Statistical mechanics of the GENERIC framework under external forcing

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The GENERIC framework provides a thermodynamically consistent approach to describe the evolution of coarse-grained variables. This framework states that the Markovian dynamic equations governing the evolution of coarse-grained variables have a universal structure that ensures energy conservation (First Law) and entropy increase (Second Law). However, the presence of external time-dependent forces can break the energy conservation law, requiring modifications to the framework's structure. To address this issue, we start from a rigorous and exact transport equation for the average of a set of coarse-grained variables derived from a projection operator technique in the presence of external forces. Under the Markovian approximation, this approach provides the statistical mechanics underpinning of the GENERIC framework under external forcing conditions. By doing so, we can account for the effects of external forcing on the system's evolution while ensuring thermodynamic consistency.

I. INTRODUCTION

Non-equilibrium statistical mechanics [1–4] is a general framework that allows one to obtain the dynamic equations of a set of coarse-grained (CG) variables from the underlying Hamiltonian dynamics of the system. This theory of coarse-graining allows one to represent a given system with less, but relevant, information. In this regard, the Mori-Zwanzig (MZ) projection operator method has been widely employed to achieve this goal [2, 5, 6]. The MZ method produces rigorous exact integro-differential transport equations for the evolution of the CG variables. As expected from an exact result, the equations are formal and, in general, untractable unless approximations are considered. The extremely useful Markovian approximation can be taken when the CG variables display an evolution with two distinct time scales. In this case, the formally exact integro-differential equations become ordinary differential equations which are much more tractable. More importantly, only for levels of descriptions which are Markovian, a thermodynamic structure emerges. This structure is known as GENERIC (for General Equation for Non-Equilibrium Reversible Irreversible Coupling) and proposes a universal form for descriptions of systems that obey the First and Second Laws of thermodynamics [3, 7]. The framework was introduced phenomenologically [8, 9], while its statistical mechanics foundation was given shortly after [10] by using the MZ projection operators technique for the case of isolated systems with time independent Hamiltonians that conserve the energy. GENERIC unifies virtually all the different theories and models based on ordinary and partial differential equations used in the CG description of matter, ranging from kinetic theory [9, 11], to Navier-Stokes hydrodynamics [10], colloidal systems [12], polymer physics [13, 14], electrochemical cells [15], viscoplastic solids [16], relativistic liquids [17], to quantum field theory [18] to name a few. A comprehensive list of examples of theories with the GENERIC structure may be found in [19].

Most of the existing research with the MZ projection operator approach has primarily focused on systems with time-independent Hamiltonians, and there has been relatively limited investigation into extending this method to encompass time-dependent Hamiltonians, which are crucial for describing the system's interaction with external fields. Notable recent exceptions are given in Refs. [20–22]. Observe that Grabert described and solved the problem of deriving the CG dynamic equations in the presence of external fields in Sec 6.2 of [1], under the assumption that the coupling of the external forces with the system is through the CG variables. te Vrugt and Wittowski [20] have extended Grabert's result to the more general case in which the coupling is not necesarily through the CG variables. This implies memory functions that depend on the present t and past t' times not in the form $t - t'$, leading to more complicated dynamic equations. Also recently, Schilling and co-workers [21] have considered the problem of CG in the presence of time-dependent forcing in a classical setting. They find essentially Grabert's result, and offer an interesting alternative interpretation in terms of an augmented phase space.

In this paper, we consider the problem of coarse-graining with external forcing, with the primary goal of establishing a connection with the GENERIC framework. Although the GENERIC framework has been considered for externally driven systems in terms of thermodynamic and geometric arguments [7, 23–25], the statistical mechanics foundation, and the link with the projection operator framework for externally forced systems are still lacking. We begin with the formal, exact integro-differential transport equation presented in Grabert's textbook for the evolution of CG variables in the presence of external forces. We then specify the assumptions required to recover the GENERIC framework in the presence of external fields, and show that all the GENERIC properties of the building blocks entering the

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dynamic equations are satisfied. The main modifications to the GENERIC framework for closed systems arise from the dependence of the energy and friction matrix on the external forcing. However, the other two building blocks, namely entropy and the reversible matrix, retain the same form as in the absence of external forcing. In the case of external forcing, energy is no longer conserved, and the First Law illustrates how energy increases as a result of the time-dependent external forces. On the other hand, entropy consistently increases, reflecting the Second Law.

In this paper, we also discuss the validity of the Onsager-Casimir reciprocity [26–28] for the *state dependent* friction matrix, an issue that was not considered in Grabert's textbook. There is large recent interest in understanding Onsager-Casimir reciprocity in systems very far from equilibrium [29–36]. We show how the generalized time reversibility conditions discovered by Bonella *et al.* for equilibrium transport coefficients [29] are further generalized to the state-dependent friction matrix encountered in the theory of coarse-graining.

The paper is organized as follows. In Sec. II we review the microscopic Hamiltonian description with external forcing. In Sec. III we present the exact equation goverining the averages of the CG variables, obtained with the method of projection operators. In Sec. IV we discuss the Markovian approximation, while in Sec. V we show how the Markovian transport equation for the averages can be written in the GENERIC format, with the usual GENERIC properties for the different building blocks. In Sec. VI, we consider the more detailed level of description given by the probability distribution of the CG variables, and obtain the corresponding Fokker-Planck Equation that governs its evolution. We investigate in Sec. VII the role of symmetries on the functional form of the building blocks, and conclude in Sec VIII.

II. THE MICROSCOPIC LEVEL

In Classical Statistical Mechanics the state of a system is given by the microstate $z = \{\mathbf{q}_i, \mathbf{p}_i, i = 1 \cdots N\}$ comprising all the coordinates and momenta of the N particles that constitute the system. We assume that the microscopic evolution of the system is well described with a Hamiltonian that may depend explicitly on time due to the action of external forces, this is

$$\hat{H}(z, \phi_t) = \hat{H}^{(0)}(z) - \phi_t^T \cdot \hat{C}(z) \tag{1}$$

where the unperturbed time-independent Hamiltonian $\hat{H}^{(0)}(z)$ is the sum of the kinetic energy and the potential energies of interaction between the particles and with any time-independent external potential. The last term in (1) represents the action of a time-dependent external forcing on the system. We will refer to ϕ_t as *the protocol* and $\hat{C}(z)$ as *the coupling functions*. Both $\phi_t, \hat{C}(z)$ are, in general, vectors with N_ϕ components, and the superscript T denotes the transpose. We will denote a function that depends on time in any of the two forms $f(t)$ or f_t, the latter used to alleviate notation.

The evolution of the microstate gives a trajectory z_t in phase space. This trajectory obeys Hamilton's equations, that can be written in compact form as

$$\frac{d}{dt} z_t = J \cdot \frac{\partial \hat{H}}{\partial z}(z_t, \phi_t) \tag{2}$$

where J is the skew-symmetric symplectic matrix. Alternatively, we may write Hamilton's equations (2) in the form

$$\frac{d}{dt} z_t = i\mathcal{L}(\phi_t)\hat{z}(z_t) \tag{3}$$

where the time-dependent Liouville operator is

$$i\mathcal{L}(\phi_t) = -\frac{\partial \hat{H}}{\partial z}(z, \phi_t) \cdot J \cdot \frac{\partial}{\partial z} = i\mathcal{L}_t \tag{4}$$

This operator is referred to as the p-Liouvillian in [37] and as the Liouville operator in the Schroedinger picture in [20]. Operators acting on phase functions are denoted in this paper with caligraphic symbols $i\mathcal{L}, \mathcal{U}, \mathcal{I}$, etc. Note that the Liouville operator is a differential operator that acts on phase functions, denoted in this paper with circumflexed symbols like $\hat{A}(z)$. In Eq (3), $\hat{z}(z)$ is the identity function in phase space, that is, the vector valued function that takes any microstate z onto itself.

The adjoint $\mathcal{O}^\dagger$ of an operator $\mathcal{O}$ is defined as the operator satisfying

$$\int dz \hat{F}(z) \mathcal{O}^\dagger \hat{G}(z) = \int dz \hat{G}(z) \mathcal{O} \hat{F}(z) \tag{5}$$

for arbitrary phase functions $\hat{F}(z), \hat{G}(z)$. The Liouville operator is anti-adjoint [38], this is

$$\int dz \hat{F}(z) i\mathcal{L}_t \hat{G}(z) = -\int dz \hat{F}(z) i\mathcal{L}_t \hat{G}(z) \tag{6}$$

For an arbitrary time independent phase function $\hat{F}(z)$ the time derivative of the composed function $\hat{F}(z_t)$ is given by

$$\frac{d}{dt} \hat{F}(z_t) = \frac{\partial \hat{F}}{\partial z}(z_t) \cdot \frac{d}{dt} z_t = i\mathcal{L}_t \hat{F}(z_t) \tag{7}$$

where we have used the chain rule and Hamilton's equations (2). The action of the Liouville operator on the Hamiltonian is

$$i\mathcal{L}_t \hat{H}(z_t, \phi_t) = -\frac{\partial \hat{H}}{\partial z}(z_t, \phi_t) \cdot J \cdot \frac{\partial \hat{H}}{\partial z}(z_t, \phi_t) = 0 \tag{8}$$

because the symplectic matrix J is a skew symmetric matrix. The explicit time-dependence of the Hamiltonian

implies that

$$\frac{d}{dt}\hat{H}(z_t,\phi_t) = -\hat{C}(z_t)\cdot\frac{d\phi_t}{dt} \tag{9}$$

For time-independent Hamiltonians where $\dot{\phi}_t = 0$, the Hamiltonian is conserved by the dynamics.

Even though Hamilton's equations give a unique solution given an initial condition, the precise specification of the initial microstate in a system with many degrees of freedom is impossible in practice. It is necessary to introduce statistical assumption on the initial conditions. The uncertainty in the initial conditions is described with a probability distribution $\rho_0(z)$ in phase space. The deterministic evolution of microstates leads to a time-dependent probability distribution $\rho_t(z)$ that obeys the Liouville equation [38]

$$\partial_t\rho_t(z) = -i\mathcal{L}(\phi_t)\rho_t(z) \tag{10}$$

that reflects the property of conservation of the volume in phase space of Hamiltonian systems [38]. We will refer to the solution $\rho_t(z)$ of the Liouville equation with initial condition $\rho_0(z)$ as the Liouville ensemble.

III. THE CG LEVEL OF DESCRIPTION

At a CG level of description, the system is represented with a set of CG variables $\hat{A}(z) = \{\hat{A}_\mu(z), \mu = 1\cdots M\}$, which are phase functions that characterize *grosso modo* the system at the selected level of description. The objective of the theory of coarse-graining is to obtain closed equations for the average of the CG variables. The time-dependent average of the CG variables is defined in terms of the Liouville ensemble as

$$a_t = \int dz\hat{A}(z)\rho_t(z) \tag{11}$$

The time derivative of the average of the CG variables is given by

$$\dot{a}_t = \int dz\rho_t(z)i\mathcal{L}_t\hat{A}(z) \tag{12}$$

where we have used the Liouville's equation (10) and the anti-adjoint property (6). Of course, (12) is not a proper dynamic equation for a_t because the right hand side is not a function of a_t, and this equation is not a *closed* equation for the averages. The strategy to close this equation is to formally express $\rho_t(z)$ in terms of another ensemble $\overline{\rho}_t(z)$, the *relevant ensemble*, that it is fully determined by the averages a_t. The merit of the projection operator method is to show that this is possible. The method starts by noting that one can convert any Liouville ensemble into a relevant ensemble with the help of an operator $\mathcal{P}_t^\dagger$

$$\overline{\rho}_t(z) = \mathcal{P}_t^\dagger\rho_t(z) \tag{13}$$

This operator is defined as [1]

$$\mathcal{P}_t^\dagger\eta(z) = \overline{\rho}_t(z)\mathrm{Tr}[\eta] + \frac{\partial\overline{\rho}_t}{\partial a(t)}(z)\mathrm{Tr}\left[(\hat{A}-a(t))\eta\right] \tag{14}$$

where $\eta(z)$ is an arbitrary density in phase space. If we require that the relevant ensemble $\overline{\rho}_t(z)$ provides the same averages (11) computed with the Liouville ensemble $\rho_t(z)$, this is

$$a_t = \int dz\hat{A}(z)\overline{\rho}_t(z) \tag{15}$$

then $\mathcal{P}_t^\dagger\overline{\rho}_t = \overline{\rho}_t$, and the operator is a projector. Observe that the time dependence of the projector arises from the corresponding dependence on the relevant ensemble which, ultimately, is due to the evolution of the thermodynamic forces λ_t or averages a_t. For this reason, we will also denote the projector with $\mathcal{P}_\lambda$ or $\mathcal{P}(a)$, depending on the context.

We show in Appendix B that the Liouville ensemble is rigorously expressed in terms of the present and past values of the relevant ensemble in the form

$$\rho_t(z) = \overline{\rho}_t(z) - \int_0^t dt'\mathcal{G}^\dagger[t,t',a,\phi]\mathcal{Q}_{t'}^\dagger i\mathcal{L}(\phi_{t'})\overline{\rho}_{t'}(z) \tag{16}$$

Here the complementary projector is $\mathcal{Q}_t^\dagger = \mathcal{I} - \mathcal{P}_t^\dagger$, and the adjoint of the projected evolution operator is defined as

$$\mathcal{G}^\dagger[t,t',a,\phi] = \exp_+\left\{\int_{t'}^t d\tau i\overline{\mathcal{L}}_\tau^\dagger\right\} \tag{17}$$

The time ordered exponential is defined through the series expansion

$$\exp_+\left\{\int_0^t d\tau i\overline{\mathcal{L}}_\tau^\dagger\right\} \equiv \sum_{n=0}^\infty\int_0^t d\tau_1\cdots\int_0^{\tau_{n-1}} d\tau_n i\overline{\mathcal{L}}_{\tau_1}^\dagger\cdots i\overline{\mathcal{L}}_{\tau_n}^\dagger \tag{18}$$

where the time argument of the operators increases from right to left. The adjoint of the projected Liouville operator is defined as

$$i\overline{\mathcal{L}}_\tau^\dagger \equiv -\mathcal{Q}^\dagger(a_\tau)i\mathcal{L}(\phi_\tau)\mathcal{Q}^\dagger(a_\tau) \tag{19}$$

A crucial assumption in order to arrive at (16) is that the initial ensemble $\rho_0(z)$ is of the relevant form, i.e.

$$\rho_0(z) = \overline{\rho}_0(z) \tag{20}$$

This means, in particular, that the initial ensemble is fully characterized by the value of the averages a_0 of the CG variables at the initial time. This seems a natural requirement when looking for equations where the initial values of the CG variables determine the subsequent evolution but, in fact, requires an initial preparation of the system in a particular way.

The remarkable equation (16) relates the Liouville ensemble $\rho_t(z)$ with the relevant ensemble $\overline{\rho}_t(z)$ at present and past times. Because the relevant ensemble is, in turn, fully determined by the value of the CG variables, (16) can be used to obtain a closed equation for the CG variables themselves. Therefore, the only two assumptions needed to obtain a closed equation for the averages are: i) the relevant ensemble gives the correct averages (15), and ii) the initial ensemble is of the relevant form (20). The actual form of the relevant ensemble is not specified yet and this gives, in principle, freedom to obtain different closed transport equations. In practice, though, one aims at representations that will admit simple approximations. We argue that this favours a particular definition of the relevant ensemble through the Maximum Entropy Principle.

A. The relevant ensemble from the Maximum Entropy Principle

Up to now, the only requirement we have about the relevant ensemble $\overline{\rho}_t(z)$ is that it depends on the average a_t and that it reproduces the average, see (15). We could take a pure epistemological approach and pose the following question: If the average a_t is the only information we have about the relevant ensemble, which is the "best" way to represent such information? This question is answered by the Maximum Entropy Principle (MEP) [39, 40] that maximizes the Gibbs-Jaynes entropy functional

$$\mathcal{S}[\rho] = -k_B \int dz \rho(z) \ln \frac{\rho(z)}{\rho_c} \tag{21}$$

where k_B is Boltzmann constant and ρ_c is a constant that makes the argument of the logarithm dimensionless, but is otherwise unimportant. The maximization is done subject to the constraint (15) and leads, through an standard calculation [39, 40] to the generalized canonical ensemble

$$\overline{\rho}_\lambda(z) = \rho_c \frac{e^{-\lambda\cdot\hat{A}(z)}}{Z(\lambda)} \tag{22}$$

The Lagrange multipliers λ are also known as conjugate variables or thermodynamic forces, see below. The normalization of (22) is given by the dimensionless partition function defined as

$$Z(\lambda) \equiv \int dz \rho_c e^{-\lambda\cdot\hat{A}(z)} \tag{23}$$

We will denote the average of an arbitrary phase function $\hat{G}(z)$ with respect to the relevant ensemble as

$$\langle \hat{G} \rangle^\lambda \equiv \int dz \overline{\rho}_\lambda(z) \hat{G}(z) \tag{24}$$

The conjugate parameters λ are selected in such a way that the average of the CG variables with the relevant ensemble is identical to the average with respect to the Liouville ensemble, this is

$$\left\langle \hat{A} \right\rangle^{\lambda_t} = a_t \tag{25}$$

By introducing the dimensionless thermodynamic potential as[1]

$$F(\lambda) = -\ln Z(\lambda) \tag{26}$$

we may express the condition (25) as

$$\frac{\partial F}{\partial \lambda}(\lambda) = a \tag{27}$$

Eqs. (27) are a system of M equations that allow to obtain the M Lagrange multipliers λ as a function of the M averages a. Note that the solution is unique, this is, for every a there is one and only one set of Lagrange multipliers λ. The proof of this reduces to show that the dimensionless thermodynamic potential (26) is a concave function of its arguments. [41–43].

The entropy of the level of description given by the CG variables is *defined* as the result of evaluating the Gibbs-Jaynes entropy functional at its maximum value given by the relevant ensemble. The result is

$$\overline{S}(a) \equiv \mathcal{S}[\overline{\rho}] = k_B \left(-F(\lambda) + \lambda a\right) \tag{28}$$

where λ is understood as the function $\lambda(a)$ of a that solves (27). Therefore, the entropy at the level of description determined by the averages of the CG variables $\hat{A}$ is (minus) the Legendre transform of the dimensionless thermodynamic potential. The derivatives of the entropy, known as thermodynamic forces, are given by the conjugate variables

$$\frac{\partial \overline{S}}{\partial a}(a) = k_B \lambda(a) \tag{29}$$

That the particular definition (28) of the entropy is a sensible one requires, of course, to show that this entropy has the properties we expect for it, in particular that it is subject to the Second Law $\frac{d\overline{S}}{dt}(a_t) \geq 0$. This will be shown once the closed equations for the average of the CG variables are derived.

The relevant ensemble (22) obtained from the MEP is the best ensemble, from an epistemological point of view, that captures the macroscopic information. However, there is an aditional physical argument that makes the particular form (22) plausible. Observe that the equilibrium ensemble of a Hamiltonian system with the property of *mixing* is a function of the microstate through the

[1] The dimensionless thermodynamic potential is defined without temperature prefactors as we treat the energy as a CG variable on an equal footing with the rest of CG variables.

dynamic invariants of the system [44, 45]. When the only dynamic invariant is the energy, the equilibrium ensemble is the microcanonical ensemble. If the CG variables were truly dynamic invariants of the underlying Hamiltonian system, the equilibrium ensemble that would be reached under the mixing assumption would be a microcanonical ensemble of the form

$$\rho_a^{\rm mic}(z) = \frac{\delta(\hat{A}(z)-a)}{\Omega(a)} \tag{30}$$

Under equivalence of ensembles, this generalized microcanonical ensemble gives similar results as the generalized canonical ensemble (22). In general, the CG variables are not dynamic invariants of the system, but if its dynamics is such that they are slowly varying functions, we expect that the Liouville ensemble will be very similar at all times to the quasi-equilibrium ensemble (22) of (30). In other words, the memory term in (16) is expected to be "small" for "slow" CG variables. This notion of quasi-equilibrium is at the core of the Markovian approximation to be considered later on.

B. The exact CG dynamic equation

Susbtitution of (16) with the form of the relevant ensemble (22) into (12), and a number of manipulations detailed in Appendix B, leads to the following exact dynamic equation for the average a_t of the CG variables

$$\frac{d}{dt}a_t = v(a_t,\phi_t) + \int_0^t dt' d[t,t',a,\phi]\cdot\frac{\partial \overline{S}}{\partial a}(a_{t'}) \tag{31}$$

where the reversible drift $v(a_t,\phi_t)$ and the memory kernel $d[t,t',a,\phi]$ are defined as

$$v(a_t,\phi_t) \equiv \left\langle i\mathcal{L}_t\hat{A}\right\rangle^{\lambda_t} \tag{32}$$

$$d[t,t',a,\phi] \equiv \frac{1}{k_B}\left\langle \left[\mathcal{G}[t,t',a,\phi]\mathcal{Q}_{t'}i\mathcal{L}_{t'}\hat{A}\right]\mathcal{Q}_{t'}i\mathcal{L}_{t'}\hat{A}\right\rangle^{\lambda_{t'}} \tag{33}$$

where the propagator, adjoint of (17), is

$$\begin{aligned}\mathcal{G}[t,t',a,\phi] &= \exp_-\left\{\int_{t'}^t d\tau i\overline{\mathcal{L}}_\tau\right\}\\ &= \sum_{n=0}^\infty \int_{t'}^t d\tau_1\cdots\int_{t'}^{\tau_{n-1}} d\tau_n i\overline{\mathcal{L}}_{\tau_n}\cdots i\overline{\mathcal{L}}_{\tau_1}\end{aligned} \tag{34}$$

The projected Liouville operator is defined as the adjoint of (19)

$$i\overline{\mathcal{L}}_\tau = \mathcal{Q}_\tau i\mathcal{L}(\phi_\tau)\mathcal{Q}_\tau \tag{35}$$

As opposed to the Liouville operator $i\mathcal{L}_\tau$, the projected Lioville operator $i\overline{\mathcal{L}}_\tau$ has a time dependence due to both, the external forcing ϕ_τ *and* the average a_τ. In fact, the projector operator is $\mathcal{Q}_t = \mathcal{I}-\mathcal{P}_t$ where

$$\mathcal{P}_t\hat{F}(z) = \left\langle\hat{F}\right\rangle^{\lambda_t} + \left\langle\hat{F}\delta_t\hat{A}\right\rangle^{\lambda_t}\cdot\Sigma_t^{-1}\cdot\delta_t\hat{A}(z) \tag{36}$$

is the adjoint operator of (14), where $\delta_t\hat{A}(z) = \hat{A}(z)-a_t$ denote the fluctuations over the mean at time t, and the covariance matrix is

$$\Sigma_t = \left\langle\delta_t\hat{A}\delta_t\hat{A}\right\rangle^{\lambda_t} \tag{37}$$

The projector (36) is the Kawasaki-Gunton projector [46] used in Grabert's textbook, and it is a generalization of the Mori projector [6] that uses the relevant ensemble instead of the equilibrium ensemble. The projectors $\mathcal{P}_t, \mathcal{Q}_t$ depend on the average a_t of the CG variables through $\lambda_t = \lambda(a_t)$.

The exact transport equation (31) has two terms. The first term $v(a_t,\phi_t)$ is a function of the averages a_t through the relevant ensemble, and is a function of the external forcing ϕ_t through the Liouville operator. The dissipative memory kernel $d[t,t',a,\phi]$ contains the propagator $\mathcal{G}[t,t',a,\phi]$ that involves in a rather intrincate way both, the external field and the projector $\mathcal{Q}_t$. As opposed to the microscopic evolution operator of Hamilton's equations that could, in principle, be evaluated through MD simulations, the evaluation of the propagator $\mathcal{G}[t,t',a,\phi]$ is not trivial. Because the projected dynamics involves the whole history of the averages a_τ with $t'\le\tau\le t$ and the whole protocol ϕ_τ, the memory kernel is a *functional* of the past history of the external field, and of the average of the CG variables. The transport equation (31) retains its structure even in the presence of time-dependent forcing. It closely resembles the equation derived for unforced situations [1], with the sole distinction lying in the explicit dependence of the Liouville operator on the external force.

We may compute the time derivative of the entropy when the evolution is given by the exact transport equation (31). The chain rule gives

$$\frac{d\overline{S}(t)}{dt} = \lambda_t\cdot v(a_t,\phi_t) + \int_0^t dt'\lambda_t\cdot d[t,t',a,\phi]\cdot\lambda_{t'} \tag{38}$$

The first term on the right hand side vanishes because

$$\lambda_t\cdot v(a_t,\phi_t) \overset{(32)}{=} -\int dz i\mathcal{L}_{t'}\overline{\rho}_{t'}(z) = 0 \tag{39}$$

where we use (6). This means that $v(a_t,\phi_t)$ does not contribute to entropy production and, for this reason, it is referred to as the reversible part of the dynamics. Note that the time derivative of the entropy is given by the memory part of the dynamics. It is not obvious that $\frac{d\overline{S}}{dt}(t)\ge 0$ from the exact rigorous form (33) for the memory kernel. However, we will see that under the Marko-

vian approximation the Second Law is satisfied.

IV. MARKOV APPROXIMATION

The exact integro-differential equation (31) is valid for *any* selection of the CG variables $\hat{A}(z)$. When the CG variables evolve as the result of the accumulation of many, but minuscule contributions (colisions, vibrations), the integro-differential equation (31) admits a Markovian approximation in terms of an ordinary differential equation (ODE) as we now discuss. The time series of such CG variables are "rough" due to the many small contribution, in such a way that they have an overall slow evolution in a typical time scale $\tau_{\rm mac}$, and a fast evolution of their time derivatives in a time scale $\tau_{\rm mic}$, with $\tau_{\rm mic} \ll \tau_{\rm mac}$. The projected current $\mathcal{Q}_{t'} i\mathcal{L}_{t'} \hat{A}$ involves the time derivatives of the CG variables through the action of the Liouville operator, and are expected to evolve in the fast time scale $\tau_{\rm mic}$. The memory kernel $d[t,t',a,\phi]$ defined in (33) is the correlation of the projected currents and, therefore, it is expected to decay in the time scale $\tau_{\rm mic}$, this is, $d[t'+\tau_{\rm mic},t',a,\phi]$ is vanishingly small. While the time derivatives decay in the $\tau_{\rm mic}$ time scale, the average of the CG variables $a(t)$ varies in the $\tau_{\rm mac}$ time scale. Of course, to mantain this separation of time scales under external forcing requires that the external forcing must be "not too fast". One way to appreciate this issue is by looking at Linear Response Theory that describes the evolution close to equilibrium of the averages under external forcing $\phi(t)$ [38]

$$\left\langle \hat{A} \right\rangle_t = \left\langle \hat{A} \right\rangle^{\rm eq} + \int_0^t dt' \chi(t-t')\phi(t') \tag{40}$$

where the $\chi(t)$ is the response function. For the sake of illustration, let us assume a model with an exponentially decaying response function $\chi(t) = \chi_0 e^{-\gamma(t-t')}$ and a sinusoidal external forcing $\phi(t) = \phi_0 \sin \omega t'$. In this case, we have

$$\left\langle \hat{A} \right\rangle_t = \left\langle \hat{A} \right\rangle^{\rm eq} + \chi_0 \phi_0 \frac{\omega e^{-\gamma t} + \gamma \sin(t\omega) - \omega \cos(t\omega)}{\gamma^2 + \omega^2} \tag{41}$$

This shows that the time-scale of variation of the average is, after an initial decay time, equal to the time-scale of the external forcing. If the external forcing has a frequency such that $\omega \tau_{\rm mic} \sim 1$, then $\tau_{\rm mac} \sim \tau_{\rm mic}$ and we do not have separation of time scales. Therefore, in order to have Markovian transport equations in the presence of external forcing requires the external forcings to be "sufficiently slow", as compared with the memory of the CG variables. Although (41) is a result near equilibrium and for small external fields, it clearly advocates for the case of using slow external forcing that respect the Markovian assumption in the more general case.

As the CG variables are slow in the time scale of decay of the memory, we may approximate within the time integral in (31)

$$\frac{\partial \overline{S}}{\partial a}(a_{t'}) \simeq \frac{\partial \overline{S}}{\partial a}(a_t) \tag{42}$$

leading to

$$\frac{d}{dt} a_t = v(a_t,\phi_t) + \overline{M}[t,a,\phi] \cdot \frac{\partial \overline{S}}{\partial a}(a_t) \tag{43}$$

where the dissipative or friction matrix is given by

$$\overline{M}[t,a,\phi] = \int_0^t dt' d[t,t',a,\phi] \tag{44}$$

Observe that (43) is not yet an ODE, because $\overline{M}[t,a,\phi]$ is still a very complicated functional of the history $a_{t'}$ (and protocol $\phi_{t'}$). We expect that when $t \gg \tau_{\rm mic}$ the time integral no longer depends on the upper limit of integration, because for those times the memory kernel has decayed. Therefore, we may write

$$\overline{M}[t,a,\phi] = \int_0^{\Delta t} dt' d[t,t',a,\phi] \tag{45}$$

where the upper limit of integration Δt is a time subject to

$$\tau_{\rm mic} \ll \Delta t \ll \tau_{\rm mac} \tag{46}$$

short in front of the time scale of evolution of the CG variables but sufficiently large for the memory to have faded away. The dependence on t in the friction matrix $\overline{M}[t,a,\phi]$ then comes entirely from the integrand. In addition, during the time $\tau_{\rm mic}$ in which there is contribution to the integral, both the history $a_{t'}$ and the protocol $\phi_{t'}$ take values which are almost constant and, in practice, these values can be taken to be a_t, ϕ_t, respectively. Therefore, we are entitled to substitute *all the instances* in the memory kernel where $a(t')$ and $\phi_{t'}$ occur with $a(t)$ and ϕ_t. For example, we may take the approximation $i\mathcal{L}(\phi_\tau) \simeq i\mathcal{L}(\phi_t)$ and $\mathcal{Q}_\tau \simeq \mathcal{Q}_t$ inside the time-ordered exponential (34), leading to

$$\mathcal{G}[t,t',a,\phi] \simeq e^{i\overline{\mathcal{L}}_t (t-t')} \tag{47}$$

Under the Markovian approximation we have that (31) becomes

$$\dot{a}_t \simeq v(a_t,\phi_t) + \overline{M}(a_t,\phi_t) \cdot \frac{\partial \overline{S}}{\partial a}(a_t) \tag{48}$$

where we collect the definition of all the building blocks

$$\overline{S}(a) = k_B \left[\ln \int dz \rho_c e^{-\lambda \cdot \hat{A}(z))} + \lambda a \right] \tag{49}$$

$$\lambda(a) = \frac{\partial S}{\partial a}(a) \tag{50}$$

$$v(\phi, a) = \left\langle i\mathcal{L}(\phi)\hat{A} \right\rangle^{\lambda} \tag{51}$$

$$\overline{M}(a_t, \phi_t) = \frac{1}{k_B} \int_0^{\Delta t} d\tau \left\langle \left[e^{i\overline{\mathcal{L}}_t \tau} \mathcal{Q}_t i\mathcal{L}_t \hat{A} \right] \mathcal{Q}_t i\mathcal{L}_t \hat{A} \right\rangle^{\lambda_t} \tag{52}$$

$$\langle \cdots \rangle^{\lambda} = \int dz \overline{\rho}_{\lambda}(z) \cdots \tag{53}$$

The friction matrix $\overline{M}(a_t, \phi_t)$ evaluated at a_t, ϕ_t is no longer a *functional* of the past values of $a_{t'}, \phi_{t'}$ but rather a *function* of the present values a_t, ϕ_t. Therefore, (48) is the closed ODE for the averages a_t that we were looking for. The dissipative matrix in terms of a time integral of a correlation function is known as the Green-Kubo expression for the friction matrix, which was originally formulated for systems near equilibrium. Observe, though, that the present theory is not limited to near equilibrium situations. In particular, the friction matrix depends, in general, on the state a_t of the system. Near equilibrium, where all conjugate variables λ_t corresponding to conserved variables take constant values, the friction matrix has the usual Green-Kubo form in terms of the equilibrium canonical ensemble.

The friction matrix involves the correlation of the projected currents, which are phase functions evolving under the projected dynamics $e^{i\overline{\mathcal{L}}_t \tau}$, that differs from the Hamiltonian dynamics generated by $e^{i\mathcal{L}_t \tau}$. It is usually argued [1, 5, 20] that, because the CG variables are "slow", $i\mathcal{L}_{t'}\hat{A}$ is a "small" quantity and one can perform a perturbation to second order. In many occasions, there is an explicit smallness parameter in the action of the Liouville operator on the CG variables. For conserved fields, the projected currents are in the form of a gradient, which in Fourier space are proportional to the wave vector $\mathbf{k}$. In the limit $\mathbf{k} \to 0$ the long wavelength components of the CG variables are really slow [47]. Or we may have a mass ratio for the dynamics of heavy particles that can serve as smallness parameter [48, 49]. In general, however, such a parameter is not explicit [50]. In any case, a formal expansion to second order in the number of Liouville operators shows that one can approximate the projected dynamics with the Hamiltonian dynamics and, for example,

$$\mathcal{Q}_t e^{i\overline{\mathcal{L}}_t \tau} i\mathcal{L}_t \hat{A} \simeq \mathcal{Q}_t e^{i\mathcal{L}_t \tau} i\mathcal{L}_t \hat{A} \tag{54}$$

in such a way that the friction matrix (52) can be computed, in principle, from MD simulations. The evolution operator $e^{i\mathcal{L}_t \tau}$ is that of the system under a *constant in time* external forcing in which the particular value of the constant external field is fixed to the value ϕ_t.

V. THE GENERIC STRUCTURE

In this section, we consider the assumptions that lead to the GENERIC structure of the dynamic equation. The GENERIC framework not only provides an elegant thermodynamic framework that ensures the First and Second Laws of thermodynamics, but it also reveals that the building blocks in the Markovian dynamic equation for the averages of the CG variables exhibit a set of properties. These properties *restrict* the possible functional form of the building blocks and, therefore, *increase* our modelling power. By focusing only on a few selected pieces of the building blocks, we can leave the rest fixed by the framework. Casting known evolution equations in the GENERIC form has been a fruitfull way to ensure thermodynamically consistency [3].

A. The CG energy

One of the building blocks in the GENERIC framework is the energy at the CG level of description. Consider first the case of no external forcing. The GENERIC structure emerges when the unperturbed Hamiltonian is a linear function of the CG variables, this is

$$\hat{H}^{(0)}(z) = c^T \cdot \hat{A}(z) \tag{55}$$

where c is a vector with constant entries. Despite its apparent simplicity, many examples of CG descriptions fall in this category. The full Hamiltonian (1) with the assumption (55) takes the form

$$\hat{H}_t(z) = c^T \cdot \hat{A}(z) - \phi_t^T \cdot \hat{C}(z) \tag{56}$$

The natural candidate for the CG energy is the relevant ensemble average of the Hamiltonian, this is

$$E(a_t, \phi_t) \equiv \left\langle \hat{H}_t \right\rangle^{\lambda_t} \tag{57}$$

that converts the Hamiltonian into a function of the CG variables. In fact,

$$\overline{E}(a_t, \phi_t) = c^T \cdot a_t - \phi_t^T \cdot \overline{C}(a_t) \tag{58}$$

where the relevant ensemble average of the coupling functions is

$$\overline{C}(a_t) \equiv \left\langle \hat{C} \right\rangle^{\lambda_t} \tag{59}$$

While (57) seems a natural way to define the energy at the CG level, the usefulness of this definition must be judged from the macroscopic properties that derive from it.

B. The reversible drift

When the Hamiltonian is (56), the Liouville operator (4) acting on the CG variables takes the form

$$i\mathcal{L}_t\hat{A}(z) = \hat{L}(z)\cdot c - \hat{L}^C(z)\cdot\phi_t \tag{60}$$

where we have introduced the Poisson bracket of the CG and coupling variables

$$\begin{aligned}\hat{L}_{\mu\nu}(z) &\equiv \{\hat{A}_\mu, \hat{A}_\nu\} = \frac{\partial\hat{A}_\mu}{\partial z}(z)\cdot J\cdot\frac{\partial\hat{A}_\nu}{\partial z}(z)\\ \hat{L}^C_{\mu\nu}(z) &\equiv \{\hat{A}_\mu, \hat{C}_\nu\} = \frac{\partial\hat{A}_\mu}{\partial z}(z)\cdot J\cdot\frac{\partial\hat{C}_\nu}{\partial z}(z)\end{aligned} \tag{61}$$

The reversible drift (51) becomes, with the help of (60)

$$v(a_t,\phi_t) = \overline{L}_t\cdot c - \overline{L}^C_t\cdot\phi_t \tag{62}$$

where,

$$\begin{aligned}\overline{L}(a_t) &\equiv \left\langle\hat{L}\right\rangle^{\lambda_t}\\ \overline{L}^C(a_t) &\equiv \left\langle\hat{L}^C\right\rangle^{\lambda_t}\end{aligned} \tag{63}$$

Observe that the gradient of the energy (58) is

$$\frac{\partial\overline{E}}{\partial a}(a,\phi) = c - \kappa_t\cdot\phi_t \tag{64}$$

where the matrix κ_t is defined as

$$\kappa_t \equiv \Sigma_t^{-1}\cdot\left\langle\delta_t\hat{A}\hat{C}^T\right\rangle^{\lambda_t} \tag{65}$$

Therefore, by using (64) we may write the reversible drift in the form

$$v(a_t,\phi_t) = \overline{L}(a_t)\cdot\frac{\partial\overline{E}}{\partial a} + \left(\overline{L}(a_t)\cdot\kappa_t - \overline{L}^C(a_t)\right)\cdot\phi_t \tag{66}$$

The first contribution is in the form of the GENERIC framework, i.e. an antisymmetric operator acting on the gradient of the energy. As we see below, the second contribution vanishes when the external forcing couples through the CG variables. Therefore, this second contribution accounts for the fact that the external forcing does not couple through the CG variables.

C. The external forces couple through the CG variables

Equation (66) simplifies enormously when the external force couples with the CG variables themselves. In this case, $\hat{C}(z) = \hat{A}(z)$, implying $L^C_t = L_t$ and $\kappa_t = \mathcal{I}$. The Hamiltonian (56) becomes

$$\hat{H}_t(z) = (c-\phi_t)^T\cdot\hat{A}(z) \tag{67}$$

and the CG energy (58) simplifies to

$$\overline{E}(a_t,\phi_t) = (c-\phi_t)^T\cdot a_t, \tag{68}$$

From (60), the action of the Liouville operator on the CG variables is

$$i\mathcal{L}_t\hat{A}(z) = \hat{L}(z)\cdot(c-\phi_t) \tag{69}$$

while the reversible drift simplifies to

$$v(a_t,\phi_t) = \overline{L}(a_t)\cdot\frac{\partial\overline{E}}{\partial a}(a_t,\phi_t) \tag{70}$$

Inserting (70) in (48) we obtain the dynamic equation for the averages in the form

$$\dot{a}_t = \overline{L}(a_t)\cdot\frac{\partial\overline{E}}{\partial a}(a_t,\phi_t) + \overline{M}(a_t,\phi_t)\frac{\partial\overline{S}}{\partial a}(a_t) \tag{71}$$

These equations have the GENERIC structure, in which the reversible part of the dynamics is given by a reversible operator $\overline{L}$ acting on the gradient of the energy function, while the irreversible part of the dynamics is given by a dissipative operator $\overline{M}$ acting on the gradient of the entropy. Of course, to qualify for GENERIC , a number of properties of the four building blocks need to be fulfilled, as discussed in the next subsection. Comparison with the unforced case shows that the reversible matrix $\overline{L}(a)$ and the entropy $\overline{S}(a)$ are unaffected by the presence of external forcing, while the energy $\overline{E}(a,\phi)$ and the friction matrix $\overline{M}(a,\phi)$ pick up a dependence on the external forcing.

D. Properties of the building blocks

The hallmark of the GENERIC structure is the reversible-irreversible coupling characterized by the following degeneracy of the reversible and dissipative operators

$$\begin{aligned}\overline{L}(a)\cdot\frac{\partial\overline{S}}{\partial a}(a) &= 0\\ \overline{M}(a,\phi)\cdot\frac{\partial\overline{E}}{\partial a}(a,\phi) &= 0\end{aligned} \tag{72}$$

The first property is easily proved with the definitions (61),(29), and (24)

$$\begin{aligned}\overline{L}\cdot\frac{\partial\overline{S}}{\partial a} &= \int dz\overline{\rho}_t\frac{\partial\hat{A}}{\partial z}\cdot J\cdot\frac{\partial\hat{A}}{\partial z}\cdot\lambda = -\int dz\frac{\partial\hat{A}}{\partial z}\cdot J\cdot\frac{\partial\overline{\rho}_t}{\partial z}\\ &= \int dz\overline{\rho}_t\frac{\partial^2\hat{A}}{\partial z\partial z} : J = 0\end{aligned} \tag{73}$$

where we have integrated by parts (neglecting phase space surface terms) and used that the full contraction of a symmetric and antisymetric matrix vanishes.

The second property in (72) is a consequence of the orthonormality of the projected current and the gradient of the energy

$$\left(\mathcal{Q}_t e^{i\overline{\mathcal{L}}_t\tau} i\mathcal{L}_t\hat{A}\right)\cdot\frac{\partial\overline{E}}{\partial a}=0 \tag{74}$$

which is easily proved

$$\left(\mathcal{Q}_t e^{i\overline{\mathcal{L}}_t\tau} i\mathcal{L}_t\hat{A}\right)\cdot\frac{\partial\overline{E}}{\partial a}\overset{(64)}{=}\mathcal{Q}_t e^{i\overline{\mathcal{L}}_t\tau} i\mathcal{L}_t\hat{A}\cdot(c-\phi_t)$$
$$\overset{(56)}{=}\mathcal{Q}_t e^{i\overline{\mathcal{L}}_t\tau} i\mathcal{L}_t\hat{H}_t\overset{(8)}{=}0 \tag{75}$$

By using (74) in the definition of the friction matrix (52) leads directly to the degeneracy condition of the friction matrix in (72).

Concerning the GENERIC symmetries of the reversible and irreversible operators, it is obvious from the definition of the reversible operator in terms of a Poisson bracket that the reversible operator is skew-symmetric $\overline{L}=-\overline{L}^T$. There seems to be no reason to think that the friction matrix $\overline{M}(a,\phi)$ is a symmetric matrix, although it is in many practical situations. The final requirement in the GENERIC framework is that the symmetric part of the friction matrix is positive definite. The justification for this property is based on plausibility, rather than a rigorous mathematical proof, and relies on the clear separation of time scales. Under this assumption, the conditional ensemble is an approximate stationary ensemble of the dynamics and, therefore, it is possible to use the Wiener-Khinchine theorem to show that the friction matrix is positive definite [1]. Alternatively, one my rewrite the Einstein-Helfand form of the friction matrix [51] which, being a mean square "displacement" of CG variables, is manifestly positive definite, see [52]. The arguments in [1, 52] leading to positive semi-definite character of the friction matrix remain unaltered in the presence of external fields.

Finally, a useful property of the reversible part of the dynamics is given by the Jacobi identity. Observe that the reversible part of the dynamics can be written as $\dot{A}=\{A,E\}$ with the Poisson bracket given in terms of the reversible operator L. Applying this to $\{A,B\}$ gives $\{\dot{A,B}\}=\{\{A,B\},E\}$. On the other hand, $\{\dot{A,B}\}=\{\dot{A},B\}+\{A,\dot{B}\}$. The Jacobi identity guarantees that these two time derivatives of $\{A,B\}$ are equal and thus the Poisson bracket remains unchanged during the time evolution [25]. In the case of purely reversible coarse-grained dynamics, the Jacobi identity is essential. However, coarse-grained dynamics derived from the underlying dynamics incorporate irreversible components, rendering the argument for equality of derivatives invalid. It seems very difficult to prove the Jacobi identity from the microscopic definition of the reversible operator L [3]. At present, the Jacobi identity seems to be a useful phenomenological restriction.

E. First and Second Laws

By using the properties (72) and the positive semidefinite character of the friction matrix, the time derivatives of the energy and entropy can be computed with the chain rule and one obtains

$$\frac{d}{dt}\overline{E}(a_t,\phi_t)=-a_t\cdot\dot{\phi}_t \tag{76}$$
$$\frac{d}{dt}\overline{S}(a_t)=\frac{\partial\overline{S}}{\partial a}(a_t)\cdot\overline{M}(a_t,\phi_t)\cdot\frac{\partial\overline{S}}{\partial a}(a_t)\geq 0 \tag{77}$$

The first equation is an expression of the First Law, stating that the energy changes due to the time-dependence of the external force. It is reassuring that (76) is compatible with the microscopic expression (9) when we assume that the Hamiltonian has the form (55) and the CG energy is given by (57). The second equation (77) is an expression of the Second Law, which is satisfied even in forced situations. It is a consequence of the positive semidefinite character of the symmetric part of the friction matrix, while any skew symmetric contribution to the friction matrix does not contribute to the production of entropy. We remark that the proof of the Second Law in the form (77) entirely relies on the Markovian approximation.

When the system is not subjected to any time-dependent forces, energy is conserved while entropy steadily increases. As a result, the CG variables, evolving with (71) and $\phi_t=0$, move within the submanifold of constant energy. Over time, they will eventually reach an equilibrium state within that submanifold, where entropy is maximized. However, in the presence of time-dependent external forcing, the system typically lacks a microscopic equilibrium state. In correspondence, the coarse-grained GENERIC equations (71) do not possess a definitive equilibrium state, despite the ongoing maximization of entropy, because energy is no longer conserved.

VI. THE STOCHASTIC FLAVOUR UNDER EXTERNAL FORCING

Up to now we have considered the CG theory in what could be termed as the *average flavour*[2], which is concerned with the evolution of averages $a(t)$ of CG variables. The *stochastic flavour*[3] of the theory of CG deals with the evolution of the probability distribution $P(a,t)$ that the CG variables $\hat{A}(z)$ take particular values a. This

[2] The term used by Grabert is "Statistical Thermodynamics" [1].
[3] The term used by Grabert is "The Fokker-Planck approach" [1].

probability distribution of the CG variables is defined by

$$P(a,t) = \int dz \rho_t(z) \hat{\Psi}_a(z) \tag{78}$$

where we have introduced the notation for the Dirac delta function

$$\hat{\Psi}_a(z) = \delta(\hat{A}(z) - a) \tag{79}$$

This notation emphasizes that the probability $P(a,t)$ is just the average of the distribution (79).

In order to obtain the dynamics for the probability density $P(a,t)$ we now use as CG variables $\hat{A}(z)$ the distribution function $\hat{\Psi}_a(z)$ [1, 2]. All we need to do is to "translate" all the elements appearing in the dynamic equation (48) to this new selection of variables. This is done in Appendix C, where we show that the transport equation (48) for the CG variables (79) takes the form of a Fokker-Planck Equation governing the probability distribution of the CG variables in the presence of external fields,

$$\begin{aligned}\frac{\partial}{\partial t} P(a,t) = &- \frac{\partial}{\partial a} \cdot \left[V(a,\phi_t) + M(a,\phi_t) \cdot \frac{\partial S}{\partial a}(a) \right] P(a,t) \\ &+ k_B \frac{\partial}{\partial a} \cdot M(a,\phi_t) \cdot \frac{\partial}{\partial a} P(a,t)\end{aligned} \tag{80}$$

where we have introduced the reversible drift

$$V(a,\phi) \equiv \left\langle i\mathcal{L}(\phi)\hat{A} \right\rangle^a \tag{81}$$

where the conditional expectation of an arbitrary phase function $\hat{F}(z)$ is defined as

$$\left\langle \hat{F} \right\rangle^a = \int dz \rho_a^{\text{mic}}(z) \hat{F}(z) \tag{82}$$

where the generalized microcanonical ensemble is given in (30). The "volume" of phase space compatible with the macrostate a is

$$\Omega(a) = \int dz \delta(\hat{A}(z) - a) \tag{83}$$

and the bare entropy is defined as

$$S(a) = k_B \ln \Omega(a) \tag{84}$$

The friction matrix is defined as

$$\begin{aligned}M_{\mu\nu}(a,\phi) \equiv \frac{1}{k_B} \int_0^{\Delta t} d\tau \Big\langle \Big(i\mathcal{L}(\phi)\hat{A}_\nu - \Big\langle i\mathcal{L}(\phi)\hat{A}_\nu \Big\rangle^a \Big) \\ \times e^{i\overline{\mathcal{L}}(a,\phi)\tau} \Big(i\mathcal{L}(\phi)\hat{A}_\mu - \Big\langle i\mathcal{L}(\phi)\hat{A}_\mu \Big\rangle^a \Big) \Big\rangle^a\end{aligned} \tag{85}$$

When the external field vanishes $\phi_t = 0$, (80) coincides with the FPE obtained by Green [53] and Zwanzig [5] for the unperturbed case. For the unperturbed case, the system may reach an equilibrium state. Due to the particular way in which the friction matrix appears in between the second derivatives in (80), and the properties of the building blocks discussed below, it is a simple exercise to show that the equilibrium solution is given by Einstein's equilibrium distribution function in the presence of dynamic invariants [45]

$$P^{\text{eq}}(a) = \Phi(E(a)) \exp\{k_B^{-1} S(a)\} \tag{86}$$

where the functional form of $\Phi(E)$ is fixed by the distribution of the energy at the initial time, and the normalization of $P^{\text{eq}}(a)$.

A. The generic form of the FPE

The FPE (80) can be written in the GENERIC form. Once more, the essential approximation lies in the ability to represent the Hamiltonian as a linear function of the coarse-grained variables, i.e. (55). When the CG variables are the distribution $\hat{\Psi}_a(z)$, (55) becomes

$$\hat{H}^{(0)}(z) = \int da E^0(a) \hat{\Psi}_a(z) \tag{87}$$

where we have translated $c \to E^0(a)$, and the scalar product becomes an integral over the "index" a. By performing the integral over the Dirac delta function in (87) we obtain

$$\hat{H}^{(0)}(z) = E^{(0)}(\hat{A}(z)) \tag{88}$$

this is, the unperturbed Hamiltonian is a function of the CG variables $\hat{A}(z)$ which, in general, it is non-linear. In the presence of external fields, we assume that the time-dependent Hamiltonian can be expressed in terms of the selected CG variables, this is

$$\hat{H}_t(z) = E^{(0)}(\hat{A}(z)) + E^{(1)}(\hat{A}(z), \phi_t) \tag{89}$$

This allows to define the CG energy function as

$$E(a,t) = E^0(a) + E^1(a,\phi_t) \tag{90}$$

which is the sum of the energy function $E^0(a)$ of the unperturbed system and the energy function $E^1(a,\phi_t)$ describing the action of the time-dependent external forcing. We will usually assume a forcing of the form

$$E^1(a,\phi_t) = -a \cdot \phi_t \tag{91}$$

One consequence of (89) is that the gradient of the Hamiltonian in phase space is given from the chain rule as

$$\frac{\partial \hat{H}_t}{\partial z}(z) = \frac{\partial E}{\partial a}(\hat{A}(z), \phi_t) \cdot \frac{\partial \hat{A}}{\partial z}(z) \tag{92}$$

This implies that the action of the Liouville operator (4) on the CG variables is

$$\begin{aligned} i\mathcal{L}(\phi_t)\hat{A}(z) &= \frac{\partial \hat{A}}{\partial z}(z)\cdot J\cdot \frac{\partial H_t}{\partial z}(z) \\ &= \frac{\partial \hat{A}}{\partial z}(z)\cdot J\cdot \frac{\partial \hat{A}}{\partial z}(z)\cdot \frac{\partial E}{\partial a}(\hat{A}(z),\phi_t) \\ &\overset{(61)}{=} \hat{L}(z)\cdot \frac{\partial E}{\partial a}(\hat{A}(z),\phi_t) \end{aligned} \tag{93}$$

By using (93) in the reversible drift (C15), and the fact that within the conditional expectation we may substitute $\hat{A}(z)$ with a, we get the following expression for the reversible drift

$$V(a,\phi_t) = L(a)\cdot \frac{\partial E}{\partial a}(a,\phi_t) \tag{94}$$

where the reversible operator defined as

$$L(a) \equiv \left\langle \hat{L} \right\rangle^a \tag{95}$$

is the conditional expectation of the Poisson bracket of the CG variables (61). By using (94) in the FPE (80) we obtain

$$\partial_t P(a,t) = -\frac{\partial}{\partial a}\cdot\left[L(a)\cdot\frac{\partial E}{\partial a}(a,\phi_t) + M(a,\phi_t)\cdot\frac{\partial S}{\partial a}(a) + k_B\frac{\partial\cdot M}{\partial a}(a,\phi_t)\right]P(a,t) + k_B\frac{\partial}{\partial a}\frac{\partial}{\partial a} : M(a,\phi_t)P(a,t) \tag{96}$$

The FPE (96), and the microscopic definition of all its building blocks are the main results of this section. When the external field vanishes $\phi_t = 0$, this equation coincides with the FPE obtained by Öttinger [10]. The comparison of the FPE (96) with the corresponding unperturbed FPE reveals that the reversible operator $L_{\mu\nu}(a)$ is unmodified but the energy picks up the natural dependence on the time-dependent external field. On the other hand, the entropy is unmodified by the time-dependent external field, but the friction matrix $M_{\mu\nu}(a,\phi_t)$ acquires an implicit dependence on the external field.

Associated to the Fokker-Planck Equation (96) there is a Stochastic Differential Equation that, in the Ito interpretation [54], has the form

$$\begin{aligned} da_t = L(a)\cdot\frac{\partial E}{\partial a}(a_t,\phi_t)dt + M(a,\phi_t)\cdot\frac{\partial S}{\partial a}(a_t)dt \\ + k_B\frac{\partial\cdot M}{\partial a}(a_t,\phi_t)dt + d\tilde{a}_t \end{aligned} \tag{97}$$

where the stochastic term $d\tilde{a}$ is a linear combination of independent increments of the Wiener proces, this is,

$$d\tilde{a}(t) = B(a_t)\cdot dW(t) \tag{98}$$

and the amplitude of the noise is determined by the Fluctuation-Dissipation theorem in the form

$$B\cdot B^T = M^S \tag{99}$$

where the superscript S denotes the symmetric part of the matrix.

B. Properties of the building blocks

The GENERIC properties of the building blocks described for the average flavour also hold for the stochastic flavor, with minor modifications. These properties are demonstrated in Appendix C 1.

The first property is the reversibility condition

$$L(a)\cdot\frac{\partial S}{\partial a}(a) + k_B\frac{\partial}{\partial a}\cdot L(a) = 0 \tag{100}$$

that links the functional form of the reversible operator $L(a)$ with the functional form of the bare entropy function $S(a)$. The reversibility condition is a strong restriction on the functional forms, and it is very helpful when modelling these building blocks. The reversibility condition (100) also holds in the unforced case [3, 10]. Note that the entropy function is typically of the order Nk_B where N is the (usually very large) number of particles in the system. Therefore, the first term in (100) is overwhemly larger than the second one. Under these conditions, one obtains the approximate, albeit accurate in most occasions, GENERIC degeneracy condition

$$L(a)\cdot\frac{\partial S}{\partial a}(a) = 0 \tag{101}$$

The degeneracy conditions on the friction matrix are

$$\begin{aligned} M(a,\phi_t)\cdot\frac{\partial E}{\partial a}(a,\phi_t) = 0 \\ M^T(a,\phi_t)\cdot\frac{\partial E}{\partial a}(a,\phi_t) = 0 \end{aligned} \tag{102}$$

These degeneracy conditions of the friction matrix are proved in Appendix C 1. Another important GENERIC property is that the symmetric part of the fric-

tion matrix (C20) is positive semi-definite. This is an automatic consequence of the corresponding property for the average flavour. As we have mentioned, a rigorous proof that the friction matrix $M(a,t)$ is a positive semi-definite function seems to be difficult. However, if it is not, the whole meaning of the Fokker-Planck approach becomes dubious [10]. We will always assume that the dissipative matrix is positive semi-definite, where the semi character is due to the degeneracy (102).

C. The First Law

Consider the average of the energy $E(a,\phi_t)$ performed with the solution $P(a,t)$ of the FPE (96)

$$\overline{E}_t = \int da E(a,\phi_t) P(a,t) \tag{103}$$

The time derivative of the average energy is given by

$$\frac{d}{dt}\overline{E}_t = \int da P(a,t)\frac{\partial E}{\partial t}(a,\phi_t) + \int da E(a,\phi_t)\frac{\partial P}{\partial t}(a,t) \tag{104}$$

The second term turns out to vanish exactly. To see this, use the FPE (96) and integrate by parts

$$\begin{aligned}&\int da E(a,\phi_t)\frac{\partial P}{\partial t}(a,t)\\ &= \int da \frac{\partial E}{\partial a}\cdot\left[\left[L\cdot\frac{\partial E}{\partial a} + M\cdot\frac{\partial S}{\partial a}\right]P - M\cdot\frac{\partial}{\partial a}P\right]\\ &= 0\end{aligned} \tag{105}$$

that vanishes because of the antisymmetry of L and the degeneracy (100). Therefore, the variation of the total energy (90),(91) of the system is given by

$$\frac{d}{dt}\overline{E}_t = \int da P(a,t) a\cdot\dot{\phi}_t = a_t\cdot\dot{\phi}_t \tag{106}$$

If the external forcing is time-independent, then total energy is conserved. Note that we may be interested not in the average change of the *total* energy but only in the actual change of the energy of the unperturbed system, discounting the energy due to the coupling, this is, from (90)

$$\left\langle \hat{H}^{(0)}\right\rangle_t = \left\langle \hat{H}_t + \hat{A}\cdot\phi_t\right\rangle_t \tag{107}$$

By using (106), the time derivative of this energy is given by

$$\frac{d}{dt}\left\langle \hat{H}^{(0)}\right\rangle_t = \dot{a}_t\cdot\phi_t \tag{108}$$

The right hand side is interpreted as the work per unit time done by the external forcing on the system, and it has the form of "velocity times force", i.e. power.

D. The Second Law

The entropy of a given level of description is obtained by inserting the relevant ensemble given by (C5) in the Appendix into the Gibbs-Jaynes entropy functional (21), leading to the result

$$S[P_t] = -k_B\int da P(a,t)\ln\frac{P(a,t)}{\Omega(a)} \tag{109}$$

We show that this entropy functional has a time derivative that is always positive or zero when the probability distribution $P(a,t)$ obeys the FPE (80). The proof follows the same steps as the proof of the H-theorem for a FPE given in [54]. By using the chain rule we have

$$\begin{aligned}\frac{d}{dt}S[P_t] &= \int da\frac{\delta S}{\delta P(a,t)}\partial_t P(a,t)\\ &= -k_B\int da\left[\ln\frac{P(a,t)}{\Omega(a)}+1\right]\frac{\partial}{\partial a}\\ &\times\cdot\left[V(a,\phi_t)P(a,t) + M(a,\phi_t)\Omega(a)\cdot\frac{\partial}{\partial a}\frac{P(a,t)}{\Omega(a)}\right]\end{aligned} \tag{110}$$

By integrating by parts (and assuming that any surface term vanishes), we have

$$\begin{aligned}\frac{d}{dt}S[P_t] &= k_B\int da P(a,t)V(a,\phi_t)\cdot\frac{\partial}{\partial a}\left[\ln\frac{P(a,t)}{\Omega(a)}+1\right]\\ &+ k_B\int da P(a,t)\\ &\times\frac{\partial}{\partial a}\cdot\left[\ln\frac{P(a,t)}{\Omega(a)}+1\right]M(a,\phi_t)\cdot\left[\frac{\partial}{\partial a}\ln\frac{P(a,t)}{\Omega(a)}\right]\end{aligned} \tag{111}$$

The reversible term does not change the entropy functional because

$$\begin{aligned}&\int da P(a,t)V(a,\phi_t)\cdot\frac{\partial}{\partial a}\left[\ln\frac{P(a,t)}{\Omega(a)}+1\right]\\ &= \int da\Omega(a)V(a,\phi_t)\cdot\frac{\partial}{\partial a}\frac{P(a,t)}{\Omega(a)}\\ &= -\int da\frac{P(a,t)}{\Omega(a)}\frac{\partial}{\partial a}\cdot V(a,\phi_t)\Omega(a) = 0\end{aligned} \tag{112}$$

where in the last equality we have integrated by parts and have used the reversibility condition (100). The reversibility condition (100) receives its name from the fact that the reversible drift does not contribute to the entropy production, as (112) shows. Therefore, (111) becomes

$$\begin{aligned}\frac{d}{dt}S[P_t] &= k_B\int da P(a,t)\\ &\times\left[\frac{\partial}{\partial a}\ln\frac{P(a,t)}{\Omega(a)}\right]\cdot M^S(a,\phi_t)\cdot\left[\frac{\partial}{\partial a}\ln\frac{P(a,t)}{\Omega(a)}\right]\geq 0\end{aligned} \tag{113}$$

where only the symmetric part of the friction matrix matters. This time derivative is always positive because the symmetric part of the friction matrix is positive semi-definite, and the probability density $P(a,t)$ is also positive. This means that the entropy functional (109) always increases.

The entropy functional $S[P_t]$ defined in (109) and the bare entropy function $S(a)$ defined in (84) are different objects, and despite names, only the entropy functional is a monotonously increasing function of time. The evolution of the bare entropy $S(a)$ (84) is due to the evolution of the CG variables according to the SDE (97). By using Ito calculus, we may compute the stochastic increment of the bare entropy as

$$dS = \frac{\partial S}{\partial a}\cdot da + \frac{1}{2}\frac{\partial^2 S}{\partial a \partial a} : dada \tag{114}$$

and neglecting terms of order higher than dt. By using the SDE (97) and the Fluctuation-Dissipation theorem (99), Ito calculus lead to the SDE

$$\begin{aligned} dS(t) = &\frac{\partial S}{\partial a}\cdot M \cdot \frac{\partial S}{\partial a} dt \\ &+ k_B \frac{\partial}{\partial a}\cdot\left[M(a)\cdot\frac{\partial S}{\partial a}\right] dt + \frac{\partial S}{\partial a}\cdot d\tilde{a} \end{aligned} \tag{115}$$

The first term satisfies

$$\frac{\partial S}{\partial a}\cdot M \cdot \frac{\partial S}{\partial a} \geq 0 \tag{116}$$

because the symmetric part of the friction matrix is positive definite, and shows that $S(t)$ is "typically" growing in time. However, neither the second term nor the third stochastic term have definite character and, therefore, the function $S(t)$ is not ensured to increase monotonously in time. When fluctuations are negligible, the second and last terms of (115) are small and, then, the bare entropy $S(a(t))$ satisfies approximately a Second Law. This is consistent with the fact that for small fluctuations, $P(a,t)$ is highly peaked at the average, and the entropy functional (109) is numerically similar, up to a constant to the bare entropy function.

E. Comparison of the average and stochastic flavours

We have considered the two flavours of this CG theory, the average flavour concerned with the averages of the CG variables, and the stochastic flavour concerned with its probability distribution. The building blocks have similar structure, but its actual functional dependence on the state is different in general, and that is the reason of using the notation $\overline{E}, \overline{S}, \overline{L}, \overline{M}$ in the average flavour, and E, S, L, M in the stochastic flavour. This issue is known as renormalization of transport coefficients due to thermal fluctuations [1, 55]. When fluctuations are very small, i.e the probability distribution is highly peaked, we have equivalence of the generalized microcanonical (30) and canonical (22) ensembles leading to similar functional forms for the building blocks. Another way to appreciate this is by looking at the SDE (97). The width of the probability distribution scales with k_B and the limit of small fluctuations can be taken formally by neglecting terms of order k_B in (97). This convert the SDE (97) into an ODE identical to the transport equation (71) for the averages.

VII. SYMMETRIES

The GENERIC properties (72) in the average flavour or (100),(102) in the stochastic flavour constrain the functional form of the building blocks. Because the building blocks are state dependent in general, and usually need to be modelled, the GENERIC properties constitute a very useful guide to recover thermodynamically consistent models. In addition to the GENERIC properties, there are a number of additional properties that originate from the symmetries of the Hamiltonian dynamics, which are also very helpful when modelling the building blocks [3]. We consider here two symmetries: time reversal symmetry and orthogonal symmetry. We present the results here and refer their demonstration to appendices A 3 and D 3, respectively

A. Time reversal symmetry

Time reversal symmetry leads to Onsager-Casimir reciprocity for the friction matrix. While the original proofs of Onsager-Casimir reciprocity were given for near equilibrium situations [26–28], and the demonstration for arbitrary far from equilibrium situations under no external forcing is given in Grabert's textbook, we have not been able to find such a demonstration for the case of i) arbitrary far from equilibrium situations with state dependent friction matrix, ii) under external forcing. For this reason, we present the derivation in Appendix A 3.

We assume that the CG variables have a well-defined parity under time reversal, this is

$$\hat{A}(\epsilon\cdot z) = \varepsilon_{\mathsf{T}}\cdot\hat{A}(z) \tag{117}$$

The matrix ϵ is diagonal with ± 1 in the diagonal, and it reverses the sign of the momentum, this is, if $z = (q,p)$ then $\epsilon\cdot z = (q,-p)$. The matrix ε_{T} is diagonal with entries ± 1 that reflects the time reversal behaviour of the CG variables. Under assumption (117), we show in Appendix A 3 that the different building blocks satisfy

the properties

$$\overline{E}(\varepsilon_{\mathsf{T}}\cdot a, \varepsilon_{\mathsf{T}}\cdot\phi) = E(a,\phi) \tag{118}$$
$$\overline{S}(\varepsilon_{\mathsf{T}}\cdot a) = \overline{S}(a) \tag{119}$$
$$\overline{L}(\varepsilon_{\mathsf{T}}\cdot a) = -\varepsilon_{\mathsf{T}}\cdot\overline{L}(a)\cdot\varepsilon_{\mathsf{T}} \tag{120}$$
$$\overline{M}(\varepsilon_{\mathsf{T}}\cdot a, \varepsilon_{\mathsf{T}}\cdot\phi) = \varepsilon_{\mathsf{T}}\cdot\overline{M}^{T}(a,\phi)\cdot\varepsilon_{\mathsf{T}} \tag{121}$$

Identical symmetry properties hold for the building blocks E, S, L, M in the stochastic flavour.

The symmetry property (121) of the friction matrix is the Onsager-Casimir reciprocity that it is here shown to be valid even for state dependent friction matrices. These properties limit the functional form of the different building blocks. A most obvious case is when all the CG variables are even under time-reversal, so ε_{T} is the identity matrix. In this case, $\overline{L}(a) = 0$, i.e. there is no reversible evolution of the dynamics, while the friction matrix is symmetric [4].

B. Orthogonal symmetry

When the unperturbed Hamiltonian is invariant under rotations and inversions, another set of symmetries reflect in the building blocks. We introduce the notation

$$\mathsf{R}\cdot z = (\mathsf{R}\cdot\mathbf{q}_1, \cdots, \mathsf{R}\cdot\mathbf{q}_N, \mathsf{R}\cdot\mathbf{p}_1, \cdots \mathsf{R}\cdot\mathbf{p}_N) \tag{122}$$

where R is an orthogonal matrix $\mathsf{R}\cdot\mathsf{R}^T = 1$. This orthogonal matrix may be a rotation ($\det\mathsf{R} = 1$) or an improper rotation ($\det\mathsf{R} = -1$). Improper rotations are also referred to as rotoinversions. Any improper rotation can be decomposed as the product of a proper rotation around a unit axis, and a mirror reflection through a plane normal to the axis and passing through the origin. We assume that the unperturbed Hamiltonian is invariant under such a transformation and that the CG variables are vectors or tensors that transform in the well-known form under orthogonal transformations, this is

$$\hat{H}^{(0)}(\mathsf{R}\cdot z) = \hat{H}^{(0)}(z)$$
$$\hat{A}(\mathsf{R}\cdot z) = \varepsilon_{\mathsf{R}}\cdot\hat{A}(z) \tag{123}$$

where ε_{R} is an $M\times M$ constant block matrix whose entries are given by the elements of the orthogonal matrix R arranged in a convenient form. We show in Appendix D 3 that the building blocks satisfy the following symmetry relations

$$\overline{E}(\varepsilon_{\mathsf{R}}\cdot a, \varepsilon_{\mathsf{R}}\cdot\phi) = \overline{E}(a,\phi) \tag{124}$$
$$\overline{S}(\varepsilon_{\mathsf{R}}\cdot a) = \overline{S}(a) \tag{125}$$
$$\overline{L}(\varepsilon_{\mathsf{R}}\cdot a) = \varepsilon_{\mathsf{R}}\cdot\overline{L}(a)\cdot\varepsilon_{\mathsf{R}}^{T} \tag{126}$$
$$\overline{M}(\varepsilon_{\mathsf{R}}\cdot a, \varepsilon_{\mathsf{R}}\cdot\phi) = \varepsilon_{\mathsf{R}}\cdot\overline{M}(a,\phi)\cdot\varepsilon_{\mathsf{R}}^{T} \tag{127}$$

Identical symmetry properties hold for the building blocks E, S, L, M in the stochastic flavour. These symmetries limit strongly the functional form of the building blocks. For example, consider the case that the CG variables are vectors. In this case, the entropy is a rotationally invariant function that can only depend on the modulus of the vector. This is a huge simplification, as it reduces a function of three variables to a function of only one variable. If the CG variable is a symmetric tensor, the entropy can only depend on the invariants of the tensor, say its eigenvalues (simplifying from six to three variables). In the absence of external forcing and for an isotropic system, the symmetry (127) of the friction matrix leads to Curie's Principle, that states that variables of different tensorial character do not couple, as discussed in detail in [56].

C. Generalized time reversal

There is recent interest in generalizations of Onsager-Casimir reciprocity [29–36]. In particular, the question of the validity of Onsager reciprocity in the presence of broken time-reversal symmetry, as in the case of spatially dependent magnetic fields has been considered in Ref. [36]. Recall that Casimir [28] generalized Onsager reciprocity [26, 27] for systems in the presence of external magnetic fields, and had to reverse the sign of the magnetic field to account for the underlying broken time-reversal symmetry. That this is not necessary, and that Onsager reciprocity is still valid without reversing the sign of the magnetic field, was first observed by Bonella et al. [29]. Following this lead, Carbone and Rondoni have found the most general symmetry leading to Onsager symmetry [34]. We show that this general symmetry is, in fact, a combination of the time reversal symmetry and the orthogonal symmetry discussed above. The crucial observation in Appendix A 3 is that the only two conditions that ensure microscopic reversibility of Hamiltonian trajectories are i) the anticommutation of the symplectic matrix J and the time-reversal matrix ϵ, and ii) the unperturbed Hamiltonian is invariant under time reversal. It is possible to generalize the argument leading to microscopic reversibility by considering the most general $6N\times 6N$ matrix that anticommute with the symplectic matrix J, this is

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{pmatrix} + \begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{128}$$

[4] Any skew-symmetric contribution to the friction matrix, if any, should arise from the presence of CG variables odd under time reversal.

where we have written the unknown matrix in block form. The condition (128) implies $\mathsf{C} = \mathsf{B}$ and $\mathsf{D} = -\mathsf{A}$, i.e. the anticommuting matrix has the following block form

$$\begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{B} & -\mathsf{A} \end{pmatrix} \tag{129}$$

where A, B are $3N \times 3N$ matrices. The action of this matrix on positions and momenta is

$$\begin{aligned} q' &= \mathsf{A} \cdot q + \mathsf{B} \cdot p \\ p' &= \mathsf{B} \cdot q - \mathsf{A} \cdot p \end{aligned} \tag{130}$$

To leave invariant the kinetic energy of the Hamiltonian, i.e. $(p')^2 = p^2$ we should have necesarily, $\mathsf{B} = 0$ and $\mathsf{A}^T \cdot \mathsf{A} = 1$, implying that the latter is an orthogonal matrix, with $\det \mathsf{A} = \pm 1$. Therefore, the most general transformation in phase space that leads to the property of microscopic reversibility has a matrix with constant identical 6×6 blocks of the form

$$\begin{pmatrix} \mathsf{R} & 0 \\ 0 & -\mathsf{R} \end{pmatrix} \tag{131}$$

for an arbitrary orthogonal matrix R. If we introduce the operators $\mathcal{T}, \mathcal{R}$ acting on an arbitrary phase space function $\hat{F}(z)$

$$\begin{aligned} \mathcal{T}\hat{F}(z) &= \hat{F}(\epsilon \cdot z) \\ \mathcal{R}\hat{F}(z) &= \hat{F}(\mathsf{R} \cdot z), \end{aligned} \tag{132}$$

then the transformation (131) corresponds to $\mathcal{TR}$. The associated symmetry of the solutions of Hamilton's equation is a combination of (A34) and (A45) in Appendix A. For a time-independent external force with $\phi_t = \phi_0$, this combination leads to

$$\mathcal{TR} e^{i\mathcal{L}(\epsilon \cdot \epsilon_{\mathsf{R}} \cdot \phi_0)t} (\mathcal{TR})^{-1} = e^{-i\mathcal{L}(\phi_0)t} \tag{133}$$

This operator identity reflects how the solution of Hamilton's equation behave under a simultaneous inversion of velocities and rotoinversions of the axis. Notably, the permutations of the axis are elements of the orthogonal group $O(3)$, meaning they can be expressed as combinations of rotations and inversions. As a result, the swaps discussed in Ref. [34] are specific examples of this combined symmetry. The combined symmetry reflects also on a symmetry of the friction matrix, result from combining (121),(127)

$$M(\varepsilon_{\mathsf{R}} \cdot \varepsilon_{\mathsf{T}} \cdot a, \varepsilon_{\mathsf{R}} \cdot \varepsilon_{\mathsf{T}} \cdot \phi) = \varepsilon_{\mathsf{R}} \cdot \varepsilon_{\mathsf{T}} \cdot M^T(a, \phi) \cdot \varepsilon_{\mathsf{T}}^T \cdot \varepsilon_{\mathsf{R}}^T \tag{134}$$

When ϕ is due to an external magnetic field $\varepsilon_{\mathsf{T}} \cdot \phi = -\phi$. Of course, we can always find a rotoinversion such that $\varepsilon_{\mathsf{R}} \cdot \varepsilon_{\mathsf{T}} \cdot \phi = \phi$, and therefore, the magnetic field will have the same sign in both sides of (134).

VIII. CONCLUSION

In this paper, we consider the statistical mechanics foundations of the GENERIC framework in the presence of external forces. We begin with Grabert's formulation of non-equilibrium statistical mechanics, which uses projection operators to produce exact closed integro-differential equations for the evolution of the average and probability distribution of CG variables. When the equations neglect memory effects, and only then, they display the beautiful and powerful GENERIC thermodynamic structure. We demonstrate that the GENERIC structure, originally given for isolated systems, is preserved even for time-dependent external forces, assuming that the external forces couple with the Hamiltonian through the CG variables [1]. Although this assumption is not essential, it simplifies the resulting dynamics by avoiding additional terms in the equation of motion. As compared to the unforced case, we demonstrate that the reversible operator L and the entropy S are unaffected by the external forcing, while the irreversible operator M and the energy E depend on the external forces. In view of the fact that the GENERIC degeneracy of the friction matrix is mantained in the forced case, it is natural that both energy and friction matrix depend on the external forces. We also show that the forced dynamics satisfies the Second Law, with entropy monotonously increasing in time, regardless of the actual time-dependence of the external forcing. Moreover, the First Law naturally emerges to account for time-dependent forces. When the forces are time-independent, the original GENERIC framework with energy conserving dynamics is recovered [10].

We emphasize the pivotal role of the Markovian approximation in obtaining this thermodynamic structure. In particular, the positive character of the friction matrix and its Onsager-Casimir properties can only be justified in the limit of clear separation of time scales. In order to not compromise the Markovian approximation, the present theory is limited to slow external fields, with time scales comparable or larger than the typical time scale of evolution of the CG variables. It remains an open problem to justify a thermodynamic structure for non-Markovian descriptions. The point of view taken by GENERIC is that if a description is non-Markovian, one has to think harder to find additional CG variables that could lead to a Markovian more detailed description of the system [3].

The theory is not limited to near equilibrium situations and, in particular, it displays a state-dependent friction matrix that goes beyond Linear Irreversible Thermodynamics [56]. We show that Onsager-Casimir reciprocity relations for the *state-dependent* friction matrix also hold in the presence of external forces, an issue not contemplated in Grabert's textbook. We show that the combination of the Onsager-Casimir reciprocity with rotational/mirror symmetries gives the general time reversibility conditions discussed recently in the literature [29–36]. Understanding Onsager-Casimir reciprocity for

state-dependent friction matrices should have an impact in the field of stochastic thermodynamics [57–62]. Although the definition of work is straightforward in the present GENERIC framework, defining heat as it appears in stochastic thermodynamics requires considering a composite system, which consists of the system of interest in contact with a thermal bath. The bath is just another inert large system, which is coarse-grained by taking only the bath Hamiltonian as the CG variable. Formulating stochastic thermodynamics in a GENERIC framework appears to be a promising avenue that could provide all the GENERIC benefits to the field.

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Appendix A: MICROSCOPIC LEVEL

In this appendix, we review Hamiltonian dynamics in order to analyze microscopic reversibility, and orthogonal invariance in the presence of a time-dependent external force. Although these concepts should be well-known, presenting them here helps to establish the necessary notation, and prepares us to examine their implications within the context of CG descriptions.

1. Formal solution

We introduce the flow map in phase space as

$$z_t = \hat{\Phi}_{[t,\phi]}(z) \tag{A1}$$

that maps any microstate z at time $t = 0$ with the corresponding microstate z_t evolved with Hamilton's equations under the influence of the protocol ϕ_t. We use the detailed notation with square brackets to denote that the solution of Hamilton's equations is a *functional* of the protocol. The flow map can be understood as a change of variables that depends on the parameter t. Incompressibility of the Hamiltonian flow in phase space implies that the Jacobian of this change of variables is unity [38]. Observe that the property of incompressibility is respected even when there is an external time-dependent forcing.

We introduce the evolution operator $\mathcal{U}_{[t,\phi]}$, whose effect on an arbitrary phase function $\hat{F}(z)$ is to compose the phase function with the flow map

$$\mathcal{U}_{[t,\phi]}\hat{F}(z) = \hat{F}\left(\hat{\Phi}_{[t,\phi]}(z)\right) \tag{A2}$$

in such a way that the solution (A1) of Hamilton's equation with initial condition z_0 at $t = 0$ can be written as

$$z_t = \mathcal{U}_{[t,\phi]}\hat{z}(z_0) \tag{A3}$$

Here, $\hat{z}(z)$ is the identity function in phase space, that is, the vector valued function that takes any microstate z onto itself. Observe that Hamilton's equations (3) can be written in the form

$$\frac{d}{dt}z_t = \mathcal{U}_{[t,\phi]}i\mathcal{L}_t\hat{z}(z_0) \tag{A4}$$

which implies the following differential equation for the evolution operator

$$\partial_t\mathcal{U}_{[t,\phi]} = \mathcal{U}_{[t,\phi]}i\mathcal{L}_t \tag{A5}$$

with initial condition

$$\mathcal{U}_{[0,\phi]} = \mathcal{I} \tag{A6}$$

where $\mathcal{I}$ is the identity operator. As can be checked by explicit differentiation, this equation is solved with the well-known time-ordered exponential defined in terms of the infinite Dyson series

$$\begin{aligned}\mathcal{U}_{[t,\phi]} &= \exp_-\left\{\int_0^t d\tau i\mathcal{L}(\phi_\tau)\right\} \\ &\equiv \sum_{n=0}^{\infty}\int_0^t d\tau_1\cdots\int_0^{\tau_{n-1}} d\tau_n i\mathcal{L}(\phi_{\tau_n})\cdots i\mathcal{L}(\phi_{\tau_1})\end{aligned} \tag{A7}$$

where $0 \le t$ and all the integration variables are ordered according to $0 \le \tau_n \le \tau_{n-1} \le \cdots \le \tau_1 \le t$. The order of the operators is such that time decreases from right to left. In Ref. [20], the time ordered exponential $\exp_-$ is denoted as $\exp_R$. The need to use time ordered exponentials comes from the fact that due to its time-dependence, the Liouville operator operator does not commute at different times $i\mathcal{L}(\phi_t)i\mathcal{L}(\phi_{t'}) \neq i\mathcal{L}(\phi_{t'})i\mathcal{L}(\phi_t)$.

2. The inverse evolution

By definition, the inverse $\mathcal{U}^{-1}_{[t,\phi]}$ of the operator $\mathcal{U}_{[t,\phi]}$ satisfies

$$\mathcal{U}_{[t,\phi]}\mathcal{U}^{-1}_{[t,\phi]} = \mathcal{I} \tag{A8}$$

where $\mathcal{I}$ is the identity operator. To get a formal expansion of the inverse operator, we first obtain a differential equation by differentiation of (A8) with respect to t and rearranging. One arrives at

$$\partial_t\mathcal{U}^{-1}_{[t,\phi]} = -\mathcal{U}^{-1}_{[t,\phi]}\partial_t\mathcal{U}_{[t,\phi]}\mathcal{U}^{-1}_{[t,\phi]} \tag{A9}$$

Inserting (A5) in this equation gives the differential equation

$$\partial_t \mathcal{U}^{-1}_{[t,\phi]} = -i\mathcal{L}_t \mathcal{U}^{-1}_{[t,\phi]} \tag{A10}$$

As can be checked by term-by-term differentiation, the solution of this differential equation with initial condition $\mathcal{U}^{-1}_{[0,\phi]} = \mathcal{I}$ is

$$\begin{aligned}\mathcal{U}^{-1}_{[t,\phi]} &= \exp_+\left\{-\int_0^t d\tau i\mathcal{L}_\tau\right\} \\ &\equiv \sum_{n=0}^{\infty}(-1)^n \int_0^t d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n i\mathcal{L}(\phi_{\tau_1})\cdots i\mathcal{L}(\phi_{\tau_n})\end{aligned} \tag{A11}$$

where the time argument of the Liouville operator increases from right to left. It can be shown that the action of the inverse operator on a phase function is

$$\mathcal{U}^{-1}_{[t,\phi]}\hat{F}(z) = \hat{F}\left(\hat{\Phi}^{-1}_{[t,\phi]}(z)\right) \tag{A12}$$

where the inverse flow map is defined through

$$\hat{\Phi}^{-1}_{[t,\phi]}\left(\hat{\Phi}_{[t,\phi]}(z)\right) \equiv \hat{z}(z) \tag{A13}$$

this is, the composition of the inverse flow map with the flow map gives the identity function. The evolution operator is unitary, this is, its adjoint is the inverse [38].

3. Time reversibility symmetry

We introduce the time reversal operator $\mathcal{T}$ which is defined through its action on an arbitrary function $\hat{F}(z)$

$$\mathcal{T}\hat{F}(z) = \hat{F}(\epsilon\cdot z) \tag{A14}$$

where the matrix ϵ is diagonal with ± 1 in the diagonal, and that reverse the sign of the momentum. This is, if $z = (q, p)$ then $\epsilon\cdot z = (q, -p)$. The time reversal operator is an involution $\mathcal{T}^2 = 1$. Note that the time reversal matrix ϵ and the symplectic matrix J anticommute

$$\epsilon\cdot J = -J\cdot\epsilon \tag{A15}$$

This simple fact has as a profound consequence that Hamilton's equations are invariant under time reversal, as shown below.

The time reversal operator $\mathcal{T}$ and the derivative operator $\frac{\partial}{\partial z_j}$ do not commute because

$$\begin{aligned}\frac{\partial}{\partial z_j}\mathcal{T}\hat{F}(z) &= \frac{\partial}{\partial z_j}\hat{F}(\epsilon\cdot z) = \hat{F}_k(\epsilon\cdot z)\epsilon_{kj} \\ &= \epsilon_{jk}\mathcal{T}\hat{F}_k(z) = \epsilon_{jk}\mathcal{T}\frac{\partial}{\partial z_k}\hat{F}(z)\end{aligned} \tag{A16}$$

where we follow the notation $\hat{F}_k(\epsilon\cdot z)$ for the partial derivative of $\hat{F}(z)$ with respect to z_k evaluated at $\epsilon\cdot z$. Because $\hat{F}(z)$ is arbitrary, we have

$$\frac{\partial}{\partial z_j}\mathcal{T} = \epsilon_{jk}\mathcal{T}\frac{\partial}{\partial z_k} \tag{A17}$$

where sum over repeated indices is implied. Therefore, the operators do not commute due to the presence of ϵ_{jk}.

We assume that the coupling functions have well-defined parity under time inversion, this is

$$\hat{C}(\epsilon\cdot z) = \varepsilon_{\mathsf{T}}\cdot\hat{C}(z) \tag{A18}$$

were ε_{T} is a diagonal matrix with ± 1 in the diagonal, according to the parity of the coupling function. This matrix satisfies $\varepsilon^2_{\mathsf{T}} = 1$. The unperturbed Hamiltonian is invariant under the time reversal operator $\hat{H}^{(0)}(z) = \hat{H}^{(0)}(\epsilon\cdot z) = \mathcal{T}\hat{H}^{(0)}(z)$ and, therefore, the Hamiltonian (1) satisfies

$$\hat{H}(\epsilon\cdot z, \varepsilon_{\mathsf{T}}\cdot\phi_t) = \hat{H}(z, \phi_t) \tag{A19}$$

that can be written as

$$\mathcal{T}\hat{H}(z, \phi_t) = \hat{H}(z, \varepsilon_{\mathsf{T}}\cdot\phi_t) \tag{A20}$$

and shows that the action of the time reversal operator on the Hamiltonian is just to change the time signature of the external field.

The time reversal behaviour of the derivatives of the Hamiltonian are easily obtained by applying the operator $\frac{\partial}{\partial z_i}$ to both sides of (A19). We have

$$\begin{aligned}\frac{\partial}{\partial z_i}\hat{H}(\epsilon\cdot z, \varepsilon_{\mathsf{T}}\cdot\phi_t) &= \frac{\partial}{\partial z_i}\hat{H}(z, \phi_t) \\ \epsilon_{ik}\hat{H}_k(\epsilon\cdot z, \varepsilon_{\mathsf{T}}\cdot\phi_t) &= \hat{H}_i(z, \phi_t)\end{aligned} \tag{A21}$$

where we introduce the notation $\hat{H}_i$ to denote the partial derivative of the Hamiltonian with respect to the i-th component of z. In terms of the time reversal operator the derivatives of the Hamiltonian transform according to

$$\mathcal{T}H_i(z, \phi_t) = \epsilon_{ij}H_j(z, \varepsilon_{\mathsf{T}}\cdot\phi_t) \tag{A22}$$

We now consider the effect of time reversal on the Liouville operator. By applying the Liouville operator on a time reversed function we have

$$\begin{aligned}i\mathcal{L}_t\mathcal{T}\hat{F}(z) &= -\hat{H}_i(z, \phi_t)J_{ij}\frac{\partial}{\partial z_j}\hat{F}(\epsilon\cdot z) \\ &= -\hat{H}_i(z, \phi_t)J_{ij}\epsilon_{jk}\hat{F}_k(\epsilon\cdot z) \\ &= \hat{H}_i(z, \phi_t)\epsilon_{ij}J_{jk}\hat{F}_k(\epsilon\cdot z)\end{aligned} \tag{A23}$$

In the last equality in (A23) we have used the anti-commutativity (A15). By inserting (A21) into (A23)

gives

$$i\mathcal{L}_t\mathcal{T}\hat{F}(z) = \hat{H}_j(\epsilon\cdot z, \varepsilon_{\mathsf{T}}\cdot\phi_t)J_{jk}\hat{F}_k(\epsilon\cdot z)$$
$$= -\mathcal{T}i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{F}(z) \tag{A24}$$

Because the function $\hat{F}(z)$ is arbitrary,

$$i\mathcal{L}(\phi_t)\mathcal{T} = -\mathcal{T}i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t) \tag{A25}$$

This shows that the Liouville operator and the time reversal operator anticommute, provided that we change accordingly the time signature of the protocol. The property (A25) is a direct consequence of the anticommutativity (A15). This anticommutativity is also reflected at the level of evolution operators. It is easy to show, by using (A25) and the Dyson expansion (A7) that

$$\exp_-\left\{\int_0^t d\tau i\mathcal{L}(\phi_\tau)\right\}\mathcal{T}\hat{F}(z)$$
$$= \mathcal{T}\exp_-\left\{-\int_0^t d\tau i\mathcal{L}(\varepsilon\cdot\phi_\tau)\right\}\hat{F}(z) \tag{A26}$$

In a similar way,

$$\exp_+\left\{\int_0^t d\tau i\mathcal{L}(\varepsilon\cdot\phi_\tau)\right\}\mathcal{T}\hat{F}(z)$$
$$= \mathcal{T}\exp_+\left\{-\int_0^t d\tau i\mathcal{L}(\phi_\tau)\right\}\hat{F}(z) \tag{A27}$$

where also the position of the parity matrix ε has changed.

Next we introduce the reverse protocol as

$$\phi^R(\tau) \equiv \varepsilon\cdot\phi(t-\tau) \tag{A28}$$

We include the parity matrix ε that tells how the coupling functions change under time reversal. Imagine that we conduct an "experiment" with an initial condition z and let evolve the system with Hamilton's equations until t under this reverse protocol. The corresponding evolution operator is

$$\mathcal{U}_{[t,\phi^R]} = \exp_-\left\{\int_0^t d\tau i\mathcal{L}(\phi^R_\tau)\right\}$$
$$= \sum_{n=0}^{\infty}\int_0^t d\tau_1\cdots\int_0^{\tau_{n-1}} d\tau_n i\mathcal{L}(\phi^R_{\tau_n})\cdots i\mathcal{L}(\phi^R_{\tau_1}) \tag{A29}$$

By performing the change of variables $\tau_n \to \tau'_n = t-\tau_n$ for all n gives

$$\mathcal{U}_{[t,\phi^R]} = \sum_{n=0}^{\infty}\int_0^t d\tau'_1\cdots\int_{\tau'_{n-1}}^t d\tau'_n i\mathcal{L}(\varepsilon\cdot\phi_{\tau'_n})\cdots i\mathcal{L}(\varepsilon\cdot\phi_{\tau'_1}) \tag{A30}$$

Observe that the times are now in the order $t \geq \tau'_1 \geq \tau'_2 \geq \cdots \geq \tau'_n \geq 0$. Following a standard procedure, we swap the order of the variables of integration. For example, the second order term is

$$\int_0^t d\tau_1\int_{\tau_2}^t d\tau_2 i\mathcal{L}(\varepsilon\cdot\phi_{\tau_2})\cdots i\mathcal{L}(\varepsilon\cdot\phi_{\tau_1})$$
$$= \int_0^t d\tau_1\int_0^{\tau_1} d\tau_2 i\mathcal{L}(\varepsilon\cdot\phi_{\tau_2})\cdots i\mathcal{L}(\varepsilon\cdot\phi_{\tau_1}) \tag{A31}$$

where a further renaming of dummy variables $\tau_1 \to \tau_2$ has been performed. Proceeding in a similar way for all orders, we conclude that

$$\mathcal{U}_{[t,\phi^R]} = \exp_+\left\{\int_0^t dti\mathcal{L}(\varepsilon\cdot\phi_t)\right\} \tag{A32}$$

where we have taken into account the ordering of the operators in order to use the definition (A11) for the time ordered exponential. By comparing (A32) with (A11), we see the close connection (up to a sign) of $\mathcal{U}_{[t,\phi^R]}$ with the inverse operator $\mathcal{U}^{-1}_{[t,\phi]}$. In fact, by using (A27) we obtain

$$\mathcal{U}_{[t,\phi^R]}\mathcal{T} \overset{(A32)}{=} \exp_+\left\{\int_0^t dti\mathcal{L}(\varepsilon\cdot\phi_t)\right\}\mathcal{T}$$
$$\overset{(A27)}{=} \mathcal{T}\exp_+\left\{-\int_0^t dti\mathcal{L}_t\right\} \tag{A33}$$

By using (A11) we arrive at the following statement about time reversibility at the level of the evolution operators

$$\mathcal{U}_{[t,\phi^R]}\mathcal{T} = \mathcal{T}\mathcal{U}^{-1}_{[t,\phi]} \tag{A34}$$

This property of time reversibility may be more trans-

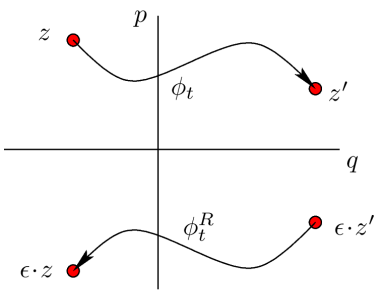

FIG. 1: The microstate z evolves forward under the protocol ϕ_t starting at $t=0$ and reaching at t the microstate $z' = \hat{\Phi}_{[t,\phi]}(z)$. If we change the sign of the momenta to produce $\epsilon\cdot z'$ and evolve this microstate *forward* in time from $t=0$ to t under the reverse protocol ϕ^R_t we will arrive, according to microscopic reversibility, at $\hat{\Phi}_{[t,\phi^R]}(\epsilon\cdot z') = \epsilon\cdot z$. If we record on a film the evolution from $z \to z'$ (the upper trajectory) and run the film backwards, we will observe the lower trajectory from $\epsilon\cdot z' \to \epsilon\cdot z$.

parent in terms of the flow map $\hat{\Phi}_{[t,\phi]}(z) = \mathcal{U}_{[t,\phi]}\hat{z}(z)$,

$$\Phi_{[t,\phi^R]}(\epsilon\cdot z) = \epsilon\cdot\hat{\Phi}^{-1}_{[t,\phi]}(z) \tag{A35}$$

This can also be written as

$$\hat{\Phi}_{[t,\phi^R]}\left(\epsilon\cdot\hat{\Phi}_{[t,\phi]}(z)\right) = \epsilon\cdot z \tag{A36}$$

In Fig. 1 we explain in words the meaning of the microscopic reversibility condition (A36) in the presence of an external time-depending forcing.

Finally, if the external field is constant in time $\phi_t = \phi_0$, the microscopic reversibility property (A34) reduces to

$$e^{i\mathcal{L}(\varepsilon\cdot\phi)}\mathcal{T} = \mathcal{T}e^{-i\mathcal{L}(\phi)} \tag{A37}$$

4. Orthogonal symmetry

We now discuss what is the effect of rotating or inverting the axis of coordinates on the solutions of Hamilton's equation. Introduce the operator $\mathcal{R}$ whose action on an arbitrary phase space function $\hat{F}(z)$ is

$$\mathcal{R}\hat{F}(z) = \hat{F}(\mathsf{R}\cdot z) \tag{A38}$$

where

$$\mathsf{R}\cdot z = (\mathsf{R}\cdot\mathbf{q}_1, \cdots, \mathsf{R}\cdot\mathbf{q}_N, \mathsf{R}\cdot\mathbf{p}_1, \cdots \mathsf{R}\cdot\mathbf{p}_N) \tag{A39}$$

and R is an orthogonal matrix $\mathsf{R}\mathsf{R}^T = 1$. This orthogonal matrix may be a rotation ($\det\mathsf{R} = 1$) or an improper rotation ($\det\mathsf{R} = -1$). Improper rotations are also referred to as rotoinversions. We assume that the unperturbed Hamiltonian is invariant under such a transformation, this is $\mathcal{R}\hat{H}^{(0)}(z) = \hat{H}^{(0)}(z)$. In addition, we assume that the CG variables are vectors or tensors that transform in the well-known form under rotations, this is

$$\hat{A}(\mathsf{R}\cdot z) = \varepsilon_{\mathsf{R}}\cdot\hat{A}(z) \tag{A40}$$

where ε_{R} is an $M\times M$ constant block matrix whose entries are given by the rotation matrix R in a convenient form. The effect of this operator on the forced Hamiltonian is

$$\mathcal{R}\hat{H}(z,\phi_t) = \mathcal{R}\left(\hat{H}^{(0)}(z) - \hat{A}^T(z)\cdot\phi_t\right) = \hat{H}(z,\varepsilon^T_{\mathsf{R}}\cdot\phi_t) \tag{A41}$$

Observe that the $6N\times 6N$ matrix made of the N blocks

$$\begin{pmatrix} \mathsf{R} & 0 \\ 0 & \mathsf{R} \end{pmatrix} \tag{A42}$$

commutes with the symplectic matrix J. This implies, by following identical steps as those leading to (A25) that

$$i\mathcal{L}(\phi)\mathcal{R} = \mathcal{R}i\mathcal{L}(\varepsilon^T_{\mathsf{R}}\cdot\phi) \tag{A43}$$

The property (A43) implies the following property of the Hamiltonian evolution operator

$$\begin{aligned}&\exp_-\left\{\int_0^t d\tau i\mathcal{L}(\phi_\tau)\right\}\mathcal{R}\hat{F}(z)\\ &= \mathcal{R}\exp_-\left\{\int_0^t d\tau i\mathcal{L}(\varepsilon_{\mathsf{R}}\cdot\phi_\tau)\right\}\hat{F}(z)\end{aligned} \tag{A44}$$

as can be easily seen by considering the expansion of the time-ordered exponential. When applied to the identity function, this implies

$$\begin{aligned}&\exp_-\left\{\int_0^t d\tau i\mathcal{L}(\phi_\tau)\right\}\hat{z}(z)\\ &= \mathcal{R}\exp_-\left\{\int_0^t d\tau i\mathcal{L}(\varepsilon^T_{\mathsf{R}}\cdot\phi_\tau)\right\}\mathcal{R}\hat{z}(z)\end{aligned} \tag{A45}$$

In words, this means that if we start the dynamics in a microstate z and evolve it with an external forcing ϕ_t, the final microstate is the same as if we start from the rotated/rotoinverted microstate $\mathcal{R}z$, evolve it with the external forcing $\varepsilon^T_{\mathsf{R}}\cdot\phi_\tau$, and then rotate/rotoinvert it. This is the expected behaviour of the dynamic trajectories when we rotate/rotoinvert the axis of coordinates.

Appendix B: THE PROJECTION OPERATOR METHOD

In this appendix we derive the relationship (16) between the Liouville ensemble and the relevant ensemble, and the exact transport equation (31) for the average of CG variables given in the main text. This appendix follows closely Grabert's textbook [1] and it is reproduced for the sake of completeness, and notational convenience.

1. The projection and its properties

The method starts by introducing the operator (14) whose action on arbitrary density $\eta(z)$ in phase space is

$$\mathcal{P}^\dagger_t\eta(z) = \overline{\rho}_t(z)\mathrm{Tr}[\eta] + \frac{\partial\overline{\rho}_t}{\partial a(t)}(z)\mathrm{Tr}\left[(\hat{A} - a(t))\eta\right] \tag{B1}$$

Observe that this projector depends on time only through the time-dependence of the average a_t, and when necessary we will write

$$\mathcal{P}_t = \mathcal{P}(a_t) \tag{B2}$$

When applied to the Liouville ensemble, and using (11), the operator gives

$$\overline{\rho}_t(z) = \mathcal{P}^\dagger_t\rho_t(z) \tag{B3}$$

If we require (15) stating that the relevant ensemble $\overline{\rho}_t(z)$ provides the same averages (11) computed with the Li-

ouville ensemble $\rho_t(z)$ then

$$\mathcal{P}_t^\dagger \overline{\rho}_t(z) = \overline{\rho}_t(z) \tag{B4}$$

An explicit calculation shows that it satisfies

$$\mathcal{P}_t^\dagger \mathcal{P}_{t'}^\dagger = \mathcal{P}_t^\dagger \tag{B5}$$

When $t = t'$ this property shows that $\mathcal{P}_t^\dagger$ is idempotent. The operator $\mathcal{P}_t^\dagger$ also satisfies the commutation property

$$\mathcal{P}_t^\dagger \partial_t \rho_t(z) = \partial_t \mathcal{P}_t^\dagger \rho_t(z) \tag{B6}$$

The adjoint $\mathcal{P}_t$ of the operator $\mathcal{P}_t^\dagger$ is defined through

$$\mathrm{Tr}\left[\hat{F}\mathcal{P}_t^\dagger \eta\right] = \mathrm{Tr}\left[\eta \mathcal{P}_t \hat{F}\right] \tag{B7}$$

and has the explicit form

$$\mathcal{P}_t \hat{F}(z) = \mathrm{Tr}[\overline{\rho}_t \hat{F}] + (\hat{A}(z) - a(t))\mathrm{Tr}\left[\frac{\partial \overline{\rho}_t}{\partial a(t)}\hat{F}\right] \tag{B8}$$

An explicit calculation shows that it satisfies

$$\mathcal{P}_{t'}\mathcal{P}_t = \mathcal{P}_t \tag{B9}$$

The complementary projection is defined as

$$\mathcal{Q}_t \equiv 1 - \mathcal{P}_t \tag{B10}$$

and it satisfies

$$\mathcal{Q}_{t'}\mathcal{Q}_t = \mathcal{Q}_{t'} \tag{B11}$$

This projector is self-adjoint with respect to the relevant ensemble, this is,

$$\left\langle \hat{F}\mathcal{P}_t \hat{G}\right\rangle^{\lambda_t} = \left\langle \hat{G}\mathcal{P}_t \hat{F}\right\rangle^{\lambda_t} \tag{B12}$$

for arbitrary phase functions $\hat{F}(z), \hat{G}(z)$.

2. The Liouville ensemble in terms of the relevant ensemble

We start by writting the Liouville ensemble in terms of the relevant ensemble

$$\rho_t(z) = \overline{\rho}_t(z) + \delta\rho_t(z) \tag{B13}$$

where $\delta\rho_t(z)$ is the so called irrelevant part of the ensemble and is defined through this equation. The objective is now to express the irrelevant part $\delta\rho_t(z)$ in terms of the relevant part $\overline{\rho}_t(z)$. From (B3), (B10), the irrelevant part of the ensemble is

$$\delta\rho_t(z) = \mathcal{Q}_t^\dagger \rho_t(z) \tag{B14}$$

We can now follow the standard derivation in which one obtains two equations, one for the time derivatives of the relevant part

$$\begin{aligned}\partial_t \overline{\rho}_t(z) &= \partial_t \mathcal{P}_t^\dagger \rho_t = -\mathcal{P}_t^\dagger i\mathcal{L}(\phi_t)\rho_t \\ &= -\mathcal{P}_t^\dagger i\mathcal{L}(\phi_t)(\mathcal{P}_t^\dagger + \mathcal{Q}_t^\dagger)\rho_t \\ &= -\mathcal{P}_t^\dagger i\mathcal{L}(\phi_t)\overline{\rho}_t - \mathcal{P}_t^\dagger i\mathcal{L}(\phi_t)\delta\rho_t\end{aligned} \tag{B15}$$

and a similar equation for the irrelevant part

$$\begin{aligned}\partial_t \delta\rho_t(z) &= \partial_t \mathcal{Q}_t^\dagger \rho_t = -\mathcal{Q}_t^\dagger i\mathcal{L}(\phi_t)\rho_t \\ &= -\mathcal{Q}_t^\dagger i\mathcal{L}(\phi_t)(\mathcal{P}_t^\dagger + \mathcal{Q}_t^\dagger)\rho_t \\ &= -\mathcal{Q}_t^\dagger i\mathcal{L}(\phi_t)\overline{\rho}_t - \mathcal{Q}_t^\dagger i\mathcal{L}(\phi_t)\delta\rho_t\end{aligned} \tag{B16}$$

The formal solution of the differential equation (B16) is given by

$$\begin{aligned}\delta\rho_t(z) &= \mathcal{G}^\dagger[t,0,a,\phi]\delta\rho_0(z) \\ &\quad - \int_0^t dt' \mathcal{G}^\dagger[t,t',a,\phi]\mathcal{Q}_{t'}^\dagger i\mathcal{L}_{t'}\overline{\rho}_{t'}\end{aligned} \tag{B17}$$

where the adjoint of the projected evolution operator is defined in (17). As mentioned in the main text, we assume that the initial ensemble is of the relevant form and, therefore, $\delta\rho_0(z) = 0$. Then (B17) becomes

$$\rho_t(z) = \overline{\rho}_t(z) - \int_0^t dt' \mathcal{G}^\dagger[t,t',a,\phi]\mathcal{Q}_{t'}^\dagger i\mathcal{L}_{t'}\overline{\rho}_{t'} \tag{B18}$$

which is equation (16) in the main text.

3. When the relevant ensemble is the generalized canonical ensemble

The result (B17) does not depend on the explicit form of the relevant ensemble. In particular the projector (B1), (B8) are general. When we use, however, the generalized canonical ensemble (22) the projectors becomes

$$\begin{aligned}\mathcal{P}_t^\dagger \eta(z) &= \overline{\rho}_t(z)\left(\mathrm{Tr}[\eta] + \delta_t\hat{A}(z)\cdot\Sigma_t^{-1}\mathrm{Tr}\left[\delta_t\hat{A}\eta\right]\right) \\ \mathcal{P}_t\hat{F}(z) &= \left\langle\hat{F}\right\rangle^{\lambda_t} + \left\langle\hat{F}\delta_t\hat{A}\right\rangle^{\lambda_t}\cdot\Sigma_t^{-1}\cdot\delta_t\hat{A}(z)\end{aligned} \tag{B19}$$

where $\delta_t\hat{A}(z) = \hat{A}(z) - a_t$ denote the fluctuations over the mean at time t, and the covariance matrix is

$$\Sigma_t = \left\langle\delta_t\hat{A}\delta_t\hat{A}\right\rangle^{\lambda_t} \tag{B20}$$

The projector (B19) is the Kawasaki-Gunton projector used in Grabert's textbook, and it is a generalization of the Mori projector that uses the relevant ensemble instead of the equilibrium ensemble. Observe that the

following property is satisfied for the projectors (B19)

$$\mathcal{P}_t^\dagger \left(\overline{\rho}_t(z)\hat{F}(z)\right) = \overline{\rho}_t(z)\mathcal{P}_t\hat{F}(z) \tag{B21}$$

We will need the action of the projection operator and Liouville operator on the relevant ensemble, this is

$$\begin{aligned}
&-\mathcal{P}_{t'}^\dagger i\mathcal{L}_{t'}\overline{\rho}_{t'}(z) \overset{(22)}{=} \mathcal{P}_{t'}^\dagger \left(\overline{\rho}_{t'}(z)i\mathcal{L}_{t'}\hat{A}\right)\cdot\lambda_{t'} \overset{(B19)}{=} \overline{\rho}_{t'}(z)\left(\mathrm{Tr}\left[\overline{\rho}_{t'}i\mathcal{L}_{t'}\hat{A}\right]\cdot\lambda_{t'} + \delta_{t'}\hat{A}(z)\cdot\Sigma_t^{-1}\mathrm{Tr}\left[\overline{\rho}_{t'}\delta_t\hat{A}i\mathcal{L}_{t'}\hat{A}\right]\cdot\lambda_{t'}\right)\\
&= \overline{\rho}_{t'}(z)\left(-\mathrm{Tr}\left[i\mathcal{L}_{t'}\overline{\rho}_{t'}\right] - \delta_{t'}\hat{A}(z)\cdot\Sigma_t^{-1}\mathrm{Tr}\left[\delta_t\hat{A}i\mathcal{L}_{t'}\overline{\rho}_{t'}\right]\right) = \overline{\rho}_{t'}(z)\delta_{t'}\hat{A}(z)\cdot\Sigma_t^{-1}\mathrm{Tr}\left[\overline{\rho}_{t'}i\mathcal{L}_{t'}\hat{A}\right]\\
&= \overline{\rho}_{t'}(z)\delta_{t'}\hat{A}(z)\cdot\Sigma_t^{-1}\cdot v_{t'}
\end{aligned} \tag{B22}$$

The effect of the complementary projector is

$$\mathcal{Q}_{t'}^\dagger i\mathcal{L}_{t'}\overline{\rho}_{t'}(z) = i\mathcal{L}_{t'}\overline{\rho}_{t'}(z) - \mathcal{P}_{t'}^\dagger i\mathcal{L}_{t'}\overline{\rho}_{t'}(z) = -\overline{\rho}_{t'}(z)i\mathcal{L}_{t'}\hat{A}(z)\cdot\lambda_{t'} + \overline{\rho}_{t'}(z)\delta_{t'}\hat{A}(z)\cdot\Sigma_t^{-1}\cdot v_{t'} \tag{B23}$$

Inserting this result in (B18) leads to

$$\rho_t(z) = \overline{\rho}_t(z) + \int_0^t dt'\mathcal{G}^\dagger[t,t',a,\phi]\left(\overline{\rho}_{t'}(z)\left(\mathcal{Q}_{t'}i\mathcal{L}_{t'}\hat{A}\right)\right)\cdot\lambda_{t'} \tag{B24}$$

We can now use this expression for the Liouville ensemble in the definition (11) of the average of the CG variables. By using Liouville's theorem (10) and an integration by parts, we obtain

$$\frac{d}{dt}a_t = \int dz\rho_t(z)i\mathcal{L}_t\hat{A}(z) = \left\langle i\mathcal{L}_t\hat{A}\right\rangle^{\lambda_t} + \int_0^t dt'\left\langle\left(\mathcal{G}[t,t',a,\phi]i\mathcal{L}_t\hat{A}\right)\left(\mathcal{Q}_{t'}i\mathcal{L}_{t'}\hat{A}\right)\right\rangle^{\lambda_{t'}}\cdot\lambda_{t'} \tag{B25}$$

where the operator $\mathcal{G}[t,t',a,\phi]$ is the adjoint of $\mathcal{G}^\dagger[t,t',a,\phi]$ and it is given by

$$\mathcal{G}[t,t',a,\phi] = \exp_-\left\{\int_{t'}^t d\tau i\mathcal{L}_\tau\mathcal{Q}_\tau\right\} \tag{B26}$$

This is (31) in the main text.

Appendix C: FROM THE AVERAGE FLAVOUR TO THE STOCHASTIC FLAVOUR

In this appendix, we consider explicitly the derivation of the stochastic flavour, which is obtained from the average flavour when we use the distribution function $\hat{\Psi}_a(z)$ as CG variable. The time-dependent average of this distribution is the probability $P(a,t)$. First, the relevant ensemble $\overline{\rho}_t$ appearing in the average $\langle\cdot\rangle^{\lambda_t}$ is given by (22) that now takes the form

$$\overline{\rho}_t(z) = \frac{\rho_c}{Z[\lambda]}e^{-\int da\lambda_a(t)\hat{\Psi}_a(z)} \tag{C1}$$

where $Z[\lambda]$ is the normalization

$$Z[\lambda] = \int dz\rho_c e^{-\int da\lambda_a(t)\hat{\Psi}_a(z)} \tag{C2}$$

and it is a functional of the Lagrange multipliers $\lambda_a(t)$ conjugate to $\hat{\Psi}_a(z)$. By performing the integral over a over the Dirac delta function $\hat{\Psi}_a(z)$ we obtain

$$\overline{\rho}_t(z) = \frac{\rho_c}{Z[\lambda]}\exp\left\{-\lambda_{\hat{A}(z)}(t)\right\} \tag{C3}$$

The Lagrange multipliers are fixed by the requirement that the relevant ensemble average of $\Psi_a(z)$ is the known probability $P(a,t)$. This gives the condition

$$P(a,t) = \frac{\Omega(a)}{Z[\lambda]}\exp\left\{-\lambda_a(t)\right\} \tag{C4}$$

and the relevant ensemble (C3) in the stochastic flavour becomes

$$\overline{\rho}_t(z) = \rho_c\frac{P(\hat{A}(z),t)}{\Omega(\hat{A}(z))} \tag{C5}$$

The entropy is defined as the result of evaluating the Gibbs-Jaynes entropy functional (21) at the relevant en-

semble (C5) which now takes the form

$$S[P_t] = -k_B \int da P(a,t) \ln \frac{P(a,t)}{\Omega(a)} \tag{C6}$$

and the conjugate variable (29), is now

$$\lambda_a(t) = \frac{1}{k_B}\frac{\delta S[P_t]}{\delta P(a,t)} = -\ln\frac{P(a,t)}{\Omega(a)} - 1 \tag{C7}$$

The average with the relevant ensemble (C5) becomes

$$\left\langle \hat{F} \right\rangle^{\lambda_t} = \int da P(a,t) \left\langle \hat{F} \right\rangle^{a} \tag{C8}$$

where we introduce the conditional expectation as

$$\left\langle \hat{F} \right\rangle^{a} = \frac{1}{\Omega(a)} \int dz \hat{\Psi}_a(z) \hat{F}(z) \tag{C9}$$

Let us go now for the projector $\mathcal{Q}_t = 1 - \mathcal{P}_t$, where the projector is given by (36). The average $\langle (\hat{A}_\nu - a_\nu(t))\hat{F}\rangle^{\lambda(t)}$ in the projector (36) is

$$\begin{aligned}
&\langle (\hat{\Psi}_a - P(a,t))\hat{F}\rangle^{\lambda(t)} \\
&= \int da'' \frac{P(a'',t)}{\Omega(a'')} \int dz \hat{\Psi}_{a''}(z)(\hat{\Psi}_a(z) - P(a,t))\hat{F}(z) \\
&= \int da'' P(a'',t) \left[\delta_{aa''} \left\langle \hat{F} \right\rangle^{a''} - \left\langle \hat{F} \right\rangle^{a''} P(a,t) \right] \\
&= (P(a,t) - P(a,t)) \left\langle \hat{F} \right\rangle^{a''} = 0
\end{aligned} \tag{C10}$$

where we have denoted the Dirac delta with $\delta_{aa''} = \delta(a - a'')$. Therefore, the projector (36) takes the form

$$\mathcal{P}_t \hat{F}(z) = \int da P(a,t) \langle \hat{F} \rangle^a \tag{C11}$$

Finally, let us consider the form of the time derivatives when $\hat{A}_\mu \to \hat{\Psi}_a(z)$. By using the chain rule, we have

$$i\mathcal{L}_t \hat{\Psi}_a(z) = -\frac{\partial}{\partial a} \hat{\Psi}_a(z) \cdot i\mathcal{L}_t \hat{A}(z) \tag{C12}$$

and the action of the projector on the time derivative is

$$\mathcal{Q}_t i\mathcal{L}_t \hat{\Psi}_a(z) - \frac{\partial}{\partial a}\hat{\Psi}_a(z) \cdot \left[i\mathcal{L}_t \hat{A}(z) - \left\langle i\mathcal{L}_t \hat{A} \right\rangle^a \right] \tag{C13}$$

The reversible term (51) will take the form

$$\begin{aligned}
v(a_t,\phi_t) &\overset{(C12)}{=} -\left\langle \frac{\partial}{\partial a} \hat{\Psi}_a(z) \cdot i\mathcal{L}_t \hat{A}(z) \right\rangle^{\lambda(t)} \\
&\overset{(C8)}{=} -\frac{\partial}{\partial a} \cdot \int da' P(a',t) \left\langle \hat{\Psi}_a i\mathcal{L}_t \hat{A} \right\rangle^{a'} \\
&= -\frac{\partial}{\partial a} \cdot V(a_t,\phi_t) P(a,t)
\end{aligned} \tag{C14}$$

where

$$V(a,\phi) \equiv \left\langle i\mathcal{L}(\phi)\hat{A} \right\rangle^a \tag{C15}$$

The friction matrix (52) becomes, after substituting $\hat{A}_\mu$ with $\hat{\Psi}_a$ and using (C12)

$$d_{aa'}(a_t,\phi_t) = \frac{\partial}{\partial a'_\nu}\frac{\partial}{\partial a_\mu} \int da'' \frac{1}{k_B} \int_0^{\Delta t} d\tau \left\langle \hat{\Psi}_a \left(i\mathcal{L}_t \hat{A}_\nu - \left\langle i\mathcal{L}_t \hat{A}_\nu \right\rangle^{a'} \right) e^{i\overline{\mathcal{L}}_t \tau} \hat{\Psi}_a i\mathcal{L}_t \hat{A}_\mu \right\rangle^{a''} P(a'',t) \tag{C16}$$

Under the Markovian approximation, in which the CG variables hardly change during the decay time of the memory kernel, we may "drag $\hat{\Psi}_a$ outside the evolution operator"

$$e^{i\overline{\mathcal{L}}_t \tau} \hat{\Psi}_{a'} i\mathcal{L}_t \hat{A}_\mu \simeq \hat{\Psi}_{a'} e^{i\overline{\mathcal{L}}_t \tau} i\mathcal{L}_t \hat{A}_\mu \tag{C17}$$

and then

$$\begin{aligned}
M_{aa'}(a_t,\phi_t) &= \frac{\partial}{\partial a'_\nu}\frac{\partial}{\partial a_\mu} \int da'' \frac{1}{k_B} \int_0^{\Delta t} d\tau \left\langle \hat{\Psi}_a \hat{\Psi}_{a'} \left(i\mathcal{L}_t \hat{A}_\nu - \left\langle i\mathcal{L}_t \hat{A}_\nu \right\rangle^{a} \right) e^{i\overline{\mathcal{L}}_t \tau} i\mathcal{L}_t \hat{A}_\mu \right\rangle^{a''} P(a'',t) \\
&= \frac{\partial}{\partial a_\nu}\frac{\partial}{\partial a'_\mu} \int da'' \delta_{aa''}\delta_{a'a''} M_{\mu\nu}(\phi_t, a'') P(a'',t) = \frac{\partial}{\partial a_\nu} k_B M_{\mu\nu}(a,\phi_t) P(a,t) \left(\frac{\partial}{\partial a'_\mu} \delta_{aa'} \right)
\end{aligned} \tag{C18}$$

where we have introduced the friction matrix

$$M_{\mu\nu}(a,\phi) \equiv \frac{1}{k_B} \int_0^{\Delta t} d\tau \left\langle \left(i\mathcal{L}(\phi)\hat{A}_\nu - \left\langle i\mathcal{L}(\phi)\hat{A}_\nu \right\rangle^a \right) e^{i\overline{\mathcal{L}}(a,\phi)\tau} i\mathcal{L}(\phi)\hat{A}_\mu \right\rangle^a \tag{C19}$$

This can be cast in terms of an auto-correlation matrix

$$M_{\mu\nu}(a,\phi) \equiv \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(i\mathcal{L}(\phi)\hat{A}_\nu - \left\langle i\mathcal{L}(\phi)\hat{A}_\nu \right\rangle^a \right) e^{i\overline{\mathcal{L}}(a,\phi)\tau} \left(i\mathcal{L}(\phi)\hat{A}_\mu - \left\langle i\mathcal{L}(\phi)\hat{A}_\mu \right\rangle^a \right) \right\rangle^a \tag{C20}$$

The irreversible part $\overline{M}_{\mu\nu}\lambda_\nu$ of the dynamics in (48) when we use the friction matrix (C18) and the conjugate variables (C7) takes the form

$$\begin{aligned} &-\int da' \frac{\partial}{\partial a_\nu} k_B M_{\mu\nu}(a,\phi_t) P(a,t) \left(\frac{\partial}{\partial a'_\mu}\delta_{aa'} \right) \left[\ln \frac{P(a',t)}{\Omega(a')} - 1 \right] = \frac{\partial}{\partial a_\nu} k_B M_{\mu\nu}(a,\phi_t) P(a,t) \frac{\partial}{\partial a_\mu} \left[\ln \frac{P(a',t)}{\Omega(a')} - 1 \right] \\ &= \frac{\partial}{\partial a_\nu} k_B M_{\mu\nu}(a,\phi_t) \frac{\partial}{\partial a_\mu} P(a,t) - \frac{\partial}{\partial a_\nu} M_{\mu\nu}(a,\phi_t) P(a,t) \frac{\partial S}{\partial a_\mu}(a) \end{aligned} \tag{C21}$$

where the bare entropy $S(a)$ is defined as

$$S(a) \equiv k_B \ln \Omega(a) \tag{C22}$$

By collecting the reversible (C14) and irreversible (C21) parts of the dynamics (48) we end up with the FPE (80) in the main text.

1. Properties of building blocks in the stochastic flavour

While the properties of the building blocks in the stochastic flavour are inherited from those in the average flavour, it is worth detailing them to highlight some differences. The reversibility condition (100) is a consequence of the following sequence of identities

$$0 \overset{(6)}{=} \mathrm{Tr}[i\mathcal{L}_t \hat{\Psi}_a] \overset{\text{ch.rule}}{=} -\frac{\partial}{\partial a}\cdot \mathrm{Tr}[\hat{\Psi}_a i\mathcal{L}_t \hat{A}] \overset{(C15)}{=} -\frac{\partial}{\partial a}\cdot V(a,\phi_t)\Omega(a) \overset{(84)}{=} \frac{1}{k_B}\left[k_B \frac{\partial}{\partial a}\cdot V(a,\phi_t) + V(a,\phi_t)\cdot \frac{\partial S}{\partial a} \right] \tag{C23}$$

This condition links the form of the reversible drift with the form of the thermodynamic forces given by the derivatives of entropy. This condition helps in practice to evaluate parts of the drift term in terms of the thermodynamic forces.

From this reversibility condition we may get the degeneracy condition in GENERIC

$$0 \overset{(94),(C23)}{=} \frac{1}{k_B}\left[k_B \frac{\partial}{\partial a}\cdot L \cdot \frac{\partial E}{\partial a} + \frac{\partial S}{\partial a}\cdot L \cdot \frac{\partial E}{\partial a} \right] = \frac{1}{k_B}\left[k_B \frac{\partial}{\partial a}\cdot L + \frac{\partial S}{\partial a}\cdot L \right]\cdot \frac{\partial E}{\partial a} \tag{C24}$$

which holds if

$$L(a)\cdot \frac{\partial S}{\partial a}(a) + k_B \frac{\partial}{\partial a}\cdot L(a) = 0 \tag{C25}$$

The first degeneracy of the friction matrix (102) is proved as follows

$$\begin{aligned} M_{\mu\nu}(a,\phi_t)\frac{\partial E}{\partial a_\nu}(a,\phi_t) &\overset{(C20)}{=} \frac{\partial E}{\partial a_\nu}(a,\phi_t)\frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(e^{i\overline{\mathcal{L}}_t\tau}\mathcal{Q}i\mathcal{L}_t\hat{A}_\mu \right) \mathcal{Q}i\mathcal{L}_t\hat{A}_\nu \right\rangle^a \\ &= \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(e^{i\overline{\mathcal{L}}_t\tau}\mathcal{Q}i\mathcal{L}_t\hat{A}_\mu \right) \mathcal{Q}i\mathcal{L}_t\hat{A}_\nu \frac{\partial E}{\partial a_\nu}(\hat{A},\phi_t) \right\rangle^a \overset{(92)}{=} \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(e^{i\overline{\mathcal{L}}_t\tau}\mathcal{Q}i\mathcal{L}_t\hat{A}_\mu \right) \mathcal{Q}i\mathcal{L}_t\hat{H} \right\rangle^a \\ &\overset{(8)}{=} 0 \end{aligned} \tag{C26}$$

where we have used in the second identity that the conditional expectation (82) of a function of CG variables satisfies

$\left\langle F(\hat{A})\right\rangle^a = F(a)$. The second degeneracy condition in (102) can be proved as follows

$$\begin{aligned}\frac{\partial E}{\partial a_\mu}(a,\phi_t)M_{\mu\nu}(a,\phi_t) &= \frac{\partial E}{\partial a_\mu}(a,\phi_t)\frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(e^{i\overline{\mathcal{L}}_t\tau}\mathcal{Q}i\mathcal{L}_t\hat{A}_\mu\right)\mathcal{Q}i\mathcal{L}_t\hat{A}_\nu\right\rangle^a \\ &= \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \frac{\partial E}{\partial a_\mu}(\hat{A},\phi_t)\left(e^{i\overline{\mathcal{L}}_t\tau}\mathcal{Q}i\mathcal{L}_t\hat{A}_\mu\right)\mathcal{Q}i\mathcal{L}_t\hat{A}_\nu\right\rangle^a \\ &\simeq \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(e^{i\overline{\mathcal{L}}_t\tau}\mathcal{Q}i\mathcal{L}_t\hat{A}_\mu\frac{\partial E}{\partial a_\mu}(\hat{A},\phi_t)\right)\mathcal{Q}i\mathcal{L}_t\hat{A}_\nu\right\rangle^a \\ &= \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left(e^{i\overline{\mathcal{L}}_t t'}\mathcal{Q}i\mathcal{L}_t\hat{H}\right)\mathcal{Q}i\mathcal{L}_t\hat{A}_\nu\right\rangle^a \overset{(8)}{=} 0 \end{aligned} \tag{C27}$$

where in the third line we have assumed that within the time-scale of the memory kernel, the gradient of the energy is almost constant, and can go inside the evolution operator.

Appendix D: TIME REVERSIBILITY AT THE CG LEVEL

1. Time reversibility in the average flavour

Let us discuss the effect of time reversibility on the different terms of the transport equation (48). We will assume that the CG variables have a well-defined parity under time reversal, this is

$$\mathcal{T}\hat{A}(z) = \hat{A}(\epsilon\cdot z) = \varepsilon_{\mathsf{T}}\cdot\hat{A}(z) \tag{D1}$$

were ε_{T} is a diagonal matrix with ± 1 in the diagonal, according to the parity of each CG variable.

We start with the time reversal properties of the partition function

$$\begin{aligned}Z(\lambda) &\overset{(23)}{=} \int dz\rho_c e^{-\lambda^T\cdot\hat{A}(\epsilon\cdot z)} \\ &\overset{(D1)}{=} \int dz\rho_c e^{-\lambda^T\cdot\varepsilon_{\mathsf{T}}\cdot\hat{A}(z)} = Z(\varepsilon_{\mathsf{T}}\cdot\lambda)\end{aligned} \tag{D2}$$

where in the first equality we have considered the change of variables $z\to\epsilon\cdot z$ that has unit Jacobian. According to (26), (27), the averages with respect to the relevant ensemble are obtained as

$$a(\lambda) = -\frac{\partial \ln Z(\lambda)}{\partial\lambda} \tag{D3}$$

and, therefore, they satisfy the following symmetry

$$a(\varepsilon_{\mathsf{T}}\cdot\lambda) = \varepsilon_{\mathsf{T}}\cdot a(\lambda) \tag{D4}$$

that just reflects the parity (D1) of the CG variables. As a consequence of all the above, the relevant ensemble satisfies

$$\overline{\rho}_\lambda(\epsilon\cdot z) = \frac{\rho_c}{Z(\lambda)}e^{-\lambda^T\cdot\hat{A}(\epsilon\cdot z)} = \frac{\rho_c}{Z(\varepsilon_{\mathsf{T}}\cdot\lambda)}e^{-\lambda^T\varepsilon_{\mathsf{T}}\cdot\hat{A}(z)} = \overline{\rho}_{\varepsilon_{\mathsf{T}}\cdot a}(z) \tag{D5}$$

The CG energy function is defined in (57)

$$\begin{aligned}E(a_t,\phi_t) &= \int dz\overline{\rho}_{\lambda_t}(z)\hat{H}(z,\phi_t) = \int dz\overline{\rho}_{\lambda_t}(\epsilon\cdot z)\hat{H}(\epsilon z,\phi_t) \\ &\overset{(D5)(A19)}{=} \int dz\overline{\rho}_{\varepsilon_{\mathsf{T}}\cdot\lambda_t}(z)\hat{H}(z,\varepsilon_{\mathsf{T}}\cdot\phi_t) \\ &= E(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\end{aligned} \tag{D6}$$

The entropy, which is just the result of evaluating the Gibbs-Jaynes entropy at the relevant ensemble, will inherit the parity property from the relevant ensemble

$$\overline{S}(\varepsilon_{\mathsf{T}}\cdot a) = \overline{S}(a) \tag{D7}$$

and the conjugate variables satisfy

$$k_B\lambda(\varepsilon_{\mathsf{T}}\cdot a) = \frac{\partial}{\partial a}\overline{S}(\varepsilon_{\mathsf{T}}\cdot a) = \varepsilon_{\mathsf{T}}\cdot\frac{\partial\overline{S}}{\partial a}(a) = k_B\varepsilon_{\mathsf{T}}\cdot\lambda(a) \tag{D8}$$

which could also be inferred from (D4).

The reversible drift term defined in (32), when evaluated at $\varepsilon_{\mathsf{T}}\cdot a$ and $\varepsilon_{\mathsf{T}}\cdot\phi_t$ is

$$\begin{aligned}v(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi_t) &\overset{(32)}{=} \int dz\overline{\rho}_{\varepsilon_{\mathsf{T}}\cdot a}(z)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}(z) \\ &\overset{(D5)}{=} \int dz\overline{\rho}_a(\epsilon\cdot z)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}(z)\end{aligned} \tag{D9}$$

We may perform the change of variables from z to $\epsilon\cdot z$ that has unit Jacobian to get

$$\begin{aligned}v(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi_t) &= \int dz\overline{\rho}_a(z)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}(\epsilon\cdot z) \\ &\overset{(A25)}{=} -\varepsilon_{\mathsf{T}}\cdot\int dz\overline{\rho}_a(z)i\mathcal{L}(\phi_t)\hat{A}(z) \\ &\overset{(32)}{=} -\varepsilon_{\mathsf{T}}\cdot v(a,\phi_t)\end{aligned} \tag{D10}$$

From (D6) and (D10) we have

$$-\varepsilon_{\mathsf{T}}\cdot v(a,\phi) = -\varepsilon_{\mathsf{T}}\cdot\overline{L}(a,\phi)\frac{\partial E}{\partial a}(a,\phi) \tag{D11}$$

which implies that the reversible operator should transform as

$$\overline{L}(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi) = -\varepsilon_{\mathsf{T}}\cdot\overline{L}(a,\phi)\cdot\varepsilon_{\mathsf{T}} \tag{D12}$$

By using the same change of variables, the relevant ensemble average of an arbitrary function $\hat{F}$ transforms as

$$\left\langle \hat{F}\right\rangle^{\lambda} = \left\langle \mathcal{T}\hat{F}\right\rangle^{\varepsilon_{\mathsf{T}}\cdot\lambda} \tag{D13}$$

The property (D13) together with the anticommutativity (A25) show that the time-reversal operator and the projector satisfy a sort of commutativity condition

$$\mathcal{T}\mathcal{Q}(a) = \mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a)\mathcal{T} \tag{D14}$$

while the action of the time-reversal operator on the projected Liouville operator (19) gives, thanks to (A25),

$$\mathcal{T}i\overline{\mathcal{L}}(a_t,\phi_t) = -i\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\mathcal{T} \tag{D15}$$

These two properties imply

$$\mathcal{T}\mathcal{Q}(a)i\overline{\mathcal{L}}(a_t,\phi_t)\mathcal{Q}(a) = -i\mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a)\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a_t)\mathcal{T} \tag{D16}$$

and, consequently, the action of the time-reversal operator on the projected dynamics is

$$\mathcal{T}e^{i\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\tau} = e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\mathcal{T} \tag{D17}$$

as can be easily shown by using the Taylor series of the exponential. The microscopic reversibility of the projected dynamics is to be compared with the corresponding one for the Hamiltonian dynamics under a constant external force (A37).

The parity of the friction matrix (52) is obtained from

$$\begin{aligned}
\overline{M}_{\mu\nu}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t) &= \frac{1}{k_B}\int_0^{\Delta t} d\tau \left\langle \left[e^{i\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\tau}\mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a_t)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\mu\right]\mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a_t)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\nu\right\rangle^{\varepsilon_{\mathsf{T}}\cdot\lambda_t} \\
&\overset{(D13)}{=} \frac{1}{k_B}\int_0^{\Delta t} d\tau\int dz\overline{\rho}_{\lambda_t}(z)\mathcal{T}\left(\left[e^{i\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\tau}\mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a_t)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\mu(z)\right]\mathcal{Q}(\varepsilon_{\mathsf{T}}\cdot a_t)i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\nu(z)\right) \\
&\overset{(D17)}{=} \frac{1}{k_B}\int_0^{\Delta t} d\tau\int dz\overline{\rho}_{\lambda_t}(z)\left[e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\mathcal{T}\hat{A}_\mu(z)\right]\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\mathcal{T}\hat{A}_\nu(z) \\
&\overset{(D1)}{=} \varepsilon_{\mathsf{T}\mu\mu'}\frac{1}{k_B}\int_0^{\Delta t} d\tau\int dz\overline{\rho}_{\lambda_t}(z)\left[e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_{\mu'}(z)\right]\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_{\nu'}(z)\varepsilon_{\mathsf{T}\nu\nu'} \\
&\overset{(D1)}{=} \varepsilon_{\mathsf{T}\mu\mu'}\frac{1}{k_B}\int_0^{\Delta t} d\tau\int dz\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_{\mu'}(z)\left[e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\right]^\dagger\overline{\rho}_{\lambda_t}(z)\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_{\nu'}(z)\varepsilon_{\mathsf{T}\nu'\nu}
\end{aligned} \tag{D18}$$

The action of the adjoint operator is

$$\begin{aligned}
\left[e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\right]^\dagger\overline{\rho}_{\lambda_t}(z)\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_\nu(z) &= \sum_{n=0}\frac{(-1)^n}{n!}[\overline{\mathcal{L}}(a_t,\phi_t)\tau]^{n\dagger}\overline{\rho}_{\lambda_t}(z)\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_\nu(z) \\
&= \sum_{n=0}\frac{\tau^n}{n!}[\mathcal{Q}^\dagger(a_t)\mathcal{L}(\phi_t)\mathcal{Q}^\dagger]^n\overline{\rho}_{\lambda_t}(z)\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_\nu(z) \\
&= \sum_{n=0}\frac{\tau^n}{n!}[\mathcal{Q}^\dagger(a_t)\mathcal{L}(\phi_t)\mathcal{Q}^\dagger]^n\overline{\rho}_{\lambda_t}(z)\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_\nu(z)
\end{aligned} \tag{D19}$$

If we assume that the relevant ensemble does not change appreciably in the time scale of the memory

$$i\mathcal{L}(\phi_t)\overline{\rho}_{\lambda_t} \simeq 0 \tag{D20}$$

and use the property (B21), we have

$$\left[e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\right]^\dagger\overline{\rho}_{\lambda_t}(z)\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_\nu(z) \simeq \overline{\rho}_{\lambda_t}(z)\left[e^{i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\right]\mathcal{Q}(a_t)i\mathcal{L}(\phi_t)\hat{A}_\nu(z) \tag{D21}$$

Using this result in (D18) we conclude

$$\overline{M}_{\mu\nu}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)=\varepsilon_{\mathsf{T}\mu\mu'}\overline{M}_{\nu\mu}(a_t,\phi_t)\varepsilon_{\mathsf{T}\nu'\nu'} \tag{D22}$$

or in matrix form

$$\overline{M}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)=\varepsilon_{\mathsf{T}}\cdot\overline{M}^{T}(a_t,\phi_t)\cdot\varepsilon_{\mathsf{T}} \tag{D23}$$

where the superscript T stands for transpose. This is the Onsager-Casimir reciprocity theorem, which is valid under the Markovian assumption.

2. Time reversibility in the stochastic flavour

We consider in this section the time-reversal properties of the diferent objects appearing in the FPE (96). Consider the measure $\Omega(a)$ and evaluate

$$\Omega(\varepsilon_{\mathsf{T}}\cdot a)=\int dz\delta\left(\hat{A}(z)-\varepsilon_{\mathsf{T}}\cdot a\right)=\int dz\delta\left(\varepsilon_{\mathsf{T}}\cdot\hat{A}(z)-a\right)=\int dz\delta\left(\hat{A}(\epsilon\cdot z)-a\right)=\Omega(a) \tag{D24}$$

where in the last equation we have performed a change of variable $z'=\epsilon\cdot z$ with unit Jacobian. The conditional expectations transform according to

$$\left\langle\hat{F}\right\rangle^{\varepsilon_{\mathsf{T}}\cdot a}=\frac{1}{\Omega(\varepsilon_{\mathsf{T}}\cdot a)}\int dz\delta\left(\hat{A}(z)-\varepsilon_{\mathsf{T}}\cdot a\right)\hat{F}(z)=\frac{1}{\Omega(a)}\int dz\delta\left(\hat{A}(\epsilon\cdot z)-a\right)\hat{F}(z)=\left\langle\mathcal{T}\hat{F}\right\rangle^{a} \tag{D25}$$

The projector and time reversibility operators commute

$$\begin{aligned}\mathcal{T}\mathcal{P}\hat{F}(z)&\overset{(C11)}{=}\mathcal{T}\int dz'\frac{\delta(\hat{A}(z)-\hat{A}(z'))}{\Omega(\hat{A}(z))}\hat{F}(z')\overset{(A14)}{=}\int dz'\frac{\delta(\hat{A}(\epsilon\cdot z)-\hat{A}(z'))}{\Omega(\hat{A}(\epsilon\cdot z))}\hat{F}(z')\overset{(D1)}{=}\int dz'\frac{\delta(\varepsilon_{\mathsf{T}}\cdot\hat{A}(z)-\hat{A}(z'))}{\Omega(\hat{A}(z))}\hat{F}(z')\\&=\int dz'\frac{\delta(\hat{A}(z)-\varepsilon_{\mathsf{T}}\cdot\hat{A}(z'))}{\Omega(\hat{A}(z))}\hat{F}(z')\overset{(D1)}{=}\int dz'\frac{\delta(\hat{A}(z)-\hat{A}(\epsilon\cdot z'))}{\Omega(\hat{A}(z))}\hat{F}(z')=\int dz'\frac{\delta(\hat{A}(z)-\hat{A}(z'))}{\Omega(\hat{A}(z))}\hat{F}(\epsilon\cdot z')\\&\overset{(A14)}{=}\mathcal{P}\mathcal{T}\hat{F}(z)\end{aligned} \tag{D26}$$

The reversible matrix $L_{\mu\nu}(a)$ defined in (95) transforms according to

$$L(\varepsilon_{\mathsf{T}}\cdot a)\overset{(D25),(61)}{=}\left\langle\mathcal{T}\left\{\hat{A},\hat{A}\right\}\right\rangle^{a}=-\varepsilon_{\mathsf{T}}\cdot L(a)\cdot\varepsilon_{\mathsf{T}} \tag{D27}$$

where we have made use of the anticommutativity of ϵ and the symplectic matrix J appearing in the Poisson bracket.

The drift term satisfies

$$V(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi_t)=\left\langle i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}\right\rangle^{\varepsilon_{\mathsf{T}}\cdot a}\overset{(D25)}{=}\left\langle\mathcal{T}i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}\right\rangle^{a}\overset{(A25)}{=}-\left\langle i\mathcal{L}(\phi_t)\mathcal{T}\hat{A}\right\rangle^{a}\overset{(D1)}{=}-\varepsilon_{\mathsf{T}}\cdot V(a,\phi_t) \tag{D28}$$

Consider the memory kernel (C20), evaluated at the time-reversed variables

$$M_{\mu\nu}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\equiv\frac{1}{k_B}\int_0^{\Delta t}d\tau\left\langle\left(i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\nu-\left\langle i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\nu\right\rangle^{\varepsilon_{\mathsf{T}}\cdot a}\right)e^{i\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi_t)\tau}i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}_\mu\right\rangle^{\varepsilon_{\mathsf{T}}\cdot a} \tag{D29}$$

Note that

$$i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}\overset{(A25)}{=}-\mathcal{T}i\mathcal{L}(\phi_t)\mathcal{T}\hat{A}\overset{(D1)}{=}-\varepsilon_{\mathsf{T}}\cdot\mathcal{T}i\mathcal{L}(\phi_t)\hat{A} \tag{D30}$$

This implies

$$\left[i\mathcal{L}(\varepsilon_{\mathsf{T}}\cdot\phi_t)\hat{A}-V(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi_t)\right]\overset{(D30)(D28)}{=}-\varepsilon_{\mathsf{T}}\mathcal{T}\left[i\mathcal{L}(\phi_t)\hat{A}-V(a,\phi_t)\right] \tag{D31}$$

Inserting this result back into (D29) gives

$$M_{\mu\nu}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\equiv\varepsilon_{\mathsf{T}\mu\mu'}\varepsilon_{\mathsf{T}\nu\nu'}\frac{1}{k_B}\int_0^{\Delta t}d\tau\left\langle\mathcal{T}\left(i\mathcal{L}_t\hat{A}_{\nu'}-\left\langle i\mathcal{L}_t\hat{A}_{\nu'}\right\rangle^a\right)e^{i\overline{\mathcal{L}}(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi_t)\tau}\mathcal{T}i\mathcal{L}_t\hat{A}_{\mu'}\right\rangle^{\varepsilon_{\mathsf{T}}\cdot a}\tag{D32}$$

Using (D25) in this expression gives

$$M_{\mu\nu}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)\equiv\varepsilon_{\mathsf{T}\mu\mu'}\varepsilon_{\mathsf{T}\nu\nu'}\frac{1}{k_B}\int_0^{\Delta t}d\tau\left\langle\left(i\mathcal{L}_t\hat{A}_{\nu'}-\left\langle i\mathcal{L}_t\hat{A}_{\nu'}\right\rangle^a\right)\mathcal{T}e^{i\overline{\mathcal{L}}(a,\varepsilon_{\mathsf{T}}\cdot\phi_t)\tau}\mathcal{T}i\mathcal{L}_t\hat{A}_{\mu'}\right\rangle^a\tag{D33}$$

Because of the anticommutativity (A25) and the commutativity (D26), the efect of the time reversal operator $\mathcal{T}$ on the evolution operator is

$$\mathcal{T}e^{i\overline{\mathcal{L}}(a_t,\varepsilon_{\mathsf{T}}\phi_t)\tau}\mathcal{T}=e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\tag{D34}$$

as can be seen from the Taylor series expansion of the exponential. Using this result in (D33) gives

$$\begin{aligned}M_{\mu\nu}(\varepsilon_{\mathsf{T}}\cdot a_t,\varepsilon_{\mathsf{T}}\cdot\phi_t)&=\varepsilon_{\mathsf{T}\mu\mu'}\varepsilon_{\mathsf{T}\nu\nu'}\frac{1}{k_B}\int_0^{\Delta t}d\tau\int dz\rho_a^{\mathrm{mic}}(z)\left(i\mathcal{L}_t\hat{A}_{\nu'}-\left\langle i\mathcal{L}_t\hat{A}_{\nu'}\right\rangle^a\right)e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}i\mathcal{L}_t\hat{A}_{\mu'}\\&\overset{(5)}{=}\varepsilon_{\mathsf{T}\mu\mu'}\varepsilon_{\mathsf{T}\nu\nu'}\frac{1}{k_B}\int_0^{\Delta t}d\tau\int dzi\mathcal{L}_t\hat{A}_{\mu'}\left[e^{-i\overline{\mathcal{L}}(a_t,\phi_t)\tau}\right]^\dagger\rho_a^{\mathrm{mic}}(z)\left(i\mathcal{L}_t\hat{A}_{\nu'}-\left\langle i\mathcal{L}_t\hat{A}_{\nu'}\right\rangle^a\right)\end{aligned}\tag{D35}$$

By following analogous steps as those in (D19)-(D21) adapted to the stochastic flavour, we may write (D33) in the form

$$M(\varepsilon_{\mathsf{T}}\cdot a,\varepsilon_{\mathsf{T}}\cdot\phi)=\varepsilon_{\mathsf{T}}\cdot M^T(a,\phi)\cdot\varepsilon_{\mathsf{T}}^T\tag{D36}$$

This is the Onsager-Casimir reciprocity for the stochastic flavour.

3. Orthogonal symmetry at the CG level

Properties (A40) and (A43) reflecting orthogonal invariance have also consequences on the functional form of the different building blocks entering the transport equations (71) and (97). We consider here the stochastic flavour, and similar results hold for the average flavour. Following very similar reasoning as those leading to (D24)-(D28) we now obtain (124)-(126) in the main text. Choosing ε_{R} instead of ε in the steps from (D29) to (D36) and mutatis mutandi by taking into account that now we have the commutativity (A43) instead of the anticommutativity (A25), we arrive at the property (127) of the friction matrix.

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