[\rho^{ss}G\ \exp\{-L^-t\}F], \tag{9}$$

where the exponential operator is defined through the formal series expansion of the exponential,

$$\exp\{Lt\} = 1 + Lt + \frac{1}{2!}L^2t^2 + \cdots. \tag{10}$$

The formal solution of the FPE (1) is

$$\rho_t(z) = \exp\{Lt\}\rho_0(z), \tag{11}$$

where $\rho_0(z)$ is the distribution function at the initial time. Now, consider an arbitrary function $F(z)$ of the state variables z. The time-dependent average computed with the solution of Eq. (1) is

$$\langle F\rangle_t = \mathrm{tr}[\rho_t F] = \mathrm{tr}[F\ \exp\{Lt\}\rho_0] = \mathrm{tr}[\rho_0\ \exp\{L^+t\}F]. \tag{12}$$

This equation allows one to give an intuitive interpretation to the operator $\exp\{L^+t\}$ as a dynamic operator that evolves forward in time the function $F(z)$, allowing the averages to be computed as a averages over initial conditions.

C. Coarse-grained level

At a coarse-grained level, the system is described by a collection of relevant variables $A(z)=\{A^\mu(z),\ \mu=1,\ldots,M\}$, where M is the number of relevant 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 usual relation

$$p(\alpha,t) \equiv \int \rho_t(z)\delta[A(z)-\alpha]dz = \mathrm{tr}[\rho_t \Psi_\alpha], \tag{13}$$

where $\Psi_\alpha(z) \equiv \delta[A(z)-\alpha]$.

The objective of the theory of coarse-graining is to derive a dynamical equation for the probability $p(\alpha,t)$. If this dynamic equation is a Fokker-Planck equation, then $p(\alpha,t)$ contains all the necessary information to describe the system at the coarse-grained level [19].

D. Relevant ensemble

Consider the relative entropy functional

$$S[\rho_t] = -k_B \int dz \rho_t(z) \ln\left(\frac{\rho_t(z)}{\rho^{ss}(z)}\right), \tag{14}$$

where $\rho^{ss}(z)$ is the steady state solution of the FPE (1). By using Eq. (1), it is a standard calculation to show that $\partial_t S[\rho_t] \geq 0$ and that the maximum occurs at $\rho_t = \rho^{ss}$, provided that the diffusion tensor d_{ij} is positive definite [7], a fact that we will always assume. Therefore, any initial distribution relaxes towards the steady state distribution. The entropy functional serves also for the purpose to define the *relevant ensemble* $\bar{\rho}_t(z)$, which is a coarse-grained probability density in the detailed space of z that captures the macroscopic behavior. The relevant ensemble is defined as the ensemble that maximizes the entropy functional (14) subject to produce the distribution function (13). Therefore, we maximize without restriction the functional

$$I[\rho] = S[\rho] + \int d\alpha \lambda(\alpha,t) p(\alpha,t) + \mu \int dz \rho(z), \tag{15}$$

where $\lambda(\alpha,t)$ is a set of Lagrange multipliers, $p(\alpha,t)$ is the functional of $\rho_t(z)$ given in Eq. (13), and μ is another Lagrange multiplier used to describe the restriction of normalized densities. By equating to zero the functional derivative of $I[\rho]$, we obtain the relevant ensemble

$$\bar{\rho}_t(z) = \int p(\alpha,t)\rho_\alpha(z)d\alpha, \tag{16}$$

where the steady state *constrained ensemble* is defined as

$$\rho_\alpha(z) \equiv \frac{1}{\Omega(\alpha)} \rho^{ss}(z)\delta[A(z)-\alpha]. \tag{17}$$

Here, $\Omega(\alpha) = p^{ss}(\alpha)$ is the steady state probability density that the functions $A(z)$ take values α, this is

$$\Omega(\alpha) \equiv \int \delta[A(z)-\alpha]\rho^{ss}(z)dz. \tag{18}$$

Note that $\Omega(\alpha)$ is a measure of the submanifold $A(z)=\alpha$ of the detailed state space, and it can be intuitively understood as the "number of microstates z that are compatible with the macrostate α."

The relevant ensemble (16) satisfies

$$p(\alpha,t) = \mathrm{tr}[\bar{\rho}_t \Psi_\alpha] \tag{19}$$

to be compared with Eq. (13). In this way, the relevant ensemble $\bar{\rho}_t$ reproduces the same coarse-grained information $p(\alpha,t)$ as the actual ensemble ρ_t. Therefore, by constructing a closed dynamic equation for the relevant ensemble we will have the equation of motion for the distribution $p(\alpha,t)$ of coarse variables.

It is interesting to note that by evaluating the entropy functional (14) at the relevant ensemble (16), we get the entropy functional at the coarse-grained level. It is given by

$$S[p(\alpha,t)] = -k_B \int d\alpha p(\alpha,t) \ln\left[\frac{p(\alpha,t)}{\Omega(\alpha)}\right]. \tag{20}$$

This entropy functional at the coarse-grained level plays a crucial role in the demonstration of an H theorem at the coarse-grained level, as shown in Eq. (86) below.

E. Projection operator

We present now a projection operator P^+ such that when applied to the actual ensemble $\rho_t(z)$ it gives the relevant ensemble, this is

$$\bar{\rho}_t = P^+ \rho_t. \tag{21}$$

An appropriate definition for this projector is the following:

$$P^+ F(z) \equiv \int d\alpha \rho_\alpha(z) \mathrm{tr}[\Psi_\alpha F], \tag{22}$$

where F is an arbitrary function. We also present the adjoint projector P with respect to the unit measure

$$\mathrm{tr}[GP^+F] = \mathrm{tr}[FPG], \tag{23}$$

which has the form

$$PF = \int \langle F \rangle^\alpha \Psi_\alpha d\alpha, \tag{24}$$

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

$$\langle F \rangle^\alpha \equiv \int \rho_\alpha(z) F(z) dz. \tag{25}$$

The projector P projects any function onto a linear combination of Ψ_α. In particular,

$$P\Psi_\alpha = \Psi_\alpha. \tag{26}$$

The projector operator (24) is self-adjoint with respect to both measures $\rho^{ss}(z)$ and $\bar{\rho}_t(z)$, i.e.,

$$\mathrm{tr}[\rho^{ss} FPG] = \mathrm{tr}[\rho^{ss} GPF]$$

$$\mathrm{tr}[\bar{\rho}_t FPG] = \mathrm{tr}[\bar{\rho}_t GPF], \tag{27}$$

where F and G are arbitrary functions.

The complementary projection operator Q is defined as

$$Q \equiv 1 - P \tag{28}$$

that satisfies $QQ=Q$ and $QP=0$.

F. Closed exact dynamic equation at the coarse-grained level

Following Zwanzig [4], we may now decompose the solution of the FPE at the detailed level, Eq. (1), into a relevant

$P^+\rho_t=\bar{\rho}_t$ and irrelevant $Q^+\rho_t\equiv(1-P^+)\rho_t$ parts, write a set of two coupled equations for each part and solve the irrelevant part in terms of the relevant part. By substituting back into the equation for the relevant part one obtains

$$\partial_t\bar{\rho}_t = P^+L\bar{\rho}_t + \int_0^t duP^+L\exp\{Q^+L(t-u)\}Q^+L\bar{\rho}_u, \quad (29)$$

where, as usual, we have assumed that the distribution function ρ_t at the initial time is of the relevant form (16) [20].

By multiplying Eq. (29) with respect to $\Psi_\alpha(z)$ and integrating over z, we obtain a closed equation for $p(\alpha,t)$. This equation can be cast into the form

$$\partial_t p(\alpha,t) = \int d\alpha' V(\alpha,\alpha')p(\alpha',t) + \int_0^t du\int d\alpha' K(\alpha,\alpha';t-u)p(\alpha',u), \quad (30)$$

where we define

$$V(\alpha,\alpha') \equiv \frac{1}{\Omega(\alpha')}\mathrm{tr}[\rho^{ss}\Psi_{\alpha'}L^+\Psi_\alpha],$$

$$K(\alpha,\alpha';t-u) \equiv -\frac{1}{\Omega(\alpha')}\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}QL^-\Psi_{\alpha'}) \times(\exp\{QL^+t\}(QL^+\Psi_\alpha)]. \quad (31)$$

In order to write $K(\alpha,\alpha';t-u)$ as in Eq. (31), we have used an equation similar to Eq. (9), i.e.,

$$\mathrm{tr}[\rho^{ss}F\exp\{QL^+t\}G] = \mathrm{tr}[\rho^{ss}G\exp\{-QL^-t\}F], \quad (32)$$

which can be proved by using the series expansion of the exponential operator and using the antiadjointness of $L^\pm$ in Eq. (8) and the self-adjointness of P and Q in Eq. (27). We can work out a more explicit expression of these objects (31) by making use of the following results:

$$L^+\Psi_\alpha = -v_+^\mu\partial_\mu\Psi_\alpha + k_Bd^{\mu\nu}\partial_\mu\partial_\nu\Psi_\alpha,$$

$$L^-\Psi_\alpha = -v_-^\mu\partial_\mu\Psi_\alpha - k_Bd^{\mu\nu}\partial_\mu\partial_\nu\Psi_\alpha,$$

$$QL^+\Psi_\alpha = -\partial_\mu[\delta_\alpha v_+^\mu\Psi_\alpha - k_B\partial_\nu\delta_\alpha d^{\mu\nu}\Psi_\alpha],$$

$$QL^-\Psi_{\alpha'} = -\partial_{\mu'}[\delta_{\alpha'}v_-^{\mu'}\Psi_{\alpha'} + k_B\partial_{\nu'}\delta_{\alpha'}d^{\mu'\nu'}\Psi_{\alpha'}], \quad (33)$$

where $\partial_\mu\equiv\partial/\partial\alpha_\mu$ and we have made use of the chain rule in

$$\partial_i\Psi_\alpha = -\partial_iA^\mu\partial_\mu\Psi_\alpha. \quad (34)$$

In Eqs. (33), we have defined the following functions:

$$v_\pm^\mu \equiv L^\pm A^\mu$$

$$d^{\mu\nu} \equiv d_{ij}(\partial_iA^\mu)(\partial_jA^\nu)$$

$$\delta_\alpha v_\pm^\mu \equiv v_\pm^\mu - \langle v_\pm^\mu\rangle^\alpha$$

$$\delta_\alpha d^{\mu\nu} \equiv d^{\mu\nu} - \langle d^{\mu\nu}\rangle^\alpha. \quad (35)$$

Equations (33) follow from a direct calculation by using the explicit expressions (4), (6), (24), and (28).

With the first equation in Eq. (33), we can write the exact result

$$V(\alpha,\alpha') = -\partial_\mu[\delta(\alpha-\alpha')\langle v_+^\mu\rangle^\alpha - k_B\partial_\nu\delta(\alpha-\alpha')\langle d^{\mu\nu}\rangle^\alpha] \quad (36)$$

and, therefore, the first term in Eq. (30) becomes

$$\int d\alpha' V(\alpha,\alpha')p(\alpha,t) = -\partial_\mu\langle v_+^\mu\rangle^\alpha p(\alpha,t) + k_B\partial_\mu\partial_\nu\langle d^{\mu\nu}\rangle^\alpha p(\alpha,t). \quad (37)$$

By using the objects defined in Eq. (33), we can write the kernel $K(\alpha,\alpha',t-u)$ in Eq. (31) in the following form:

$$K(\alpha,\alpha',t-u) = -\frac{1}{\Omega(\alpha')}\partial_\mu\partial_{\mu'}\,\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}v_-^{\mu'}\Psi_{\alpha'})(\exp\{QL^+t\}\delta_\alpha v_+^\mu\Psi_\alpha)] + \frac{k_B}{\Omega(\alpha')}\partial_\mu\partial_\nu\partial_{\mu'}\,\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}v_-^{\mu'}\Psi_{\alpha'}) \times(\exp\{QL^+t\}\delta_\alpha d^{\mu\nu}\Psi_\alpha)] - \frac{k_B}{\Omega(\alpha')}\partial_\mu\partial_{\mu'}\partial_{\nu'}\,\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}d^{\mu'\nu'}\Psi_{\alpha'})(\exp\{QL^+u\}\delta_\alpha v_+^\mu\Psi_\alpha)] + \frac{k_B^2}{\Omega(\alpha')}\partial_\mu\partial_\nu\partial_{\mu'}\partial_{\nu'}\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}d^{\mu'\nu'}\Psi_{\alpha'})(\exp\{QL^+t\}\delta_\alpha d^{\mu\nu}\Psi_\alpha)]. \quad (38)$$

By inserting Eqs. (37) and (38) into the dynamic equation (30), we arrive at the following exact equation for $p(\alpha,t)$:

$$\partial_t p(\alpha,t) = -\partial_\mu\langle v_+^\mu\rangle^\alpha p(\alpha,t) + k_B\partial_\mu\partial_\nu\langle d^{\mu\nu}\rangle^\alpha p(\alpha,t) + k_B\partial_\mu\int d\alpha'\int_0^t duK_0^{\mu\mu'}(\alpha,\alpha',t-u)\Omega(\alpha')\partial_{\mu'}\frac{p(\alpha',u)}{\Omega(\alpha')} - k_B^2\partial_\mu\partial_\nu\int d\alpha'\int_0^t duK_-^{\mu\nu\mu'}(\alpha,\alpha',t-u)\Omega(\alpha')\partial_{\mu'}\frac{p(\alpha',u)}{\Omega(\alpha')} - k_B^2\partial_\mu\int d\alpha'\int_0^t duK_+^{\mu\mu'\nu'}(\alpha,\alpha',t-u)\Omega(\alpha')\partial_{\mu'}\partial_{\nu'}\frac{p(\alpha',u)}{\Omega(\alpha')} + k_B^3\partial_\mu\partial_\nu\int d\alpha'\int_0^t duK^{\mu\nu\mu'\nu'}(\alpha,\alpha',t-u)\Omega(\alpha')\partial_{\mu'}\partial_{\nu'}\frac{p(\alpha',u)}{\Omega(\alpha')}, \quad (39)$$

where we have defined the following memory kernels:

$$K_0^{\mu\mu'}(\alpha,\alpha',t-u) \equiv \frac{1}{k_B}\frac{1}{\Omega(\alpha')}\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}v_-^{\mu'}\Psi_{\alpha'}) \times(\exp\{QL^+t\}\delta_\alpha v_+^\mu\Psi_\alpha)]$$

$$K_-^{\mu\nu\mu'}(\alpha,\alpha',t-u) \equiv \frac{1}{k_B}\frac{1}{\Omega(\alpha')}\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}v_-^{\mu'}\Psi_{\alpha'}) \times(\exp\{QL^+t\}\delta_\alpha d^{\mu\nu}\Psi_\alpha)]$$

$$K_+^{\mu\mu'\nu'}(\alpha,\alpha',t-u) \equiv \frac{1}{k_B}\frac{1}{\Omega(\alpha')}\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}d^{\mu'\nu'}\Psi_{\alpha'}) \times(\exp\{QL^+t\}\delta_\alpha v_+^\mu\Psi_\alpha)]$$

$$K^{\mu\nu\mu'\nu'}(\alpha,\alpha',t-u) \equiv \frac{1}{k_B}\frac{1}{\Omega(\alpha')}\mathrm{tr}[\rho^{ss}(\exp\{QL^-u\}\delta_{\alpha'}d^{\mu'\nu'}\Psi_{\alpha'}) \times(\exp\{QL^+t\}\delta_\alpha d^{\mu\nu}\Psi_\alpha)]. \quad (40)$$

The reason for introducing the factors k_B^{-1} in these definitions will be discussed later. In order to obtain a more explicit expression for $K(\alpha,\alpha',t)$, we need to make several approximations as detailed in the next subsection.

Due to the fact that Eq. (39) is exact, it must happen that $\Omega(\alpha)$ is, actually, its stationary solution, see Eq. (18). Actually, from the definition (31) we have

$$\int d\alpha' V(\alpha,\alpha')\Omega(\alpha) = \int d\alpha'\ \mathrm{tr}[\rho^{ss}\Psi_{\alpha'}L^+\Psi_\alpha] = \mathrm{tr}[\rho^{ss}L^+\Psi_\alpha] = 0. \quad (41)$$

This implies

$$-\partial_\mu\langle v_+^\mu\rangle^\alpha\Omega(\alpha) + k_B\partial_\mu\partial_\nu\langle d^{\mu\nu}\rangle^\alpha\Omega(\alpha) = 0. \quad (42)$$

This equation ensures that $\Omega(\alpha)$ is the steady state solution of Eq. (39), as it should.

G. Markovian approximation of the coarse-grained dynamic equation

Equation (39) is a closed and exact equation for the distribution function $p(\alpha,t)$ at the coarse-grained level. It is a complicated linear integro-differential equation for $p(\alpha,t)$ and, as such, it contains exactly the same information as the original Fokker-Planck equation (1) at the detailed level. Of course, the usefulness of Eq. (39) comes from the fact that it admits, in certain circumstances, a Markovian approximation that renders it into the form of a usual FPE.

The Markovian approximation states that, if the selected relevant variables are *slow* in the time scale in which the correlation kernel $K(\alpha,\alpha';t-u)$ decays, then we can approximate the memory term in Eq. (33) as

$$\int_0^t du\int d\alpha' K(\alpha,\alpha';t-u)p(\alpha',u) = \int d\alpha' K(\alpha,\alpha')p(\alpha',t), \quad (43)$$

where we have introduced the Green-Kubo type integral operator

$$K(\alpha,\alpha') = \int_0^\tau du K(\alpha,\alpha';u). \quad (44)$$

Here, τ is a time large enough for the kernel to have decayed, but small in terms of the time scale of evolution of the probability of the relevant variables. This time τ exists, given the assumed separation of time scales between the kernel time scale and the time scale of macroscopic variables. This crucial approximation renders the memory equation into the form of a local in time integro-differential equation.

Of course, an integro-differential equation is still a complex mathematical object and we seek now additional approximations that transforms the resulting dynamical equation into a partial differential equation. To this end, we will take the additional approximations

$$\exp\{L^+Qt\}F\Psi_\alpha \approx \Psi_\alpha\exp\{L^+Qt\}F \approx \Psi_\alpha\exp\{L^+t\}QF$$

$$\exp\{L^-Qu\}F\Psi_\alpha \approx \Psi_\alpha\exp\{L^-Qu\}F \approx \Psi_\alpha\exp\{L^-u\}QF, \quad (45)$$

where F is any of the functions that appear in the kernel. The rational for this approximation is that the projected evolution operator $\exp\{L^+Q(t-u)\}$ has no effect, during the short time scale in which the kernel decays, on the relevant variables A^μ appearing inside Ψ_α. The relevant variables are slow if the Markovian approximation is valid. We have also assumed that the effect of the projection operator on the dynamics is irrelevant, as far as short time dynamics is concerned. This is a usual assumption in the derivation of Green-Kubo expressions for transport coefficients in Classical Statistical Mechanics [7]. There is no other justification of these approximations apart from this intuitive idea of separation of time scales between the kernel and the coarse-grained variables. A more rigorous approach along the lines of Ref. [12] would be certainly desirable in the present situation. However, we expect that the above approximation will be simply confirmed by such a more rigorous approach.

With the approximation (45), the time integral of the kernels in Eq. (40) becomes local in the space of coarse variables

$$\int_0^\tau du K_0^{\mu\mu'}(\alpha,\alpha',u) = \delta(\alpha-\alpha')K_0^{\mu\mu'}(\alpha)$$

$$\int_0^\tau du K_-^{\mu\nu\mu'}(\alpha,\alpha',u) = \delta(\alpha-\alpha')K_-^{\mu\nu\mu'}(\alpha)$$

$$\int_0^\tau du K_+^{\mu\mu'\nu'}(\alpha,\alpha',u) = \delta(\alpha-\alpha')K_+^{\mu\mu'\nu'}(\alpha)$$

$$\int_0^\tau du K^{\mu\nu\mu'\nu'}(\alpha,\alpha',u) = \delta(\alpha-\alpha')K^{\mu\nu\mu'\nu'}(\alpha), \quad (46)$$

where the Green-Kubo transport coefficients $K(\alpha)$ are introduced as

$$K_0^{\mu\mu'}(\alpha) \equiv \frac{1}{k_B}\int_0^\tau du\langle(\exp\{L^- u\}\delta_\alpha v_-^{\mu'})(\exp\{L^+\tau\}\delta_\alpha v_+^{\mu})\rangle^\alpha$$

$$K_-^{\mu\nu\mu'}(\alpha) \equiv \frac{1}{k_B}\int_0^\tau du\langle(\exp\{L^- u\}\delta_\alpha v_-^{\mu'})(\exp\{L^+\tau\}\delta_\alpha d^{\mu\nu})\rangle^\alpha$$

$$K_+^{\mu\mu'\nu'}(\alpha) \equiv \frac{1}{k_B}\int_0^\tau du\langle(\exp\{L^- u\}\delta_\alpha d^{\mu'\nu'})(\exp\{L^+\tau\}\delta_\alpha v_+^{\mu})\rangle^\alpha$$

$$K^{\mu\nu\mu'\nu'}(\alpha) \equiv \frac{1}{k_B}\int_0^\tau du\langle(\exp\{L^- u\}\delta_\alpha d^{\mu'\nu'})(\exp\{L^+\tau\}\delta_\alpha d^{\mu\nu})\rangle^\alpha. \quad (47)$$

We justify now the reason for introducing the factor k_B^{-1} in the definitions (40) and (47). The overall magnitude of the integrand of $K(\alpha)$ in Eq. (47) can be estimated by considering its value at time $t=0$. For example, the integrand of $K_0^{\mu\mu'}(\alpha)$ at zero time is $\langle(\delta_\alpha v_-^{\mu'})(\delta_\alpha v_+^{\mu})\rangle^\alpha$. This object is a constrained average of a covariance of the steady state solution in Eq. (1). The factor k_B^{-1} in Eq. (3) is introduced as a reminder that the width of $\rho^{\rm ss}(z)$ is on the order of k_B. Stated in less precise but illustrative words, "thermal fluctuations are on the order of k_B." Therefore, the overall magnitude of $\langle(\delta_\alpha v_-^{\mu'})(\delta_\alpha v_+^{\mu})\rangle^\alpha$ is on the order of k_B. We have introduced a factor k_B^{-1} in the definition of $K(\alpha)$ in Eq. (47) in such a way that the expected order of magnitude of $K(\alpha)$ is k_B^0.

By using Eqs. (43) and (46) in the dynamic equation (39), we arrive at a local in time partial differential equation for $p(\alpha,t)$,

$$\begin{aligned}\partial_t p(\alpha,t) = &-\partial_\mu\langle v_+^\mu\rangle^\alpha p(\alpha,t) + k_B\partial_\mu\partial_\nu\langle d^{\mu\nu}\rangle^\alpha p(\alpha,t)\\ &+ k_B\partial_\mu K_0^{\mu\mu'}(\alpha)\Omega(\alpha)\partial_{\mu'}\frac{p(\alpha,t)}{\Omega(\alpha)}\\ &- k_B^2\partial_\mu\partial_\nu K_-^{\mu\nu\mu'}(\alpha)\Omega(\alpha)\partial_{\mu'}\frac{p(\alpha,t)}{\Omega(\alpha)}\\ &- k_B^2\partial_\mu K_+^{\mu\mu'\nu'}(\alpha)\Omega(\alpha)\partial_{\mu'}\partial_{\nu'}\frac{p(\alpha,t)}{\Omega(\alpha)}\\ &+ k_B^3\partial_\mu\partial_\nu K^{\mu\nu\mu'\nu'}(\alpha)\Omega(\alpha)\partial_{\mu'}\partial_{\nu'}\frac{p(\alpha,t)}{\Omega(\alpha)}. \quad (48)\end{aligned}$$

In what follows, we will assume that the terms of order k_B^2 and k_B^3 are negligible in front of the terms of order k_B. Note that Eq. (48) is not a FPE because it contains third and fourth order derivatives of the probability density. From Pawula's theorem [21] it is known that the only meaningful equation for the probability density of a Markov process with only finite-order derivatives is the usual Fokker-Planck equation. By neglecting the terms of order higher than k_B^2 we obtain a proper Fokker-Planck equation involving only second derivatives. While k_B has physical dimensions, it should be taken as an indicator of a dimensionless reciprocal of the "system size." This is apparent from Eq. (3) where the entropy scales as the system size, leading to the standard result in equilibrium Statistical Mechanics that fluctuations scale as the inverse of the square root of the volume. While neglecting terms of high order in k_B is appropriate in Eq. (48), one should not neglect the first order terms in k_B within the evolution operator $\exp\{L^{\pm}t\}$, as this would change the stochastic nature of this evolution. The neglect of higher order terms allows us to retain fluctuation effects to first order in k_B, but not higher.

The final coarse Fokker-Planck equation can be cast in the form

$$\begin{aligned}\partial_t p(\alpha,t) = &-\partial_\mu[V^\mu(\alpha) + M^{\mu\nu}(\alpha)\partial_\nu S(\alpha)]p(\alpha,t)\\ &+ k_B\partial_\mu M^{\mu\nu}(\alpha)\partial_\nu p(\alpha,t), \quad (49)\end{aligned}$$

where we have introduced the entropy $S(\alpha)$, the drift $V^\mu(\alpha)$, and the friction matrix $M^{\mu\nu}(\alpha)$ through

$$S(\alpha) = k_B \ln\Omega(\alpha),$$

$$V^\mu(\alpha) \equiv \langle v_+^\mu\rangle^\alpha - d^{\mu\nu}(\alpha)\partial_\nu S(\alpha) - k_B\partial_\mu d^{\mu\nu}(\alpha),$$

$$M^{\mu\nu}(\alpha) \equiv \langle d^{\mu\nu}\rangle^\alpha + K_0^{\mu\nu}(\alpha). \quad (50)$$

In Appendix A, we show that the drift can be written as

$$V^\mu(\alpha) = \langle V^\mu(z)\rangle^\alpha, \quad (51)$$

where

$$V^\mu(z) \equiv \left[v_i - k_B\frac{1}{\rho^{\rm ss}}\partial_j d_{ij}\rho^{\rm ss}\right]\partial_i A^\mu. \quad (52)$$

Note that, thanks to Eq. (42), $\partial_\mu V^\mu(\alpha)\Omega(\alpha)=0$ and, therefore, $\Omega(\alpha)$ is still the steady state solution of the approximate FPE (49). In other words, the dynamics at the detailed level and at the coarse level lead to steady state distribution functions $\rho^{\rm ss}(z)$ and $p^{\rm ss}(\alpha)$, respectively, which are consistent with each other.

The FPE (49) is the desired dynamic equation for the coarse-grained level of description. Under slightly different notation, it has been obtained in Ref. [11]. If the detailed level of description is given by a purely reversible dynamics, as it happens when we are coarse-graining from the detailed atomistic dynamics, then $d^{\mu\nu}=0$ and $L^+=L^-=L$, the Liouville operator. In this case, the friction matrix has the usual Green-Kubo expression and the resulting FPE is the one first obtained by Zwanzig [4].

III. EINSTEIN-HELFAND FORM FOR $M^{\mu\nu}$

The friction matrix M in Eq. (50) contains the term $K_0^{\mu\nu}(\alpha)$ that has a Green-Kubo form involving a time integral as shown in the first Eq. (47). Perhaps the simplest example of a Green-Kubo formula is the one that expresses the diffusion coefficient D of a Brownian particle in terms of the time integral of the autocorrelation of the velocity of the Brown-

ian particle. An alternative expression for D is given by the Einstein's result $D=\langle[r(t)-r(0)]^2\rangle/2t$. Generalizations of the connection between the Green-Kubo form and the Einstein form for other transport coefficients have been given by Helfand [18]. The starting point in Helfand derivation is the deterministic equations of classical mechanics. In this section, we give the Einstein-Helfand form for the matrix M when the detailed level is stochastic. In this way, the matrix M is shown to be manifestly positive definite.

As a previous step, we show that for a system described with a FPE with a well-defined stationary solution, there is a theorem that allows to express mean square "displacements" in terms of integrals of correlation functions.

A. Theorem about diffusion processes

The two-time correlation function $\langle FG\rangle_{tt'}$ of two arbitrary functions $F(z),G(z)$ is defined as

$$\langle FG\rangle_{tt'} \equiv \overline{F(t)G(t')}, \tag{53}$$

where $F(t)=F[z(t)]$ and $G(t)=G[z(t)]$ are the functions evaluated at the stochastic realization of the process $z(t)$, and the average $\overline{\cdots}$ is over realizations of this stochastic process. An alternative but equivalent form of the correlation function in terms of the two-time probability $\rho(z,t,z',t')$ is the following:

$$\langle FG\rangle_{tt'} \equiv \int dz \int dz' F(z)G(z')\rho(z,t,z',t'). \tag{54}$$

In terms of the conditional probability $\rho(z',t'|z,t)$ of finding z' at time t', given that at time t the state was z, we have $\rho(z,t,z',t')=\rho(z,t)\rho(z',t'|z,t)$ with $t'>t$. Note that the conditional probability also satisfies the FPE (1) [19], this is

$$\partial_{t'}\rho(z',t'|z,t) = L'\rho(z',t'|z,t) \tag{55}$$

with initial condition $\rho(z',t|z,t)=\delta(z'-z)$. The prime in the operator L denotes that the derivatives in this differential operator are with respect to z'. Note that the ordering $t'>t$ is crucial in the definition of the conditional probability and the use of Eq. (55). The formal solution of Eq. (55) for the conditional probability is, therefore,

$$\rho(z',t'|z,t) = \exp\{L'(t'-t)\}\delta(z-z'). \tag{56}$$

By substitution of this solution into Eq. (54), we obtain

$$\langle FG\rangle_{tt'} = \int dz F(z)\rho(z,t)\exp\{L^+(t'-t)\}G(z). \tag{57}$$

In the steady state, when $\rho(z,t)=\rho^{ss}(z)$, the correlation in Eq. (57) is stationary (it only depends on the time difference). In this case, and after using Eq. (9), we have,

$$\langle FG\rangle^{ss}_{tt'} = \langle(\exp\{L^-t\}F)(\exp\{L^+t'\}G)\rangle^{ss} \quad t'>t, \tag{58}$$

where we have introduced the steady state average

$$\langle\cdots\rangle^{ss} = \int dz\rho^{ss}(z)\cdots. \tag{59}$$

Note that both functions in Eq. (58) are "evolved" in a different way with the dynamic operators involving L^+ or L^-.

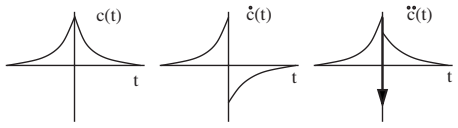

FIG. 1. Cartoon of the correlation function and its time derivatives. If the correlation has a cusp at the origin, its second time derivative has a Dirac delta function at the origin.

The origin of the asymmetry in the evolution of F and G is just the ordering $t'>t$. In the opposite case $t'<t$ we have the phase space expression

$$\langle FG\rangle_{tt'} = \langle(\exp\{L^+t\}F)(\exp\{L^-t'\}G)\rangle^{ss} \quad t'<t. \tag{60}$$

Eqs. (58) and (60) are the phase space expression of the correlation function.

We introduce now the matrix of stationary autocorrelation function of a set of variables $A^\mu(z)$, this is

$$\begin{aligned} C^{\mu\nu}(t,t') &\equiv \int dz \int dz' A^\mu(z)A^\nu(z')\rho^{ss}(z,t,z',t') \\ &= \langle(\exp\{L^-t\}A^\mu)(\exp\{L^+t'\}A^\nu)\rangle^{ss} \quad \text{if} \quad t'>t \\ &= \langle(\exp\{L^+t\}A^\mu)(\exp\{L^-t'\}A^\nu)\rangle^{ss} \quad \text{if} \quad t'<t, \end{aligned} \tag{61}$$

and also the matrix of its derivatives

$$B^{\mu\nu}(t,t') \equiv \frac{d}{dt}\frac{d}{dt'}C^{\mu\nu}(t,t'). \tag{62}$$

For $t'>t$, Eqs. (62) and (61) lead to

$$B^{\mu\nu}(t,t') = \int dz\rho^{ss}(z)[\exp(L^-t)L^-A^\mu(z)][\exp(L^+t')L^+A^\nu(z)]. \tag{63}$$

We have a similar expression for the case $t'<t$. The combination of both cases can be written as

$$\begin{aligned} B^{\mu\nu}(t,t') &= b^{\mu\nu}(t'-t) \quad \text{for} \quad t'>t \\ B^{\mu\nu}(t,t') &= b^{\nu\mu}(t-t') \quad \text{for} \quad t'<t, \end{aligned} \tag{64}$$

where

$$b^{\mu\nu}(u) \equiv \int dz\rho^{ss}(z)[L^-A^\mu(z)][\exp(L^+u)L^+A^\nu(z)] \quad u>0. \tag{65}$$

We have discussed separately the cases $t'>t$ and $t'<t$, and the question arises about what happens when $t'=t$. It turns out that the correlation matrix $C^{\mu\nu}(t,t')$ has a discontinuous first time derivative at $t=t'$ and, therefore, the matrix $B^{\mu\nu}(t,t')$ will have a delta function contribution that represents the derivative of the discontinuity, as schematically shown in Fig. 1. Let us see how this arises.

If $t'>t$, we have, from Eq. (61),

$$\frac{d}{dt'}C^{\mu\nu}(t,t') = \langle A^{\mu}(\exp\{L^{+}(t'-t)\}L^{+}A^{\nu})\rangle^{\mathrm{ss}}. \tag{66}$$

When $t \to t'$, with $t' > t$, this leads to

$$\lim_{\substack{t\to t'\\ t'>t}} \frac{d}{dt'}C^{\mu\nu}(t,t') = \langle A^{\mu}L^{+}A^{\nu}\rangle^{\mathrm{ss}}. \tag{67}$$

On the other hand, if $t' < t$ we have, from Eq. (61),

$$\frac{d}{dt'}C^{\mu\nu}(t,t') = \langle L^{-}A^{\nu}(\exp\{L^{+}(t-t')\}A^{\mu})\rangle^{\mathrm{ss}}. \tag{68}$$

When $t \to t'$, with $t' < t$, this leads to

$$\lim_{\substack{t\to t'\\ t'<t}} \frac{d}{dt'}C^{\mu\nu}(t,t') = \langle A^{\mu}L^{-}A^{\nu}\rangle^{\mathrm{ss}}. \tag{69}$$

We observe that, as a function of t, the first derivative is discontinuous at $t=t'$, in general. Therefore, in the second derivative in Eq. (62), we must account for this discontinuity by adding the term

$$\delta(t-t')\langle A^{\mu}[L^{-}-L^{+}]A^{\nu}\rangle^{\mathrm{ss}} = \delta(t-t')2k_B\langle d^{\mu\nu}\rangle^{\mathrm{ss}}, \tag{70}$$

where the equality follows from the use of Eqs. (4) and (6), the definition (35), and some integration by parts.

Now, consider the following double time integral:

$$\mathcal{B}^{\mu\nu}(\tau) \equiv \int_0^{\tau} dt \int_0^{\tau} dt' B^{\mu\nu}(t,t') = \int_0^{\tau} dt \int_0^{t} dt' b^{\nu\mu}(t-t') + \int_0^{\tau} dt \int_t^{\tau} dt' b^{\mu\nu}(t'-t) + \tau 2k_B\langle d^{\mu\nu}\rangle^{\mathrm{ss}}, \tag{71}$$

where we have taken into account the Dirac delta function contribution in Eq. (70) giving the last term in Eq. (71). By the change in variables $u=t-t'$ in the first integral and $u=t'-t$ in the second, we have

$$\begin{aligned}\mathcal{B}^{\mu\nu}(\tau) &= \int_0^{\tau} dt \int_0^{t} du b^{\nu\mu}(u) + \int_0^{\tau} dt \int_0^{\tau-t} du b^{\mu\nu}(u)\\ &= \int_0^{\tau} du b^{\nu\mu}(u) \int_u^{\tau} dt + \int_0^{\tau} du b^{\mu\nu}(u) \int_0^{\tau-u} dt\\ &\quad + \tau 2k_B\langle d^{\mu\nu}\rangle^{\mathrm{ss}} = \int_0^{\tau} du(\tau-u)(b^{\nu\mu}(u) + b^{\mu\nu}(u))\\ &\quad + \tau 2k_B\langle d^{\mu\nu}\rangle^{\mathrm{ss}}.\end{aligned} \tag{72}$$

Now, let us consider the convergence properties of these integrals. In principle, we expect that when $u \to \infty$ the two variables $L^{+}A^{\nu}$ and $L^{-}A^{\mu}$ in Eq. (65) become uncorrelated, this is

$$\lim_{u\to\infty} b^{\mu\nu}(u) = \left[\int dz \rho^{\mathrm{ss}}(z) L^{-}A^{\mu}(z)\right]\left[\int dz \rho^{\mathrm{ss}}(z) L^{+}A^{\nu}(z)\right] = 0, \tag{73}$$

where the last identity comes from the fact that $L\rho^{\mathrm{ss}}=0$. Therefore, $b^{\mu\nu}(u)$ tends to zero as u increases. We will assume that this decay is sufficiently strong in order for both integrals

$$\int_0^{\tau} du[b^{\nu\mu}(u) + b^{\mu\nu}(u)]$$

$$\int_0^{\tau} duu[b^{\nu\mu}(u) + b^{\mu\nu}(u)] \tag{74}$$

to exist in the limit $\tau \to \infty$. In this case, for sufficiently large τ, we can neglect in Eq. (72) the second integral in Eq. (74) in front of the first one, this is

$$\mathcal{B}^{\mu\nu}(\tau) \approx \tau \int_0^{\tau} du[b^{\nu\mu}(u) + b^{\mu\nu}(u)] + \tau 2k_B\langle d^{\mu\nu}\rangle^{\mathrm{ss}}. \tag{75}$$

On the other hand, by using Eq. (62), we can perform the time integrals of the time derivatives in Eq. (71),

$$\begin{aligned}\mathcal{B}^{\mu\nu}(\tau) &= \int_0^{\tau} dt \int_0^{\tau} dt' \frac{d}{dt}\frac{d}{dt'}C^{\mu\nu}(t,t')\\ &= C^{\mu\nu}(\tau,\tau) - C^{\mu\nu}(0,\tau) + C^{\mu\nu}(0,0) - C^{\mu\nu}(\tau,0).\end{aligned} \tag{76}$$

By using that, the correlation can be written in terms of averages over realizations of the stochastic process, i.e.,

$$C^{\mu\nu}(t,t') = \overline{A^{\mu}(t)A^{\nu}(t')}, \tag{77}$$

we have from Eqs. (76) and (77) that

$$\mathcal{B}^{\mu\nu}(\tau) = \overline{[A^{\mu}(\tau) - A^{\mu}(0)][A^{\nu}(\tau) - A^{\nu}(0)]}. \tag{78}$$

In summary, for sufficiently large τ we have, from Eqs. (75) and (78), the following relationship:

$$\frac{1}{2\tau}\overline{[A^{\mu}(\tau) - A^{\mu}(0)][A^{\nu}(\tau) - A^{\nu}(0)]} = k_B\langle d^{\mu\nu}\rangle^{\mathrm{ss}} + \frac{1}{2}\int_0^{\tau} du[b^{\nu\mu}(u) + b^{\mu\nu}(u)]. \tag{79}$$

This formula is a general expression that relates the mean square "displacements" of a set of phase functions A^{μ} with the time integral of the stationary correlation function $b^{\mu\nu}(u)$ defined in Eq. (65). Note that this correlation function $b^{\mu\nu}(u)$ has not a symmetric appearance in that *both* operators L^{+}, L^{-} occur in the definition of the correlation. This is clearly a consequence of the general structure of a correlation function in Eqs. (58) and (60).

B. Einstein-Helfand version of the friction matrix

The friction matrix M defined in Eq. (50) can be decomposed into a symmetric part plus an antisymmetric part. Only

the symmetric part contributes to the second derivative terms in the Fokker-Planck equation (49). The antisymmetric part may contribute to the irreversible drift term $M^{\mu\nu}\partial_\nu S$ in Eq. (49) but it will not produce any entropy production (see Sec. III C). Note that a general symmetry property of $K_0^{\nu\mu}(\alpha)$ is not obvious from its microscopic expression (46) and the possibility of having irreversible transport that does not produce entropy increase is not excluded [6].

The symmetric part of the matrix M in Eq. (50) can be written as

$$\frac{1}{2}[M^{\mu\nu}+M^{\nu\mu}]=\langle d^{\mu\nu}\rangle^{\alpha}+\frac{1}{2}\int_0^\tau du[m^{\mu\nu}(\tau,u)+m^{\nu\mu}(\tau,u)], \tag{80}$$

where, from the definition of $K_0^{\mu\nu}$ in Eq. (47), we have introduced $m^{\mu\nu}(\tau,u)$ as

$$m^{\mu\nu}(\tau,u)\equiv\frac{1}{k_B}\langle(\exp\{L^-u\}L^-A^\nu-\langle L^-A^\nu\rangle^\alpha)(\exp\{L^+\tau\}L^+A^\mu - \langle L^+A^\mu\rangle^\alpha)\rangle^\alpha. \tag{81}$$

Note that, in principle, $m^{\mu\nu}(\tau,u)$ depends on both time arguments. However, within the spirit of the approximation (45), we may safely assume that the constrained ensemble $\rho_\alpha(z)$ defined in Eq. (17) is, within the time span τ, a stationary ensemble, because it depends on the slow variables $A(z)$, which hardly change during τ under the assumption of a clear separation of time scales. Under this assumption, we have that $\langle L^+A^\mu\rangle^\alpha\approx 0$. In this way, the matrix $m^{\mu\nu}(\tau,u)$ can be further approximated by

$$m^{\mu\nu}(\tau,u)=\frac{1}{k_B}\langle(\exp\{L^-u\}L^-A^\nu)(\exp\{L^+\tau\}L^+A^\mu)\rangle^\alpha. \tag{82}$$

We see, therefore, that if we keep assuming consistently that the constrained ensemble is an approximate stationary ensemble of the dynamics generated by L, then $m^{\mu\nu}(\tau,u)$ can be approximated by $b^{\mu\nu}(\tau,u)$ defined in Eq. (65). As a consequence, Eqs. (80), (75), and (78) show that, for sufficiently large τ, we have

$$M^{\mu\nu}=\frac{1}{2k_B\tau}\overline{[A^\mu(\tau)-A^\mu(0)][A^\nu(\tau)-A^\nu(0)]}. \tag{83}$$

This is one of the main results of this paper. Expression (83) is a generalization of the Einstein-Helfand form of the transport coefficients to the case that the original detailed level of description is stochastic. In principle we can use this expression to compute the transport matrix from a stochastic simulation of the detailed level, in the same way as it is used for ordinary molecular dynamics [22].

Note that in the Einstein form, the matrix $M^{\mu\nu}$ is manifestly positive definite. Just left and right multiply Eq. (83) with an arbitrary vector u_μ to get

$$\frac{1}{2k_B\tau}\overline{\left\{\sum_\mu u_\mu[A^\mu(\tau)-A^\mu(0)]\right\}^2}, \tag{84}$$

which is always a positive quantity.

The usual argument in order to prove that a Green-Kubo friction matrix is positive definite for the case that the detailed level is Classical Mechanics is the Wiener-Kinchine theorem [7]. This theorem states that the time integral of a stationary autocorrelation matrix is always positive definite. Note, however, that Eq. (81) is not an obvious *auto*correlation in general, due to the asymmetry in the appearance of the operators L^+ and L^-. Even though the matrix $d^{\mu\nu}$ is definite positive by its very definition in Eq. (35) (and the fact that d_{ij} is itself positive definite), it is not obvious that the time integral of the correlation $b^{\mu\nu}(\tau,u)$ is positive definite. The above derivation of the Einstein-Helfand form of the transport matrix M is valid for both, deterministic and stochastic detailed dynamics and is, therefore, an alternative demonstration that the transport matrix is positive definite.

C. *H* theorem

It is possible to show that, as any other Fokker-Planck equation [19], the FPE (49) has an H theorem. The role of the H function is played by the entropy functional introduced in Eq. (20). The time derivative of $S[p(\alpha,t)]$ is given by

$$\frac{\partial}{\partial t}S[p(\alpha,t)]=-k_B\int d\alpha\frac{\delta S[p(\alpha,t)]}{\delta p(\alpha,t)}\frac{\partial}{\partial t}p(\alpha,t) =-k_B\int d\alpha\left[\ln\frac{p(\alpha,t)}{p^{\rm ss}(\alpha)}-1\right]\frac{\partial}{\partial t}p(\alpha,t). \tag{85}$$

By using the FPE (49), the fact that $p(\alpha,t)$ is normalized to 1 for all t, and a suitable integration by parts with neglect of surface terms, one is led to

$$\frac{\partial}{\partial t}S[p(\alpha,t)] =\frac{1}{2}\int d\alpha p(\alpha,t)\partial_\mu\left[\ln\frac{p(\alpha,t)}{p^{\rm ss}(\alpha)}\right]M^{\mu\nu}(\alpha)\partial_\nu\left[\ln\frac{p(\alpha,t)}{p^{\rm ss}(\alpha)}\right]\geq 0, \tag{86}$$

where the inequality is due to the fact that the matrix $M(\alpha)$ (or rather its symmetric part) is positive definite. The entropy functional is an strictly increasing function of time. It takes the maximum value (zero) at the steady state distribution function. This proves, then, that any initial distribution function obeying the Fokker-Planck equation (49) relaxes towards the steady state distribution $p^{\rm ss}(\alpha)$, which is, therefore, unique.

IV. TIME REVERSAL AND DETAILED BALANCE

In this section, we discuss the consequences of having a detailed level of description that satisfies the property of detailed balance. Under time reversal the detailed state z changes to $\bar{z}=\epsilon z$, where ϵ is a diagonal matrix that has ± 1 in the diagonal depending on the time reversal character of each component of z. The condition of *detailed balance* states that the two-time steady state probability satisfies [19]

$$\rho^{\rm ss}(z,t+\tau,z',t)=\rho^{\rm ss}(\epsilon z',t+\tau,\epsilon z,t). \tag{87}$$

This implies that under time reversal, the steady state distribution behaves as $\rho^{\rm ss}(\epsilon z)=\rho^{\rm ss}(z)$.

A remarkable property about detailed balance is that it is a feature of the system and not of the level of description considered. In other words, if the system is described at its most detailed level by a Fokker-Planck equation satisfying detailed balance, then, any coarse-grained FPE obtained from this one will also satisfy detailed balance. In particular, any FPE that is derived from Hamilton's equations of motion satisfies detailed balance.

In order to see how this remarkable property arises, let us assume that the relevant variables $A^\mu(z)$ have a well-defined parity under time reversal of z, this is

$$A(\epsilon z) = \varepsilon A(z), \tag{88}$$

where ε is a diagonal matrix that has ± 1 in the diagonal depending on the time reversal character of each relevant variable.

The two time probability distribution $p(\alpha,t,\alpha',t')$ that gives the probability density that the relevant variables take values α at time t and α' at time t' is defined in a similar way to the one time probability in Eq. (13), this is

$$p(\alpha,t,\alpha',t') \equiv \int dz \int dz' \rho(z,t,z',t') \times \delta[A(z)-\alpha]\delta[A(z')-\alpha'], \tag{89}$$

where $\rho(z,t,z',t')$ is the two time probability at the detailed level. By using the detailed balance property (87) in Eq. (89), performing the change in variables $x=\epsilon z, x'=\epsilon z'$, and using the parity properties in Eq. (88), one obtains that the coarse distribution also satisfies detailed balance, this is,

$$p^{\rm ss}(\alpha,t+\tau,\alpha',t) = p^{\rm ss}(\varepsilon\alpha',t+\tau,\varepsilon\alpha,t). \tag{90}$$

Therefore, the detailed balance property is a property of the system and not of the level of description used.

A. Coarse FPE with detailed balance

The necessary and sufficient conditions in order that the FPE (1) satisfies detailed balance are [19]

$$\epsilon_i v_i(\epsilon z) = -v_i(z) + \frac{2k_B}{\rho^{\rm ss}(z)}\partial_j d_{ij}(z)\rho^{\rm ss}(z)$$

$$d_{ij}(\epsilon z) = \epsilon_i \epsilon_j d_{ij}(z). \tag{91}$$

In this and subsequent expressions, repeated indices are summed over *except* those involving ϵ_i. Because we know from Eq. (90) that detailed balance is also satisfied at the coarse level, we should be able to demonstrate that the objects introduced in Eq. (50) for the coarse FPE (49) also satisfy the set of properties analogous to Eq. (91). The purpose of the present section is to demonstrate explicitly that this is actually the case. This should give further confidence on the obtained microscopic expressions and, in particular, to the, at first sight, counterintuitive asymmetric appearance of the L^+, L^- operators in the Green-Kubo expression.

We introduce the reversible drift v_i^R and the irreversible drift v_i^I through

$$v_i = v_i^R + v_i^I$$

$$v_i^R(z) \equiv \frac{1}{2}[v_i(z) - \epsilon_i v_i(\epsilon z)] = -\epsilon_i v_i^R(\epsilon z)$$

$$v_i^I(z) \equiv \frac{1}{2}[v_i(z) + \epsilon_i v_i(\epsilon z)] = \epsilon_i v_i^I(\epsilon z), \tag{92}$$

and then the first condition of detailed balance in Eq. (91) translates into

$$\rho^{\rm ss} v_i^I = k_B \partial_j d_{ij} \rho^{\rm ss}, \tag{93}$$

or equivalently

$$v_i^I = d_{ij}\partial_j \mathcal{S} + k_B \partial_j d_{ij}, \tag{94}$$

where the entropy $\mathcal{S}(z)$ is defined in Eq. (3).

By using the detailed balance condition (94), we can write the original FPE (1) in the form

$$\partial_t \rho_t = -\frac{\partial}{\partial z_i}\left[v_i^R + d_{ij}\frac{\partial \mathcal{S}}{\partial z_j}\right]\rho_t + k_B \frac{\partial}{\partial z_i} d_{ij} \frac{\partial}{\partial z_j}\rho_t. \tag{95}$$

As a consequence, if we insert Eq. (3) into Eq. (95), we get that the reversible drift satisfies

$$\partial_i v_i^R \rho^{\rm ss}(z) = 0. \tag{96}$$

Under the detailed balance conditions, the operators L^+, L^- defined in Eqs. (4) and (6) adopt a particularly symmetric form

$$L^+ = v_i^R(z)\partial_i + v_i^I(z)\partial_i + k_B d_{ij}(z)\partial_i\partial_j,$$

$$L^- = v_i^R(z)\partial_i - v_i^I(z)\partial_i - k_B d_{ij}(z)\partial_i\partial_j. \tag{97}$$

By using these forms for the operators, we observe that $v_\pm^\mu$ in Eq. (35), can be expressed as

$$v_\pm^\mu = v_R^\mu \pm v_I^\mu$$

$$v_R^\mu \equiv v_i^R \partial_i A^\mu$$

$$v_I^\mu \equiv v_i^I \partial_i A^\mu + k_B d_{ij}\partial_i\partial_j A^\mu. \tag{98}$$

As we will show later, v_R^μ is a macroscopic reversible drift while v_I^μ is a macroscopic irreversible drift.

B. Detailed balance at the coarser level

The Fokker-Planck equation (49) can be written in the form

$$\partial_t p(\alpha,t) = -\partial_\mu \mathcal{A}^\mu(\alpha)p(\alpha,t) + \frac{1}{2}\partial_\mu\partial_\nu \mathcal{B}^{\mu\nu}(\alpha)p(\alpha,t)$$

$$\mathcal{A}^\mu(\alpha) = \langle v_R^\mu \rangle^\alpha + M^{\mu\nu}(\alpha)\partial_\nu S(\alpha) + k_B \partial_\mu M^{\mu\nu}(\alpha)$$

$$\mathcal{B}^{\mu\nu}(\alpha) = 2k_B M^{\mu\nu}(\alpha). \tag{99}$$

We have used that $V^\mu(\alpha) = \langle v_R^\mu \rangle^\alpha$ as it is shown in the Appendix B.

The Green-Kubo matrix $K_0^{\mu\nu}(\alpha)$, as introduced in Eq. (47), has no particular symmetry and, therefore, the matrix

$M^{\mu\nu}(\alpha)$ in Eq. (50) has no symmetry either. It is convenient, therefore, to introduce the symmetric $M^{\mu\nu S}(\alpha)=[M^{\mu\nu}(\alpha)+M^{\nu\mu}(\alpha)]/2$ and antisymmetric $M^{\mu\nu A}(\alpha)=[M^{\mu\nu}(\alpha)-M^{\nu\mu}(\alpha)]/2$ parts of the friction matrix $M^{\mu\nu}(\alpha)$. In this way,

$$\mathcal{A}^{\mu}(\alpha)=\langle v_R^{\mu}\rangle^{\alpha}+M^{\mu\nu A}(\alpha)\partial_{\nu}S(\alpha)+\frac{k_B}{\Omega(\alpha)}\partial_{\mu}M^{\mu\nu S}(\alpha)\Omega(\alpha)$$

$$\mathcal{B}^{\mu\nu}(\alpha)=2k_BM^{\mu\nu S}(\alpha). \tag{100}$$

The necessary and sufficient conditions for detailed balance take the following form in terms of $\mathcal{A}^{\mu}(\alpha)$ and $\mathcal{B}_{\mu\nu}(\alpha)$ [19]:

$$\epsilon_{\mu}\mathcal{A}^{\mu}(\epsilon\alpha)=-\mathcal{A}^{\mu}(\alpha)+\frac{1}{\Omega(\alpha)}\partial_{\nu}\mathcal{B}_{\mu\nu}\Omega(\alpha)$$

$$\mathcal{B}_{\mu\nu}(\epsilon\alpha)=\epsilon_{\mu}\epsilon_{\nu}\mathcal{B}(\alpha). \tag{101}$$

Eqs. (101) are analogous to Eqs. (91) at the coarse level.

We want to prove that the properties (101) are indeed satisfied, provided that the corresponding properties (91) are satisfied too. In this way, we ensure that the detailed balance property is satisfied at both levels of descriptions, as it should.

To this end, we analyze what are the effects of the time reversal symmetry on the different objects of the FPE (49) when detailed balance holds. The parity properties of the relevant variables Eq. (88) translate into the following properties for the derivatives of the relevant variables

$$\frac{\partial A^{\mu}}{\partial z_i}(\epsilon z)=\varepsilon^{\mu}\epsilon_i\frac{\partial A^{\mu}}{\partial z_i}(z)$$

$$\frac{\partial^2 A^{\mu}}{\partial z_i\,\partial z_j}(\epsilon z)=\varepsilon^{\mu}\epsilon_i\epsilon_j\frac{\partial^2 A^{\mu}}{\partial z_i\,\partial z_j}(z). \tag{102}$$

By using the definitions (35) and the above properties, we easily arrive at the following behavior under time reversal

$$v_R^{\mu}(\epsilon z)=-\varepsilon^{\mu}v_R^{\mu}(z)$$

$$v_I^{\mu}(\epsilon z)=\varepsilon^{\mu}v_I^{\mu}(z)$$

$$v_+^{\mu}(\epsilon z)=-\varepsilon^{\mu}v_-^{\mu}(z)$$

$$d^{\mu\nu}(\epsilon z)=\varepsilon^{\mu}\varepsilon^{\nu}d^{\mu\nu}(z). \tag{103}$$

These properties justify to call v_R^{μ} the reversible drift and v_I^{μ} the irreversible drift. The steady state distribution behaves as

$$\Omega(\varepsilon\alpha)=\Omega(\alpha), \tag{104}$$

as can be easily shown from the definition (18) and a simple change in variables $z'=\epsilon z$. This equation implies that the entropy (50) satisfies

$$S(\varepsilon\alpha)=S(\alpha), \tag{105}$$

and, therefore,

$$\partial_{\mu}S(\varepsilon\alpha)=\varepsilon^{\mu}\partial_{\mu}S(\alpha). \tag{106}$$

Let us consider now the time reversal behavior of the constrained averages of Eq. (103). They are

$$\langle v_R^{\mu}\rangle^{\varepsilon\alpha}=-\varepsilon^{\mu}\langle v_R^{\mu}\rangle^{\alpha}$$

$$\langle v_I^{\mu}\rangle^{\varepsilon\alpha}=\varepsilon^{\mu}\langle v_I^{\mu}\rangle^{\alpha}$$

$$\langle v_+^{\mu}\rangle^{\varepsilon\alpha}=-\varepsilon^{\mu}\langle v_-^{\mu}\rangle^{\alpha}$$

$$\langle d^{\mu\nu}\rangle^{\varepsilon\alpha}=\varepsilon^{\mu}\varepsilon^{\nu}\langle d^{\mu\nu}\rangle^{\alpha}. \tag{107}$$

Eqs. (103) and (107) imply for the fluctuations

$$\delta_{\varepsilon\alpha}v_R^{\mu}(\epsilon z)=-\varepsilon^{\mu}\delta_{\alpha}v_R^{\mu}(z)$$

$$\delta_{\varepsilon\alpha}v_I^{\mu}(\epsilon z)=\varepsilon^{\mu}\delta_{\alpha}v_I^{\mu}(z)$$

$$\delta_{\varepsilon\alpha}v_+^{\mu}(\epsilon z)=-\varepsilon^{\mu}\delta_{\alpha}v_-^{\mu}(z). \tag{108}$$

Next, we focus on the effect of time reversal on the dynamic operators. Consider

$$\begin{aligned}L^+[F(\epsilon z)]&=\left[v_i^R\frac{\partial}{\partial z_i}+v_i^I\frac{\partial}{\partial z_i}+k_Bd_{ij}\frac{\partial}{\partial z_i}\frac{\partial}{\partial z_j}\right]F(\epsilon z)\\&=\left[-v_i^R(\epsilon z)\frac{\partial}{\partial\epsilon z_i}+v_i^I(\epsilon z)\frac{\partial}{\partial\epsilon z_i}\right.\\&\quad\left.+k_Bd_{ij}(\epsilon z)\frac{\partial}{\partial\epsilon z_i}\frac{\partial}{\partial\epsilon z_j}\right]F(\epsilon z)\\&=-[L^-F](\epsilon z).\end{aligned} \tag{109}$$

where in the second equality we have used the time reversal properties (92). In a similar way, we obtain

$$L^-[F(\epsilon z)]=-[L^+F](\epsilon z). \tag{110}$$

Consider now $L^-[v_R^{\mu}(\epsilon z)]$. On one hand, this term is equal to $-\varepsilon^{\mu}L^-[v_R^{\mu}(z)]$, where we have used Eq. (103). On the other hand, Eq. (110) shows that it is also equal to $-(L^+v_R^{\mu})(\epsilon z)$. Therefore, we conclude

$$[L^+v_R^{\mu}](\epsilon z)=\varepsilon^{\mu}[L^-v_R^{\mu}](z). \tag{111}$$

Apply L^- to this equation and use Eq. (110) to arrive

$$[L^+L^+v_R^{\mu}](\epsilon z)=-\varepsilon^{\mu}[L^-L^-v_R^{\mu}](z)$$

$$[L^+L^+L^+v_R^{\mu}](\epsilon z)=\varepsilon^{\mu}[L^-L^-L^-v_R^{\mu}](z). \tag{112}$$

By induction and the series expansion of the exponential, we can finally conclude

$$[\exp\{L^+t\}v_R^{\mu}](\epsilon z)=-\varepsilon^{\mu}[\exp\{-L^-t\}v_R^{\mu}](z). \tag{113}$$

Next, consider $L^-[v_I^{\mu}(\epsilon z)]$. On one hand, this term is, by Eq. (103), equal to $\varepsilon^{\mu}[L^-v_I^{\mu}](z)$. On the other hand, Eq. (110) implies that it is equal to $-[L^+v_I^{\mu}](\epsilon z)$. Therefore,

$$[L^+v_I^{\mu}](\epsilon z)=-\varepsilon^{\mu}[L^-v_I^{\mu}](z). \tag{114}$$

Apply L^- to this equation in succession and use Eq. (110) to obtain

$$[L^+L^+v_I^{\mu}](\epsilon z)=\varepsilon^{\mu}[L^-L^-v_I^{\mu}](z)$$

$$[L^+L^+L^+v_I^{\mu}](\epsilon z)=-\varepsilon^{\mu}[L^-L^-L^-v_I^{\mu}](z). \tag{115}$$

By induction, we conclude

$$[\exp\{L^+t\}v_I^\mu](\epsilon z) = \varepsilon^\mu[\exp\{-L^-t\}v_I^\mu](z). \quad (116)$$

Eqs. (113) and (116) imply

$$[\exp\{L^+t\}v_+^\mu](\epsilon z) = -\varepsilon^\mu[\exp\{-L^-t\}v_-^\mu](z). \quad (117)$$

Now, we have all the ingredients to discuss the time reversal of $K_0^{\mu\nu}$, which is one of the contributions to the friction matrix in Eq. (50) and it is defined in Eq. (47)

$$K_0^{\mu\nu}(\varepsilon\alpha) = \frac{1}{\Omega(\varepsilon\alpha)k_B}\int_0^\tau dt \int dz[\rho^{ss}(z)\delta(A(z)-\varepsilon\alpha)(v_-^\nu(z) - \langle v_-^\nu\rangle^{\varepsilon\alpha})\exp\{L^+t\}(v_+^\mu(z) - \langle v_+^\mu\rangle^{\varepsilon\alpha})]. \quad (118)$$

Use $\delta[A(z)-\varepsilon\alpha]=\delta[A(\epsilon z)-\alpha]$ and perform the change in variables $z'=\epsilon z$. This leads to

$$K_0^{\mu\nu}(\varepsilon\alpha) = \frac{1}{\Omega(\varepsilon)k_B}\int_0^\tau dt \int dz'[\rho^{ss}(\epsilon z')\delta(A(z')-\alpha)(v_-^\nu(\epsilon z') - \langle v_-^\nu\rangle^{\varepsilon\alpha}) \times \exp\{L^+t\}(v_+^\mu(\epsilon z') - \langle v_+^\mu\rangle^{\varepsilon\alpha})]. \quad (119)$$

Next, use the properties (104), (108), and (113) to write

$$K_0^{\mu\nu}(\varepsilon\alpha) = \frac{1}{\Omega(\alpha)k_B}\int_0^\tau dt \int dz'(\rho^{ss}(z')\delta[A(z')-\alpha] \times\{-\varepsilon^\nu[v_+^\nu(z') - \langle v_+^\nu\rangle^\alpha]\} \times [-\varepsilon^\mu \exp(-L^-t)] \times[v_-^\mu(z') - \langle v_-^\mu\rangle^\alpha]). \quad (120)$$

Now, under the assumptions used in Eq. (45) (stating that the constrained average is approximately stationary within the time span τ) and by using Eq. (9), we obtain

$$K_0^{\mu\nu}(\varepsilon\alpha) = \varepsilon^\nu\varepsilon^\mu\frac{1}{\Omega(\alpha)k_B}\int_0^\tau dt \int dz'\{\rho^{ss}(z')\delta[A(z')-\alpha] \times[v_-^\mu(z') - \langle v_-^\mu\rangle^\alpha] \times [\exp(L^+t)][v_+^\nu(z') - \langle v_+^\nu\rangle^\alpha]\}. \quad (121)$$

Therefore, from the very definition of $K_0^{\mu\nu}(\alpha)$ in Eq. (47)

$$K_0^{\mu\nu}(\varepsilon\alpha) = \varepsilon^\nu\varepsilon^\mu K_0^{\nu\mu}(\alpha). \quad (122)$$

This time reversal property implies the following transforms for the symmetric and antisymmetric parts of the friction matrix M:

$$M^{\mu\nu A}(\varepsilon\alpha) = -\varepsilon^\nu\varepsilon^\mu M^{\mu\nu A}(\alpha)$$

$$M^{\mu\nu S}(\varepsilon\alpha) = \varepsilon^\nu\varepsilon^\mu M^{\mu\nu S}(\alpha). \quad (123)$$

By collecting Eq. (106), the first equation of Eq. (107), and Eq. (123), and using them in the definitions (99), we can write

$$\epsilon_\mu\mathcal{A}^\mu(\epsilon\alpha) = -v_R^\mu(\alpha) - M^{\mu\nu A}(\alpha)\partial_\nu S(\alpha) + \frac{k_B}{\Omega(\alpha)}\partial_\nu[M^{\mu\nu S}(\alpha)\Omega(\alpha)] = -\mathcal{A}_\mu(\alpha) + \frac{1}{\Omega(\alpha)}\partial_\nu\mathcal{B}_{\mu\nu}(\alpha)\Omega(\alpha), \quad (124)$$

which is precisely the first condition in Eq. (101). The second condition of Eq. (101) is just the second equation in Eq. (123).

In summary, in this section, we have shown from the phase space definitions of the different objects appearing in the coarse-grained FPE (49) that their time reversal properties are exactly the same as those of the original detailed FPE (95). This implies that the detailed balance conditions in Eq. (101) are satisfied for the coarse FPE (49). This is quite reassuring and gives confidence to the particular asymmetric structure of the Green-Kubo formula for the friction matrix.

V. CONCLUSIONS

We have presented a derivation of the FPE that governs the coarse-grained behavior of a system that is described at a more detailed level by another FPE. The coarse FPE has been obtained previously in Refs. [14,11]. The main result of the present paper is the proof that the transport matrix of the coarse FPE is positive definite, which is a necessary requirement for the FPE to make sense. Also, we have shown that the coarse FPE satisfies the necessary and sufficient conditions for detailed balance provided that the detailed FPE also satisfies them. Finally, we have elucidated the different reversible/irreversible nature of the objects in the coarse FPE. In this doing, it becomes apparent that the structure of the Green-Kubo expression for the friction matrix contains two contributions, one that can be interpreted as the direct transfer of the detailed fluctuations to the coarse level, and a second contribution consisting of a time integral of a correlation function. This last contribution can be interpreted as the additional friction that emerges at the coarse time scale out of the evolution that at a detailed level is not seen as fluctuations but that can be regarded indeed as fluctuations on the coarse time scale [6]. The present work shows that the Einstein-Helfand form for the transport coefficients can now be used also for the case that the underlying dynamics is stochastic.

A last word on the issue of transitive coarse graining [14,23] is in order. We have considered in the present paper the coarse-graining of an already coarse-grained system. It is possible to iterate once more the process in order to obtain an even more coarse-description of the system. In that case, the effect of going from the more detailed level to the coarsest level, directly or through the passage through an intermediate level, should give the same answer. The transitivity property has been considered in Refs. [6,14], and it would be interesting to show that the Einstein-Helfand forms at each level are consistently recovered. We plan to address this issue in the future.

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APPENDIX A

In this appendix, we prove Eq. (51). Consider

$$V^{\mu}(\alpha)\Omega(\alpha) = \langle v_{+}^{\mu}\rangle^{\alpha}\Omega(\alpha) - k_B\partial_{\nu}d^{\mu\nu}(\alpha)\Omega(\alpha), \tag{A1}$$

where we have used the definitions (50). Now, use the microscopic definitions (35) and the chain rule (34) to write

$$\begin{aligned} V^{\mu}(\alpha)\Omega(\alpha) &= \mathrm{tr}[\rho^{ss}\Psi_{\alpha}(v_i\partial_i A^{\mu} + k_B d_{ij}\partial_i\partial_j A^{\mu})] \\ &\quad + k_B\,\mathrm{tr}[\rho^{ss}\partial_i A^{\mu} d_{ij}\partial_j\Psi_{\alpha}) \\ &= \mathrm{tr}[\rho^{ss}\Psi_{\alpha}v_i\partial_i A^{\mu}] + k_B\,\mathrm{tr}[\rho^{ss}d_{ij}(\partial_j\Psi_{\alpha}\partial_i A^{\mu})]\ \mathrm{bf} \\ &= \mathrm{tr}\left[\rho^{ss}\Psi_{\alpha}\left(v_i - \frac{k_B}{\rho^{ss}}\partial_j d_{ij}\rho^{ss}\right)\partial_i A^{\mu}\right]. \end{aligned} \tag{A2}$$

By dividing with $\Omega(\alpha)$, we obtain Eq. (51) in the text.

APPENDIX B

In this appendix, we show that $V^{\mu}(\alpha)=\langle v_R^{\mu}\rangle^{\alpha}$, which has been used in Eq. (99). First, we show that

$$\langle v_I^{\mu}\rangle^{\alpha}\Omega(\alpha) = k_B\partial_{\nu}\langle d^{\mu\nu}\rangle^{\alpha}\Omega(\alpha). \tag{B1}$$

This identity can be proved as follows. By using the definitions (35) and the detailed balance condition (94), we can write

$$\langle v_I^{\mu}\rangle^{\alpha}\Omega(\alpha) = \mathrm{tr}\{\rho^{ss}\Psi_{\alpha}[d_{ij}\partial_j\mathcal{S} + k_B\partial_j(d_{ij}\partial_i A^{\mu})]\}. \tag{B2}$$

Integration by parts in the second equation and using Eq. (34), we finally arrive at Eq. (B1). This equation can also be written as

$$\langle v_I^{\mu}\rangle^{\alpha} = \langle d^{\mu\nu}\rangle^{\alpha}\partial_{\nu}S(\alpha) + k_B\partial_{\nu}\langle d^{\mu\nu}\rangle^{\alpha}, \tag{B3}$$

which is the equivalent of Eq. (94) at the more coarse level. The identity (B3) allows one to obtain the drift of the coarse FPE in the very simple form

$$V^{\mu}(\alpha) = \langle v_R^{\mu}\rangle^{\alpha}. \tag{B4}$$

It is worth checking that the equilibrium distribution function $\Omega(\alpha)$ is still a solution of the FPE (99) with the drift (B4). Indeed, we need to prove that

$$\partial_{\mu}[\langle v_R^{\mu}\rangle^{\alpha}\Omega(\alpha)] = 0, \tag{B5}$$

which is the analogous of Eq. (96) at the more coarse level. By the definition of the constrained average, we have

$$\partial_{\mu}[\langle v_R^{\mu}\rangle^{\alpha}\Omega(\alpha)] = \partial_{\mu}\,\mathrm{tr}[\rho^{ss}\Psi_{\alpha}v_i^R\partial_i A^{\mu}]. \tag{B6}$$

By using Eq. (34) and an integration by parts, we get

$$\partial_{\mu}[\langle v_R^{\mu}\rangle^{\alpha}\Omega(\alpha)] = -\,\mathrm{tr}[\partial_i(\rho^{ss}v_i^R)\Psi_{\alpha}] = 0, \tag{B7}$$

where in the last identity, we have used Eq. (96).

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